DEPARTAMENT DE QUÍMICA FÍSICA TFG 25-26

NÚMERO DE TEMA	TEMA	TUTOR(S) ACADÈMIC(S) (si un és d'un altre departament, posa'l entre parèntesi)	TUTOR EXTERN (si escau)	Observaciones
3	Derivatives of polyaromatic systems: Synthesis, characterization and calculation of properties.	Begoña Milian Medina/ Rafael Ballesteros Garrido(Q.Orgánica)		
6	Photoactive Nanoparticles Prepared by Miniemulsion Polymerization	Rafael Muñoz Espí/María González Béjar(Q.Orgánica)		
7	Polysaccharide-Based Hybrid Particles as Magnetically Separable Catalysts	Rafael Muñoz Espí/Francisco F. Pérez Pla		
10	Encapsulation of Phase Change Materials through Valorization of Lignocellulosic Waste	Rafael Muñoz Espi/Mario Culebras Rubio		
16	Theoretical Analysis of Dynamical Motions in Biomolecular Motors.	Iñaki Tuñón/Jose Javier Ruiz		
18	Preparation and evaluation of the catalytic activity of sustainable nickel nanoparticle catalysts deposited on carbonized polydopamine supports.	Francisco F. Pérez Pla/Mª Angeles Úbeda Picot(Q.Inorgánica)		
20	Application of Virtual Reality and Augmented Reality in Chemistry Learning	Jesús Vicente de Julián		
21	Simulation of Membrane Proteins in the Presence of Electric Fields	Jesús Vicente de Julián		

22	Desing or Rotavirus Inhibitor Compounds	Jesús Vicente de Julián		
23	Computational Design of Titanium Metal–Organic Frameworks for Selective CO_2 Capture	Neyvis Almora Barrios		
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		
29	Dissection of the Binding Energy in Protein-Ligand of potencial 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 Guillém		
33	Separation of cobalt and nickel metals by selective electrodeposition on different types of electrodes.	Jerónimo Agrisuelas Valles/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 Valles/José Juan García Jareño		
35	Electrogeneration and characterization of poly(phenosafranine) on stainless steel.	Jerónimo Agrisuelas Valles/José Juan García Jareño		

37	Photochemistry of nitro-alkane derivatives and their role in pollution	Javier Segarra Marti/Angelo Giussani		
38	Microsolvation effects on the photophysical reactivity of DNA model systems	Javier Segarra Martí		
40	Molecular mechanism of the synthesis of N-heterocyclic carbene Fe(II) complexes studied by electronic structure methods	Antonio Fránces Monerris		
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 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: 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): 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 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 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 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 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 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)

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 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 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 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