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)
1	Analysis of Enzyme Catalytic Properties using Molecular Dynamic Simulations.	IÑAKI TUÑÓN / JOSE JAVIER RUIZ	
2	Determination of Enzymatic Mechanisms by means of Computational Simulations.	JOSE JAVIER RUIZ / IÑAKI TUÑÓN	
3	Derivatives of polyaromatic systems: Synthesis, characterization and calculation of properties.	BEGOÑA MILIAN MEDINA / (RAFAEL BALLESTEROS GARRIDO)(Q.ORGÁNICA)	
4	Theoretical study of the photophysical properties of heteroleptic Ir(III) complexes	ENRIQUE ORTI GUILLEN / ANGELO GIUSSANI	
5	Application of Functionalized Polymer Nanoparticles in Asymmetric Catalysis	RAFAEL MUÑOZ ESPI / FRANCISCO F. PÉREZ PLA	
6	Photoactive Nanoparticles Prepared by Miniemulsion Polymerization	RAFAEL MUÑOZ ESPI / (MARÍA GONZÁLEZ BÉJAR), (Q. ORGÁNICA)	
7	Polysaccharide-Based Hybrid Particles as Magnetically Separable Catalysts	RAFAEL MUÑOZ ESPI / FRANCISCO F. PÉREZ PLA	
8	Thermoregulating Polymer Coatings Containing Phase Change Materials	RAFAEL MUÑOZ ESPI	
9	Supercritical CO_2-Assisted Fabrication of Polymer Supports for Enzyme Immobilization	RAFAEL MUÑOZ ESPI / (AMPARO CHÁFER ORTEGA)(INGENIERIA QUÍMICA)	
10	Encapsulation of Phase Change Materials through Valorization of Lignocellulosic Waste	RAFAEL MUÑOZ ESPI / MARIO CULEBRAS RUBIO	
11	Lignin-based carbon materials for catalytic applications	MARIO CULEBRAS RUBIO / FRANCISCO F. PÉREZ PLA	
12	Synthesis and characterization of lignin-based nanoparticles	MARIO CULEBRAS RUBIO / RAFAEL MUÑOZ ESPI	
13	Hybrid carbon nanofibers derived from lignin for energy harvesting and storage applications	MARIO CULEBRAS RUBIO	
14	Effect of metal halide perovskite composition on the performance of light-emitting devices	DANIEL TORDERA SALVADOR	
15	Computational study of the selective oxidation of ethanol over vanadia supported catalyst	LOURDES GRACIA EDO	
16	Theoretical Analysis of Dynamical Motions in Biomolecular Motors.	IÑAKI TUÑÓN / JOSE JAVIER RUIZ	
17	Preparation and evaluation of the activity of sustainable catalysts formed by biometals deposited on porous carbon supports.	FRANCISCO F. PÉREZ PLA / (MARÍA ANGELES ÚBEDA PICOT)(Q.INORGÁNICA)	
18	Preparation and evaluation of the catalytic activity of sustainable nickel nanoparticle catalysts deposited on carbonized polydopamine supports.	FRANCISCO F. PÉREZ PLA / (MARÍA ANGELES ÚBEDA PICOT)(Q.INORGÁNICA)	
19	Effect of seed layers on the photoluminescent efficiency of metal halide perovskites	CRISTINA ROLDAN CARMONA	

20	Application of Virtual Reality and Augmented Reality in Chemistry Learning	JESÚS VICENTE DE JULIÁN ORTIZ	
21	Simulation of Membrane Proteins in the Presence of Electric Fields	JESÚS VICENTE DE JULIÁN ORTIZ	
22	Desing of Rotavirus Inhibitor Compounds	JESÚS VICENTE DE JULIÁN ORTIZ	
23	Computational Design of Titanium Metal–Organic Frameworks for Selective CO_2 Capture	NEYVIS ALMORA BARRIOS	
24	Lignin extraction from agricultural pruning waste for hydrogels preparation	MARIO CULEBRAS RUBIO / RAFAEL BALLESTEROS GARRIDO (Q.ORGÁNICA)	
25	Lignin/Cu2S Composites for Thermoelectric 3D-Printing Materials	CLARA GÓMEZ CLARI / MARIO CULEBRAS RUBIO	
26	Synthesis of thermoplastic polyurethanes with improved thermal resistance	CLARA GÓMEZ CLARI	
27	Thermoplastic polyurethanes from sustainable polycarbonatediols	CLARA GÓMEZ CLARI	
28	Insights into the thermal effects on the enzymatic degradation of polyethylene terephthalate from computational modeling	JUAN ARAGÓ MARCH	
29	Dissection of the Binding Energy in Protein-Ligand of Potential Anticancer Drugs Candidates	ALBERTO FERNÁNDEZ ALARCÓN	
30	Syntesis and Characterization of New Iron(II) Spin Crossover Coordination Polymers	CARLOS BARTUAL MURGUI /(JOSÉ ANTONIO REAL CABEZAS)(Q.INORGÁNICA)	
31	First-principles characterization of honeycomb 2D MOFs as porous conductors	JOAQUIN CALBO ROIG / ENRIQUE ORTI GUILLÉN	
32	Ion Insertion Batteries. Historical evolution, challenges and future.	JERÓNIMO AGRISUELAS VALLÉS / JOSÉ JUAN GARCÍA JAREÑO	
33	Separation of cobalt and nickel metals by selective electrodeposition on different types of electrodes.	JERÓNIMO AGRISUELAS VALLÉS / JOSÉ JUAN GARCÍA JAREÑO	
34	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	
35	Electrogeneration and characterization of poly(phenosafranine) on stainless steel.	JERÓNIMO AGRISUELAS VALLÉS / JOSÉ JUAN GARCÍA JAREÑO	
36	Corrosion rate study of steels. Effect of protective polymeric films.	JOSÉ JUAN GARCÍA JAREÑO / JERÓNIMO AGRISUELAS VALLES	
37	Photochemistry of nitro-alkane derivatives and their role in pollution	JAVIER SEGARRA MARTÍ / ANGELO GIUSSANI	
38	Microsolvation effects on the photophysical reactivity of DNA model systems	JAVIER SEGARRA MARTÍ	
39	Multiscale modelling of chemical reactivity with machine learning potentials	KIRILL ZINOVJEV	
40	Molecular mechanism of the synthesis of N-heterocyclic carbene Fe(II) complexes studied by electronic structure methods	ANTONIO FRANCÉS MONERRIS	
41	Design and development of new antimicrobial biosystems for biotechnological applications.	Mª CARMEN MARTÍNEZ BISBAL	BERNARDOS BAU(upv)

42	Determination of changes in the composition of neonatal saliva by NMR spectroscopy	Mª CARMEN MARTÍNEZ BISBAL	
43	Study of the vulnerability of atheroma plaques in cell culture samples by NMR spectroscopy	Mª CARMEN MARTÍNEZ BISBAL	
44	DNA binding energies of indole-like biomolecules	DANIEL ROCA SANJUÁN / ANTONIO FRANCÉS MONERRIS	
45	Free energies of cations and anions of nucleobases in DNA: A computational study	DANIEL ROCA SANJUÁN / JAVIER SEGARRA MARTÍ	
46	Effect of anharmonicity in the quantum-chemistry determination of absorption electronic spectra	DANIEL ROCA SANJUÁN / DAVID FRANCISCO MACIAS PINILLA	
47	Computational Modeling of the DNA unbinding dynamics of indole-like biomolecules	DANIEL ROCA SANJUÁN / (ANA MARÍA BORREGO SÁNCHEZ) (FARMACIA Y TECNOLOGÍA FARMACÉUTICA Y PARASITOLOGÍA)	
48	First principles study of a family of Layered Double Hydroxides (LDHs) for catalysis and water treatment	JOSE JAIME BALDOVI JACHAN	

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Iñaki Tuñón

ACADEMIC TUTOR 2 Jose Javier Ruiz

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Analysis of Enzyme Catalytic Properties using Molecular Dynamic Simulations.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Análisis del espacio conformacional de la proteína en estudio.
Determinación de los parámetros energéticos y geométricos más relevantes que permitan entender el comportamiento del sistema en estudio.
Determinación de poblaciones conformacionales y sus probabilidades mediante análisis de componentes principales.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se utilizarán métodos de cálculo de simulación computacional.
El estudio se realizará utilizando fundamentalmente el programa AMBER y AMBERTOOLS.
Además se usarán programas de visualización de estructuras, tal como VMD, PYMOL, etc.
Programas de análisis en PYTHON. Implementación de scripts en la plataforma Júpiter.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jose Javier Ruiz

ACADEMIC TUTOR 2 Iñaki Tuñón

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Determination of Enzymatic Mechanisms by means of Computational Simulations.

OBJECTVES / 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 del sustrato natural, estableciendo las diferentes etapas y las barreras de energía potencial.
Determinación de las barreras de energía libre.
Comparación de las propiedades cinéticas y termodinámicas del modelo construido con los datos experimentales disponibles.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se utilizarán métodos de cálculo de Química Cuántica.
El estudio se realizará utilizando fundamentalmente el programa Gaussian, con posibilidad de utilización de ORCA. Además se usarán programas de visualización de estructuras, tal como: Molden, Gaussview o VMD.
Localización de los puntos estacionarios asociados al proceso catalítico.
Determinación de la constante de velocidad para cada uno de las etapas de la reacción analizadas.
Determinación de la constante de equilibrio del sistema y evaluación respecto a valores determinados experimentalmente.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 BEGOÑA MILIAN MEDINA

ACADEMIC TUTOR 2 RAFAEL BALLESTEROS GARRIDO

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUÍMICA FÍSICA y QUÍMICA ORGÁNICA

TITLE (Mandatory in English)

Derivatives of polyaromatic systems: Synthesis, characterization and calculation of properties.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Sintetizar y caracterizar estructuras poliaromáticas heterocíclicas
- Estudiar los sistemas preparados mediante cálculos químico-cuánticos

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Síntesis orgánica,
Caracterización molecular (RMN,IR, HRMS, UV/Vis, Fluorescencia)
Cálculo de propiedades (estructura molecular y electrónica, espectros vibracional y electrónico) a nivel DFT, en vacío y en presencia de disolventes mediante modelos PCM.

IMPORTANTE: Es necesario haber cursado la asignatura Química Computacional para poder llevar a cabo este TFG.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Enrique Orti Guillen

ACADEMIC TUTOR 2 Angelo Giussani

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

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

OBJECTVES / 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

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Espí

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).

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Espí

ACADEMIC TUTOR (if needed): María González Béjar (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.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Espí

ACADEMIC TUTOR (if needed): Francisco F. Pérez 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 the 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 previoulsy 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.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Espí

ACADEMIC TUTOR (if needed):

EXTERNAL TUTOR (if needed):

Department: Physical Chemistry

TITLE (Mandatory in English)

Thermoregulating Polymer Coatings Containing Phase Change Materials

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Development of preparation strategies for polymer films and coatings from nanocapsules containing phase change materials.
- Development of experimental devices to evaluate the efficiency of the final materials.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

In this work, polymer capsules will be prepared using the miniemulsion technique. These capsules must incorporate the so-called phase change materials (PCM), which store energy in the form of latent heat when they change phase due to an increase in temperature. This energy is released when the temperature drops again.

Films containing the PCM will be formed from the polymer capsules. The characterization of the systems will be carried out using appropriate techniques, including dynamic light scattering (DLS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM), and differential scanning calorimetry (DSC), among others.

The final step will be the evaluation of the efficiency of the polymer coatings after different cycles of temperature change.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Espí

ACADEMIC TUTOR (if needed): Amparo Cháfer Ortega (Enginyeria Química)

EXTERNAL TUTOR (if needed):

Department: Physical Chemistry

TITLE (Mandatory in English)

Supercritical CO_2-Assisted Fabrication of Polymer Supports for Enzyme Immobilization

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Development of synthesis strategies for the use of supercritical CO2 as a solvent in heterogeneous phase polymerization processes aimed at preparing enzymatic supports.

- Incorporation of specific enzymes into polymer supports and study of the enzymatic activity.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The work focuses on the use of supercritical CO2 as a sustainable solvent for heterogeneous phase polymerization reactions (i.e., with the monomer dispersed in a continuous phase of supercritical CO2). The equipment for conducting experiments with supercritical fluids is located in the Department of Chemical Engineering at ETSE.

Polyacrylamide will be used as the initial polymer system, although the application of other polymers may also be evaluated. The optimal conditions for incorporating enzymes (e.g., catalase) into the polymer supports will be studied.

Once the materials have been characterized using appropriate analytical techniques (FTIR, swelling studies, thermogravimetric analysis, differential scanning calorimetry, electron microscopy), the activity of the supported enzymes will be evaluated and compared to that of free enzymes.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Rafael Muñoz-Espí

ACADEMIC TUTOR (if needed): Mario Culebras Rubio

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.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Mario Culebras Rubio

ACADEMIC TUTOR 2 Francisco Pérez Pla

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Lignin-based carbon materials for catalytic applications

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Preparación de nanopartículas de lignina cargadas con magnetita y precursores metálicos. Caracterización morfológica, estructural y de la actividad catalítica.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

La La metodología a utilizar implicará:
1. El uso de técnicas de nanoestructuración de materiales basadas en "soft template".
2. Carbonización en atmosfera contralada.
6. Análisis térmico mediante calorimetría diferencial de barrido modulada y termogravimetría de los precursores de carbono
3. Análisis morfológico mediante microscopía electrónica de barrido y transmisión

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Mario Culebras Rubio

ACADEMIC TUTOR 2 Rafael Muñoz Espí

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Synthesis and characterization of lignin-based nanoparticles

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The preparation of lignin lanoparticles loaded with various materials

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 the energy field.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Mario Culebras Rubio

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Hybrid carbon nanofibers derived from lignin for energy harvesting and storage applications

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Explore new synthetic routes to produce carbon nanostructures from lignin (nanofibers). Optimize the experimental conditions of electrospinning to control the porosity and morphology of the final material with the incorporation of metallic oxides. Carry out a comprehensive characterization of its electrical, thermal, and structural properties,

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The methodology to be used will involve:
The use of material nanostructuring techniques based on electrospinning.
Carbonization under a controlled atmosphere.T
hermal analysis of the carbon precursors using modulated differential scanning calorimetry (MDSC) and thermogravimetric analysis (TGA).
Measurement of electrical and electrochemical properties.
Morphological analysis using scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Daniel Tordera Salvador

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Department of Physical Chemistry

TITLE (Mandatory in English)

Effect of metal halide perovskite composition on the performance of light-emitting devices

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Metal halide perovskites are active materials at the forefront of the new light-emitting technologies. The composition on these materials can greatly affect the performance of the resulting light-emitting devices. In this work, the student will fabricate and characterize perovskite light-emitting devices in order to obtain highly-efficient and stable devices via the study of the composition of the perovskite. MOED group (www.moed.es) is a world leader in the preparation of optoelectronic devices with high vacuum deposition techniques.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The methodology of the project will be as follows:

1) Literature study on metal halide perovskites on light-emitting diodes.

2) Fabrication of devices by high-vacuum deposition techniques.

3) Optical (photoluminescence, quantum yield), electrical (electroluminescence, current density versus voltage and luminance) and morphological characterization of devices.

4) Writing and presentation of results.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Lourdes Gracia Edo

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Computational study of the selective oxidation of ethanol over vanadia supported catalyst

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Study of the catalytically active site of vanadium oxide in three supported catalysts (SiO_2, TiO_2, ZrO_2).
- Study of the ethanol adsorption stage, preferably through the V-O-M junction (M = Si, Ti, Zr).
- Study of the stage of hydrogen transfer from the species $V\text{-}OCH_2CH_3$ to an O atom associated with the active center.
- Comparison of activation energy and rate coefficients for the three supported models.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The chemical reactivity of supported vanadium oxides has received considerable attention due to its importance in oxidation catalysis.

The GAUSSIAN program will be used to optimize all stationary points and to perform the corresponding vibrational analysis. Calculations based on Density Functional Theory (DFT) will be performed using appropriate functionals and basis sets to describe the atoms.

The intrinsic reaction coordinate method will be carried out to describe the paths of minimum energy that connect the transition structures with the corresponding minima.

Suggestion: to have taken the subject of Computational Chemistry

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Iñaki Tuñón

ACADEMIC TUTOR 2 Jose Javier Ruiz

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Theoretical Analysis of Dynamical Motions in Biomolecular Motors.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Evaluación del espacio de conformacional del sistema biológico estudiado.
Establecimiento de los parámetros geométricos y energéticos más pertinentes que faciliten la comprensión del comportamiento del sistema en estudio.
Análisis de los movimientos dinámicos del sistema biológico analizado.
Establecimiento de poblaciones conformacionales y sus probabilidades a través del estudio de los componentes principales.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se utilizarán métodos de cálculo de simulación computacional.
El estudio se realizará utilizando fundamentalmente el programa AMBER y AMBERTOOLS.
Además se usarán programas de visualización de estructuras, tal como VMD, PYMOL, etc.
Programas de análisis en PYTHON. Implementación de scripts en la plataforma Júpiter.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Francisco F. Pérez Pla

ACADEMIC TUTOR 2 M. Ángeles Úbeda Picot

EXTERNAL TUTOR (if needed): ---

DEPARTMENT(S): Química Física y Química Inorgánica.

TITLE (Mandatory in English)

Preparation and evaluation of the activity of sustainable catalysts formed by biometals deposited on porous carbon supports.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this study is to synthesise composite materials of carbon and oxides (magnetite/SiO2) that function as an eco-friendly support for biometals. In addition, the structural characterisation of these materials will be conducted through the utilisation of various analytical techniques. The catalytic activity and stability of the prepared materials will be evaluated in relation to the reduction of 4-nitrophenol to 4-aminophenol, a reaction of environmental significance. In the final phase, the MCR (Multi Curve Resolution) mathematical procedure will be implemented to determine the kinetic constants of interest, using the Haber mechanism.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

To prepare the particles, dopamine will be polymerized on the surface of micro/nano-crystals of the oxide. This support will be impregnated with cations of the biometal, which will then be reduced by carbonization in a controlled N2 atmosphere. This methodology yields structured "core-shell" composites. After synthesis, the materials will be characterized by thermogravimetric analysis, the specific area and porosimetry will be determined from nitrogen adsorption isotherms, and morphological analysis of the particles will be performed by transmission electron microscopy. Microanalysis of the deposited biometal will be carried out by scanning electron spectroscopy. Finally, the catalytic activity of each material will be evaluated against the reduction of 4-nitrophenol to 4-aminophenol using DAD-UV-Vis and HPLC absorption measurements aimed at calculating the TOF (turnover frequency). Using the latter technique, the stability will be evaluated by measuring the TON (turnover number) and the recyclability of the material. Finally, the reaction constants of interest will be calculated using the MCR (Multi Curve Resolution) methodology using the Haber mechanism.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1	Francisco F. Pérez Pla
ACADEMIC TUTOR 2	M. Ángeles Úbeda Picot
EXTERNAL TUTOR (if needed):	--
DEPARTMENT(S):	Química Física y Química Inorgánica

TITLE (Mandatory in English)

Preparation and evaluation of the catalytic activity of sustainable nickel nanoparticle catalysts deposited on carbonized polydopamine supports.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this study is to synthesise composite materials of carbon and oxides (magnetite/SiO2) that function as an eco-friendly support for biometals. In addition, the structural characterisation of these materials will be conducted through the utilisation of various analytical techniques. The catalytic activity and stability of the prepared materials will be evaluated in relation to the reduction of 4-nitrophenol to 4-aminophenol, a reaction of environmental significance. In the final phase, the MCR (Multi Curve Resolution) mathematical procedure will be implemented to determine the kinetic constants of interest, using the Haber mechanism.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

To prepare the particles, dopamine will be polymerized on the surface of micro/nano-crystals of the oxide. This support will be impregnated with cations of the biometal, which will then be reduced by carbonization in a controlled N2 atmosphere. This methodology yields structured "core-shell" composites. After synthesis, the materials will be characterized by thermogravimetric analysis, the specific area and porosimetry will be determined from nitrogen adsorption isotherms, and morphological analysis of the particles will be performed by transmission electron microscopy. Microanalysis of the deposited biometal will be carried out by scanning electron spectroscopy. Finally, the catalytic activity of each material will be evaluated against the reduction of 4-nitrophenol to 4-aminophenol using DAD-UV-Vis and HPLC absorption measurements aimed at calculating the TOF (turnover frequency). Using the latter technique, the stability will be evaluated by measuring the TON (turnover number) and the recyclability of the material. Finally, the reaction constants of interest will be calculated using the MCR (Multi Curve Resolution) methodology using the Haber mechanism.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 CRISTINA ROLDAN CARMONA

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUIMICA FISICA

TITLE (Mandatory in English)

Effect of seed layers on the photoluminescent efficiency of metal halide perovskites

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

MOED group (https://moed.es) has been a pioneer in Spain in the use of high-efficiency, hybrid vacuum-deposited perovskites for photovoltaics. This project aims to develop efficient optoelectronic devices by investigating the use of seed layers as growth templates for vacuum-deposited metal halide perovskite semiconductors. Special emphasis will be placed on how these layers influence crystallization dynamics and photoluminescence efficiency, with the goal of optimizing film quality and light-emission performance—key parameters in both photovoltaic technologies.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1) Fabrication of metal halide perovskite semiconductors using scalable vacuum deposition techniques.

2) Baseline optical and electrical characterization of the films and corresponding photovoltaic devices.

3) Integration of organic and inorganic seed layers to guide crystallization and interface formation.

4) Investigation of photophysical processes related to film quality and photoluminescence efficiency.

5) Optimization of solar cell performance.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jesús Vicente de Julián Ortiz

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Application of Virtual Reality and Augmented Reality in Chemistry Learning

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Development of specific teaching materials on the application of virtual reality and augmented reality in chemistry teaching. This will include user manuals, interactive resources, and practical exercises. The topics covered will be stereochemistry, crystal structure, and protein structure.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Specific learning objectives will be defined for each topic (stereochemistry, crystal structure, and protein structure). These objectives will guide the design of interactive resources and exercises. Low-fidelity prototypes, such as storyboards and wireframes, will be created and iteratively refined based on feedback from the needs assessment.
Three-dimensional models, interactive simulations, and virtual labs will be created for each topic. User manuals will be developed to guide educators and students on the use of the materials. A pilot test will be conducted with a small, diverse group of students and educators. Data will be collected through observations, usage logs, and feedback questionnaires to assess usability, effectiveness, and engagement. This feedback will inform iterative design improvements, ensuring the materials are user-friendly and pedagogically sound.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jesús Vicente de Julián Ortiz

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Simulation of Membrane Proteins in the Presence of Electric Fields

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To develop a model capable of simulating the behavior of membrane proteins within an electric field, accurately representing the electrostatic interactions and conformational changes.
To apply this model to simulate the molecular dynamics of the interaction between the T-lymphocyte receptor complex and the Major Histocompatibility Complex, focusing on the influence of electric fields on the conformation changes.
To analyze the simulation data to identify key residues and interactions that are significantly affected by the presence of electric fields, providing insights into the mechanism of T-lymphocyte activation.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

System Setup: Construct detailed atomistic models of the complexes using available structural data (e.g., PDB files). Embed these complexes within a realistic membrane environment using appropriate lipid molecules. Define the electric field parameters (magnitude, direction).
Molecular Dynamics Simulations: Employ state-of-the-art molecular dynamics (MD) simulation software (e.g., NAMD, GROMACS) with appropriate force fields (e.g., CHARMM, AMBER) to simulate the system's behavior under the influence of the electric field.
Data Analysis: Analyze the simulation trajectories to characterize the conformational dynamics of the proteins and the effects of the electric field. The applicability and usefulness of virtual reality techniques for visualizing these interactions will be studied.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jesús vicente de Julián Ortiz

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Design of Rotavirus Inhibitor Compounds

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To design covalent inhibitors of the rotavirus receptor that binds to glycoproteins of intestinal epithelial cells.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Structure-based drug design techniques on the rotavirus binding domain.
Perform virtual screening of compound libraries (e.g., commercially available databases, in-house libraries) to identify potential inhibitors. Docking simulations will be used to assess the binding affinity and binding mode of candidate compounds to the receptor.
Validation of the inhibitors designed by using cell culture assay. Identify potential sources of discrepancies between simulations and experiments.
Design covalent inhibitors by incorporating electrophilic warheads into the identified candidate compounds. The warheads will be positioned to react with nucleophilic residues (e.g., lysine, serine, cysteine) within the binding site of the receptor.
Conduct molecular dynamics (MD) simulations to assess the stability and binding affinity of the designed covalent inhibitors.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Neyvis Almora Barrios

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): Alechania Misturini Morelli

DEPARTMENT(S): Department of Physical Chemistry

TITLE (Mandatory in English)

Computational Design of Titanium Metal–Organic Frameworks for Selective CO_2 Capture

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Identificar las aminas y la estabilidad de las redes metal-orgánicas de titanio (Ti-MOF) que potencialmente podrían interaccionar fuertemente entre si.

2. Estudiar la incorporación de las aminas en los Ti-MOFs a través de métodos de química computacional.

3. Estudiar la estabilidad termodinámica e identificar las interacciones directoras del sistema amina-Ti-MOFs.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Revisión bibliográfica de las aminas usadas para capturar dióxido de carbono en MOFs.
2. Estudio conformacional de las moléculas seleccionadas en el paso 1, usando técnicas computacionales. Se usaran programas de visualización de estructuras tales como Materials Studio, vmd, gdis, and gview.
3. Estudio de estabilidad de Ti-MOFs. Se optimizaran las geometrías del los cristales con técnicas de campo de fuerza implementadas en códigos tal como GULP.
4. Calculo de la energía de interacción entre las aminas y los Ti-MOFs mas estables (segun el paso 2) usando métodos de Química Clásica.
5. Calcular la energía de adsorción del CO2 en los sistemas mas estables (identificados en el paso 4) amina-Ti-MOFs
6. Comparación de los resultados teóricos con los trabajos experimentales de nuestro grupo FuniMAT (www.icmol.es/funimat).

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Mario Culebras Rubio

ACADEMIC TUTOR 2 RAFAEL BALLESTEROS GARRIDO

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Lignin extraction from agricultural pruning waste for hydrogels preparation

OBJECTVES / 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 mediate 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 alcalinos
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.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 CLARA MARIA GOMEZ CLARI

ACADEMIC TUTOR 2 MARIO CULEBRAS RUBIO

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUIMICA FISICA

TITLE (Mandatory in English)

Lignin/Cu2S Composites for Thermoelectric 3D-Printing Materials

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of the project is to synthesize and characterize Cu2S by different methods. These particles will be mixed with lignin to obtain materials with thermoelectric properties to be used in 3D printers.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project is experimental, as it involves the synthesis and chemical-physical characterization of Cu2S particles and lignin-Cu2S blends.
The student will synthesize different Cu2S particles controlling the structure to obtain good thermoelectric properties. Different porportions of Cu2S will be blended with lignin and other thermoplastic polymers to obtain inks for thermoelectric 3D materials. The physico chemical properties as well as the themoelectric properties will be characterize. 3D printing materials will be obtained an characterize.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 CLARA MARIA GOMEZ CLARI

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUIMICA FISICA

TITLE (Mandatory in English)

Synthesis of thermoplastic polyurethanes with improved thermal resistance

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this project is to obtain thermoplastic polyurethanes with improved thermal resistance by synthesizing and characterizing the thermal and mechanical properties. The solvent-free prepolymer method will be used to obtain polyurethanes based on different grades of polycarbonate diol.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project is experimental, as it involves the synthesis and chemical-physical characterization of thermoplastic polyurethanes.
The student will synthesize different polyurethanes based on polycarbonate diol as a macrodiol, controlling the proportions of the rigid segment and macrodiol. MDI will be used as an isocyanate. Plates will be obtained for chemical-physical characterization. Thermal characterization will be performed using differential scanning calorimetry and thermogravimetric analysis, molecular mass determination, and mechanical characterization of tensile and abrasion resistance properties.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 CLARA MARIA GOMEZ CLARI

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUIMICA FISICA

TITLE (Mandatory in English)

Thermoplastic polyurethanes from sustainable polycarbonatediols

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this project is to synthesize and characterize the thermal and mechanical properties, using the solvent-free prepolymer method, polyurethanes based on different grades of polycarbonate diol obtained from sustainable resources and to characterize their chemical and physical properties.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project is experimental, as it involves the synthesis and chemical-physical characterization of thermoplastic polyurethanes.
The student will synthesize different polyurethanes based on polycarbonate diol as a macrodiol, controlling the proportions of the rigid segment and macrodiol. MDI will be used as an isocyanate. Plates will be obtained for chemical-physical characterization. Thermal characterization will be performed using differential scanning calorimetry and thermogravimetric analysis, molecular mass determination, and mechanical characterization of tensile and abrasion resistance properties.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Juan Aragó March

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Insights into the thermal effects on the enzymatic degradation of polyethylene terephthalate from computational modeling

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The proposed project aims to: 1) analyze the effect of temperature on the recognition and degradation of a polyethylene terephthalate (PET) model by enzymatic action (leaf-branch compost cutinase, LCC), 2) initiate the student in the use of computational chemistry methods and calculation programs as well as in the literature search relevant to the project, and 3) instruct the student in the analysis, structuring and writing up of the research results.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

To provide a plaussible description of thermal behavior of LCC, the student will carry out:

1) A literature survey to identify and select those relevant articles that address the thermal effects on the LCC activity.

2) Classical and hybrid (quantum-classical) simulations to understand at molecular level the enzyme reaction.

3) Implementation of small programs to facilitate the analysis of the simulations.

4) Writing up the results.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Alberto Fernández Alarcón

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Deparment of Physical Chemistry

TITLE (Mandatory in English)

Dissection of the Binding Energy in Protein-Ligand of Potential Anticancer Drugs Candidates

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Objetivo General
Que el estudiante se sumerja en los métodos relacionados con las química computacional, en particular en aquellos centrados en el estudio de la densidad electrónica, y su aplicación en el diseño de medicamentos basado en el estudio por fragmentos.
Objetivos particulares
Analizar, mediante las herramientas de la topología química cuántica de la densidad electrónica, las interacciones no covalentes que dan origen a la formación de complejos proteína-ligando de fármacos con potencial uso en el tratamiento del cáncer.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

El estudio de la topología química cuántica (QCT), mediante el análisis de la función de onda (WFN), permite la recuperación de conceptos químicos fundamentales y una detallada descripción de la naturaleza de la interacción entre estas entidades. Una limitación de la QCT es el número de átomos, pero el diseño de fármacos basado en fragmentos nos da la posibilidad de aplicar la QCT al estudio de complejos proteína-ligante. El proyecto se basa en la búsqueda bibliográfica de los agentes anticancerígenos más prometedores para, después de una optimización geométrica en el marco de la teoría del funcional de la densidad (DFT), obtener la WFN del ligando, el sitio activo de la proteína y el complejo proteína-ligando. El análisis de la WFN mediante metodologías como AIM (átomos en moléculas), IQA (átomos cuánticos interactuantes) y NCI (Interacciones No Covalentes) permitan describir la naturaleza de la interacción –atractiva o repulsiva, iónica o covalente,

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Carlos Bartual Murgui (Dpto. Química Física)

ACADEMIC TUTOR 2 José Antonio Real Cabezos (Dpto. Química Inorgánica)

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

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

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Este trabajo tiene como objetivo introducir al estudiante en la transición de espín en compuestos de hierro(II), mediante la síntesis y caracterización de nuevos polímeros de coordinación 2D con ligandos π-aceptores. Se busca desarrollar materiales multifuncionales que combinen propiedades como transición de espín, fluorescencia, porosidad o comportamiento huésped-anfitrión, con aplicaciones potenciales en sensores o materiales inteligentes.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

El trabajo comenzará con una revisión bibliográfica mediante el uso de bases de datos científicas accesibles desde la UV. A continuación, se llevará a cabo la síntesis de ligandos y complejos metálicos mediante técnicas de química orgánica y métodos de difusión lenta líquido-líquido. Los compuestos obtenidos se caracterizarán mediante espectroscopía IR, difracción de rayos X (monocristalina y en polvo), análisis termogravimétrico (TGA), medidas de adsorción (isotermas) y determinación de la susceptibilidad magnética.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Joaquín Calbo Roig

ACADEMIC TUTOR 2 Enrique Ortí Guillén

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Department of Physical Chemistry

TITLE (Mandatory in English)

First-principles characterization of honeycomb 2D MOFs as porous conductors

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo principal de este trabajo es establecer relaciones de estructura–propiedad en una familia de redes metal-orgánicas (MOFs) bidimensionales con arquitectura tipo panal (honeycomb), explorando modificaciones químicas que permitan guiar el diseño racional de nuevos materiales porosos con conductividad eléctrica. En particular, se analizará el impacto de:
1. El metal de transición empleado como nodo inorgánico.
2. La naturaleza del grupo anclaje del ligando orgánico.
3. El grado de conjugación π del sistema molecular orgánico.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Revisión bibliográfica sobre MOFs 2D de tipo honeycomb construidos a partir de ligandos basados en anillos de benceno, trifenileno y trinaftileno, caracterizados experimental o teóricamente en la literatura.
2. Optimización y análisis estructural de los sistemas cristalinos propuestos, mediante cálculos de tipo DFT (Density Functional Theory).
3. Análisis de estabilidad estructural, si procede, considerando configuraciones alternativas de apilamiento entre capas vecinas (autoensamblaje).
4. Caracterización teórica de las propiedades electrónicas mediante el cálculo de la estructura de bandas, densidad de estados, análisis de cargas y densidad de spin.
5. Evaluación de propiedades de transporte, mediante el cálculo de masas efectivas y/o acoplamientos electrónicos entre unidades electroactivas, como indicadores clave del comportamiento conductor.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR 2 José Juan García Jareño

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

Ion Insertion Batteries. Historical evolution, challenges and future.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Obtain updated information on the current and future status of ionic insertion batteries.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Bibliographic study of different types of ionic insertion.
2. Bibliographic study of problems generated with battery use and recycling.
3. Bibliographic study of battery charging speed and capacity and their evolution.
4. Writing the TFG report

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR 2 José Juan García Jareño

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

Separation of cobalt and nickel metals by selective electrodeposition on different types of electrodes.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Optimization of experimental conditions for cobalt and nickel electrodeposition.
Evaluation of the electrodeposit performance.

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

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jerónimo Agrisuelas Vallés

ACADEMIC TUTOR 2 José Juan García Jareño

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

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

OBJECTVES / 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

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 José Juan García Jareño

ACADEMIC TUTOR 2 Jerónimo Agrisuelas Vallés

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

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

OBJECTVES / 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.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 José Juan García Jareño

ACADEMIC TUTOR 2 Jerónimo Agrisuelas Vallés

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química-Física

TITLE (Mandatory in English)

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

OBJECTVES / 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

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Javier Segarra Martí

ACADEMIC TUTOR 2 Angelo Giussani

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Photochemistry of nitro-alkane derivatives and their role in pollution

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Iniciación en el uso de métodos de cálculo de la química cuántica para el estado excitado y su interpretación, introducidos en el curso de química computacional.
- Investigar la estructura nuclear y electrónica, y los caminos de desactivación y fotodegradación de la reacción R-NO2 + hv --> R· + ·NO2.
- Extraer el papel del tamaño de la cadena de alcanos R y como afecta ésta a la fotodegradación.
- Se instruya en el análisis, estructuración y redacción de los resultados de la investigación.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

La formación de NO y NO2 es una de las principales causas de la contaminación atmosférica proveniente de derivados de nitro-compuestos. En este TFG se propone caracterizar el mecanismo detrás de la fotodegradación de compuestos nitroalcanos como modelos representativos de esta clase de reacciones, siguiendo el plan:

1) Búsqueda bibliográfica para identificar propiedades nucleares y electrónicas del nitrometano tanto teórica como experimentalmente.
2) Determinación de propiedades electrónicas y espectroscópicas de diferentes nitroalcanos mediante los métodos teóricos CASSCF/CASPT2.
3) Análisis de los resultados obtenidos y comparativa espectroscópica con los resultados experimentales encontrados en la bibliografía, a modo de proveer de una descripción atomística de dicha reacción de fotodegradación.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Javier Segarra Martí

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Physical Chemistry

TITLE (Mandatory in English)

Microsolvation effects on the photophysical reactivity of DNA model systems

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- To understand how microsolvation affects the UV-Vis radiation absorption in DNA/RNA chromophores and the ensuing reactivity, which is key to rationalising their photostability
- To introduce the student to the field of computational chemistry, particularly to the simulation of electronic excited states and their interpretation, including spectroscopy and reactivity
- To gain data handling competencies, including parsing and curating data using basic programming tools like Python

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

DNA/RNA nucleobases (Ade, Cyt, Thy, Ura, and Gua) encode our genetic material and are key to life. However, exposure to UV-Vis radiation has been linked with deleterious societal concerns like skin cancer/melanoma. While the effects of UV-Vis radiation on our genetic lexicon are well understood in the gas phase, it remains unclear how the biological media in which DNA is embedded affects the photophysics of the nucleobases. This project proposes modelling simple DNA/RNA systems under different microsolvation conditions to understand how specific solvent positioning may affect reactivity, and whether a systematic increase in microsolvation can bridge the gap with the photo-properties in the condensed phase. To do this, the following plan will be followed:

1) In-depth search of the literature for the different models and experiments available
2) Modelling the UV-Vis absorption spectrum and excited state relaxation pathways of selected microsolvated DNA/RNA species
3) Analyse the results obtained and contrast them against results found in the literature

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Kirill Zinovjev

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Multiscale modelling of chemical reactivity with machine learning potentials

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The project will be dedicated to training a multiscale machine learning / molecular mechanics (ML/MM) model for a chemical reaction (to be chosen together with the student). It will involve performing quantum chemical (QM) calculations, ML model training and molecular dynamics (MD) simulations to obtain reaction free energy profiles.
Specific objectives:
- Obtain initial training set for the ML model training by performing QM calculations
- Train the ML potential and the embedding model
- Obtain reaction free energy profile
- Evaluate model performance by comparing to reference QM/MM calculations

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

QM calculations (ORCA)
Machine Learning (PyTorch, MACE)
Molecular Dynamics (OpenMM)
Data Analysis (Python)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Antonio Francés Monerris

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Dep. Química Física

TITLE (Mandatory in English)

Molecular mechanism of the synthesis of N-heterocyclic carbene Fe(II) complexes studied by electronic structure methods

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This project aims to identify the molecular mechanism, i.e. involved electronic states, atom reorganization, driving forces, influence of the ligand, etc. that take place during the synthesis of Fe(II) complexes bearing N-heterocyclic carbene ligands. These complexes are of high interest in the production of photoactive devices in general, such as green technologies like solar energy storage.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry and Inorganic Chemistry. The subject Computational Chemistry is strongly advised. Quantum chemistry software will be used to determine the energy profiles of each reaction step, including relaxed potential energy surfaces and coordinate interpolations, among others.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 M.Carmen Martínez Bisbal

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): Andrea Bernardos Bau

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Design and development of new antimicrobial biosystems for biotechnological applications.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Design, synthesis, characterization and validation of new antimicrobial systems against specific microorganisms. Objective 1: Design and synthesis of new materials containing bioactive molecules for the elimination of microorganisms. Objective 2: Bioactive molecules-controlled release from the antimicrobial systems detected by 1H-NMR spectroscopy. Specific objective 3: In vitro validation of new nanoparticles containing bioactive molecules against pathogens such us Botritis cinerea, Escherichia coli and Staphylocos aureus, among others.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

One of the strategies for the development of these new antimicrobial materials is the design of hybrid systems loaded with bioactive molecules or functionalized with biomolecules, controlling the release of bioactive molecules. Organic-inorganic hybrid systems will be prepared with "molecular gates" loaded with bioactive compounds, and functionalized on the external surface with organic molecules. The release of active substances will be carried out by the presence of suitable stimuli such as enzymes exogenated by different pathogens using NMR techniques.
Then antimicrobial assays will be developed for the in vitro validation of new antimicrobial materials containing bioactive molecules against pathogens such us Botrytis cinerea, Escherichia coli and Staphylocos aureus, among others.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 M.Carmen Martínez Bisbal

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Determination of changes in the composition of neonatal saliva by NMR spectroscopy

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This work aims to study the impact of the type of breastfeeding on the saliva of newborns using nuclear magnetic resonance spectroscopy (NMR).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Samples (neonatal saliva) will be prepared for the acquisition of NMR spectra.
Once the NMR spectra are acquired, they will be processed and the signals will be integrated.
Then the signals integrated in the different spectra will be studied statistically to determine the differences in the metabolic profile.
Likewise, the resonances that undergo changes according to the lactation received will be identified.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 M.Carmen Martínez Bisbal

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

Study of the vulnerability of atheroma plaques in cell culture samples by NMR spectroscopy

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Determination of differences in NMR spectra in cell culture samples from atheroma plaques from patients.

Relation of these differences to vulnerability of plaques and determination of their potential as a diagnostic support tool for atheroma plaque vulnerability.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Atheroma plaques from patients (symptomatic > vulnerable plaque; asymptomatic > stable, non-vunerable plaque) have already been obtained, cells from plaques (vascular smooth muscle cell, VSMC) obtained and cultured, and NMR spectra acquired.

In this work 1D proton spectra with suppression of the water signal from VSMC cell cultures will be processed and analysed. The published literature on the subject and metabolomics databases will be consulted for the assignment of resonances.

Once the main resonances have been identified, the signals present in the spectra will be integrated and will undergo univariate and/or multivariate statistical study. An attempt will be made to determine the discriminating variables (biomarkers) to identify samples (VSMC cells) from vulnerable and stable atheroma plaques.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): Antonio Francés Monerris

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

DNA binding energies of indole-like biomolecules

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Binding free energies of ligands in DNA allow to analyze the stability of the complexation with nucleic acids and to quantify the relative population of such ligands in DNA with respect to the surrounding aqueous environment. In this proposal, the student will determine the binding free energies of indole-like biomolecules, such as melanin monomers, serotonin, melatonin, and tryptophan, and their dioxetane derivatives. These dioxetane molecules are harmful for the normal cellular functioning because they can induce DNA damage.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry. Molecular dynamics simulations will be performed using Newton mechanics and molecular potentials to explore all the relevant conformational space of the complex and the unbound system connecting both of them to obtain the free energy change. Enhanced sampling techniques will be also used to accelerate the exploration.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): Javier Segarra Martí

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

Free energies of cations and anions of nucleobases in DNA: A computational study

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

The ionization potentials and electron affinities of DNA nucleobases in the gas phase and aqueous solution is well determined both experimentally and theoretically. However, in the environment of nucleic acids, such property is not well known despite its relevance to understand the role of nucleobase cations and anions in the physiological conditions.

In this proposal, the student will use statistical thermochemistry and quantum chemistry to determine the free energies of the cations and anions of nucleobases with respect to the neutral systems in the DNA environment. The implications for the biological functions of nucleic acids will be also discussed.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry, or in the Double Degree of Chemistry and Physics in the subject Elements of Physical Chemistry. Hybrid methods combining quantum and classical mechanics will be used. Molecular dynamics simulations will be also performed to obtain the free energy change in the process of transforming a neutral nucleobase into a cation or anion in the DNA environment.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): David Francisco Macias Pinilla

EXTERNAL TUTOR (if needed):

Department: Química Física

TITLE (Mandatory in English)

Effect of anharmonicity in the quantum-chemistry determination of absorption electronic spectra

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Determining the absorption electronic spectra by computational chemistry is useful for short-lived or unstable molecular systems difficult to capture experimentally. Most of the common approaches in computational chemistry consider the effects of nuclear vibrations by the harmonic modelling. However, for low-frequency modes, anharmonicities might give play an important role, especially at the red-tail of the electronic spectra.

The goal of this proposal is to implement anharmonic corrections in current models and evaluate the effect of such corrections in the computed spectra. Molecules of interest in atmospheric chemistry will be choosen for such purpose

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry, or in the Double Degree of Chemistry and Physics in the subject Elements of Physical Chemistry. Quantum chemistry calculations will be done to determine the vibrational wave functions with and without anharmonicities. They will be used to compute excitation energies and associated oscillator strengths and subsequently the spectra.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Daniel Roca Sanjuán

ACADEMIC TUTOR (if needed): Ana María Borrego Sánchez

EXTERNAL TUTOR (if needed):

Department: Química Física (DRS) y Farmacia y Tecnología Farmacéutica y Parasitología (AMBS)

TITLE (Mandatory in English)

Computational Modeling of the DNA unbinding dynamics of indole-like biomolecules

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

Under the conditions of immflamation and oxydative stress, in the human body, indole-like biomolecules, such as melanin monomers, serotonin, melatonin, and tryptophan, can undergo chemical transformations giving rise to dioxetane derivatives. These dioxetanes are harmful for the normal cellular functioning because they can induce DNA damage.

One important step to understand how harmful are the mentioned dioxetanes for damagind our genetic code is to determine the binding properties to the nucleic acids because in order to produce DNA damage these molecules must first bind the DNA structure. This will we the goal of the present proposal: to determine the mechanism, energetics and time that for the

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

The student will use the knowledge acquired in the Degree in Chemistry, in particular, in the subjects of Physical Chemistry II and III and Computational Chemistry. Molecular dynamics simulations will be performed using Newton mechanics and molecular potentials to simulate the dynamics of the interaction between the dioxetanes and DNA. Enhanced sampling techniques will be also used to accelerate the simulation and integrate Newton's equations untill the micro- and mili-seconds time scale.

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jose Jaime Baldovi Jachan

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Física

TITLE (Mandatory in English)

First principles study of a family of Layered Double Hydroxides (LDHs) for catalysis and water treatment

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Caracterizar estructuralmente una familia representativa de LDH y determinar con precisión sus propiedades electrónicas

2. Calcular los perfiles de energía libre de reacción para estudiar mecanismos catalíticos relevantes

3. Evaluar el potencial de LDH de Mn y Co para la activación de radicales en procesos de descontaminación de aguas

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Revisión bibliográfica de LDHs para procesos catalíticos y tratamiento de aguas.

2. Generación de diferentes estructuras aleatorias variando la concentración relativa entre ambas especies metálicas (Ni1-xFex, Co1-xFex y Mn1-xFex) manteniendo las simetrías propias del sistema.

3. Construcción de diagramas de energía libre para mecanismos catalíticos, identificación de etapas limitantes y cálculo de sobrepotenciales teóricos.

4. Modelado estructural de LDH basados en Mn y Co, incluyendo configuraciones con diferentes proporciones metálicas y sustituciones isoestructurales, así como la optimización de superficies activas y análisis de su estabilidad