

DEPARTAMENT DE QUÍMICA INORGÀNICA

NÚMERO	TEMA	TUTOR(S) ACADÈMIC(S) (si un és d'un altre departament, posa'l entre parèntesi)	TUTOR EXTERN (si escau)
1	Iron based molecular switches as advanced materials for storage and display information	Ana Belén Gaspar Pedrós	
2	Synthesis and characterisation of photocatalysts for energy conversion reactions based on hetroestructures of Layeres Double Hydroxides (LDHs) and graphene	Antonio Luis Ribera Hermano	
3	Synthesis of Layered-Double-Hydroxides (LDHs) based photocatalysts for Energy Conversion Reactions using Non-Conventional Methods	Antonio Luis Ribera Hermano	
4	Evaluation of the Biological Activity of Metal Complexes with Heterocyclic Diamines	Begoña Verdejo Viu	
5	Chromium-substituted polyoxomolybdates: synthetic strategies, structural diversity and applications	Carlos Giménez Saiz	
6	Chromium-substituted polyoxotungstates: synthetic strategies, structural diversity and applications	Carlos Giménez Saiz	
7	Systematic study of the gas-solid phase reactivity of transition metal-containing Metal organic Frameworks (MOFs)	Carlos J. Gómez García - Sam Benmansour Souilamas	
8	Cobalt (II) pyrazolate MOFs with coordination vacancies: dynamics and stability of monovalent species	Carlos Martí Gastaldo	
9	Porous chiral frameworks built from helical Fe(II)-Pyrazolate chains	Carlos Martí Gastaldo	
10	Crystal growth of layered selenides for new atomically thin ferroelectric materials	Efrén Navarro Moratalla	
11	Synthesis of layered hydroxides as new candidates for quantum spin liquids	Efrén Navarro Moratalla	
12	Design and synthesis of bioMOFs and their application in environmental remediation	Emilio Pardo Marín	
13	Encapsulation of quantum dots in hybrid matrices and study of the optical properties	Emilio Pardo Marín	
14	Host-guest chemistry of metal-organic frameworks (MOFs) and their use in water remediation	Emilio Pardo Marín	
15	Catalytic applications of self-assembled hydrolytic metallocages	Enrique García-España Monsonís	

16	Tripodal polyamines for nucleic acid recognition	Enrique García-España Monsonís	
17	Luminiscent Nanocomposites without the inclusion of fluorophores	Enrique García-España Monsonís	
18	Antioxidant applications of liposome encapsulated polyamine metal complexes	Enrique García-España Monsonís - Teresa Albelda Gimeno	
19	Synthesis of Novel Fluorescent Polyamine Ligands and Evaluation of the Antioxidant Activity of Their Metal Complexes	Estefanía Delgado Pinar - José Miguel Llinares Belenguer (Química Orgánica)	
20	Current status and perspectives of iridium complexes as possible anti-cancer agents	Francisco José Martínez Lillo	
21	High entropy layered double hydroxides for green hydrogen production	Gonzalo Abellán Sáez	
22	Meta-Layered Hydroxides for energy Storage	Gonzalo Abellán Sáez	
23	Preparation of Electrode Materials Based on Two-Dimensional Materials for Green Hydrogen Production	Gonzalo Abellán Sáez	Eduarne Nuin
24	Synthesis of Perilenebisimides for Functionalization of Two-Dimensional Materials	Gonzalo Abellán Sáez	Eduarne Nuin
25	Exploring the Ti-based synthesis of Layered Double Hydroxides	Gonzalo Abellán Sáez - Rebeca Martínez Haya (Dept. Ingeniería Química ETSE)	
26	Two-dimensional Phosphorene: discharge agents for intercalated black phosphorous compounds	Gonzalo Abellán Sáez - Rebeca Martínez Haya (Dept. Ingeniería Química ETSE)	
27	Mesoporous MOFs for large molecule encapsulation	Guillermo Mínguez Espallargas - Jorge Salinas Uber	
28	Metalloligand-based MOFs	Guillermo Mínguez Espallargas - Jorge Salinas Uber	
29	Optimizing the properties of metal halide perovskites for photovoltaic applications	Hendrik Jan, Bolink	
30	Development of MOF-Based Electrocatalysts for Nitrate Reduction	Isabel Abánades Lázaro - Joaquín Soriano López	
31	Sustainable synthesis of mesoporous fertilizers from rice production waste	Jamal El Haskouri Bennagi	
32	Rice Revaluation: New Materials for a Sustainable Future	Jamal El Haskouri Bennagi - Miriam Benítez Serra	
33	Metal-Organic Frameworks Composites for Environmental Applications	Jesús Ferrando Soria	

34	Shaping of Metal-Organic Frameworks for Environmental Applications	Jesús Ferrando Soria	
35	Evaluation of intermolecular interactions in the formation of molecular crystals	Joan Cano Boquera	
36	Theoretical Reflections on the Spin Crossover Phenomenon	Joan Cano Boquera	
37	Developing ligands to target G-Quadruplexes	Jorge González García	Cristina Galiana Roselló
38	Identification of putative G-Quadruplexes forming sequences involved in candida	Jorge González García	Cristina Galiana Roselló
39	Strategies for degrading RNAs	Jorge González García	Ariadna Bargiela Schonbrunn
40	The Spin Crossover Phenomenon in Iron (II) Complexes	José Antonio Real Cabezos - Carlos Bartual Murgui (Química Física)	
41	Development of materials for agricultural applications	Jose Vicente Ros Lis	
42	Development of sustainable strategies for chemical synthesis	Jose Vicente Ros Lis	
43	Development of Semiconductor Thin Films via Physical Vapor Deposition Methods for Application in Optoelectronic Devices	Kassio Zanoni	
44	Preparation and evaluation of the catalytic activity of sustainable iron nanoparticle catalysts deposited on carbonized polydopamine supports	M ^a Ángeles Úbeda Picot - Francisco F. Pérez Pla (Química Física)	
45	Colloidal synthesis of 2D materials based on pnictogen elements	Matteo Andrea Lucherelli - Gonzalo Abellán	
46	Production of metal-doped carbon nano onions (CNOs) for energy applications	Matteo Andrea Lucherelli - Gonzalo Abellán	
47	Thin-film photodetectors based on unconventional semiconductors	Michele Sessolo	
48	Multifunctional spin crossover compounds	Miguel Clemente León	
49	Sustainable synthesis of reticular porous materials	Mónica Giménez Marqués	
50	Mechanochemically functionalised porous silicas: a sustainable strategy	Pedro José Amorós del Toro	
51	Mesoporous silicas with ultra-large pores for delivery applications	Pedro José Amorós del Toro	
52	In-Situ Synthesis of NiOx Films for Efficient Hole Transport Layer in Perovskite Solar Cells	Rafael Abargues López	
53	In-Situ Synthesis of SnO2 Films for Electron Transport Material in Perovskite Solar Cell	Rafael Abargues López	
54	In-Situ synthesis of transparent electrically conducting polymers for Perovskite-based Photovoltaics and LEDs	Rafael Abargues López	
55	Lead-Free Double Perovskites Nanocomposite for Photodetectors, Photocatalysis and Memristors	Rafael Abargues López	

56	Luminiscent Nanocomposites for High-Efficiency and Large-Area LEDs	Rafael Abargues López	
57	Synthesis of 0D perovskite nanocrystals for optoelectronic devices	Rafael Abargues López	
58	Structural and Anti-oxidant properties of Metal coomplexes with small azamacrocycles	Salvador Blasco Llopis - Begoña Verdejo Viu	
59	Exploring the performance of known MOFs based on copper for diverse vapour capture	Sam Benmansour Souilamas	
60	Investigating the reactivity of known zinc MOFs towards different vapour and gases	Sam Benmansour Souilamas	
61	Synthesis and characterisation of new metal complexes using anilato organic ligands and transition metals	Sam Benmansour Souilamas	
62	Synthesis of Ultrastable Metal-Organic Frameworks Based on azolate-Type Ligands	Sergio Tatay Aguilar	
63	Solvent-free synthesis of stable azolate metal-organic frameworks	Víctor Rubio Giménez	

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Ana Belén Gaspar Pedrós

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): ICMOL (Institute of Molecular Science); Inorganic Chemistry

TITLE (Mandatory in English)

Iron based molecular switches as advanced materials for storage and display information

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The research goal of this proposal is the synthesis of iron based molecular materials exhibiting electronic bi-stability driven by an electrical field. An iron molecular switch addressable by electronic means will impact on the potential technological applications of iron based molecular materials in electronic devices.

To be sensitive to electrical fields the iron molecular switch must be asymmetric and possess a high dipole moment. This molecular architecture will be achieved by exploiting the versatility and functionality of organic and coordination chemistry.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1- Designing the proposed system. After an adequate bibliographic work, the choice of the metallic salt, the monomeric or polynuclear nature of the compound to synthesise, the selection of the peripheral and bridging ligands and the solvents will be made at this stage. In many cases the ligands are not commercially available and will require a previous synthetic organic chemistry.

2- Synthesis. The preparation of the compounds will be carried out using techniques of solution chemistry in inert atmosphere. The crystallogenesis of the compounds will depend on the nature of the solid to be synthesised. Typically, it will require slow evaporation in an argon stream or the use of H-shaped diffusion vessels. Elemental analytical characterisation, electronic microscopy (polymetallic systems), thermal analysis, IR spectroscopy, etc. will be done.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Antonio L. Ribera Hermano

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Synthesis and characterisation of photocatalysts for energy conversion reactions based on heterostructures of Layered Double Hydroxides (LDHs) and graphene

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- * Síntesis de heteroestructuras a partir de hidróxidos dobles laminares (LDHs) y grafeno para reacciones como reducción de CO₂, disociación del agua (water splitting) y fijación de nitrógeno.
- * Los catalizadores preparados se caracterizarán mediante las técnicas habituales para este tipo de materiales (PDRX, análisis elemental, SEM, TG, etc.) así como técnicas más específicas (espectroscopía UV-Vis, electroquímica, etc.).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- * Síntesis. A) Sintetizar los sistemas LDH precursores que contengan los metales de transición elegidos, optimizando la composición química de los mismos y el método de síntesis: i) método tradicional de coprecipitación a pH constante; ii) método de precipitación homogénea con ARRr como generadores de pH básico; iii) método hidrotermal con Urea; iv) método solvotermal en metanol que permita el control morfológico del material para conseguir morfologías especiales; v) método con disolventes que dificultan el apilamiento para obtener materiales con pocas capas. B) Obtener grafeno a partir de compuestos ricos en carbono. C) Preparar heteroestructuras a partir de LDH y grafeno por métodos "in situ" que garanticen una adecuada interfase entre los precursores
- * Caracterización. Las heteroestructuras preparadas serán caracterizadas mediante técnicas convencionales (difracción de RX, análisis elemental, SEM, etc.) así como por técnicas más específicas, como espectroscopia UV-Vis y sobre todo una exhaustiva caracterización electroquímica para el estudio de los centros activos.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Antonio L. Ribera Hermano

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Synthesis of Layered-Double-Hydroxides (LDHs) based photocatalysts for Energy Conversion Reactions using Non-Conventional Methods.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- * Síntesis de fotocatalizadores basados en hidróxidos dobles laminares (LDHs) utilizando métodos no-convencionales, para reacciones como reducción de CO₂, disociación del agua (water splitting) y fijación de nitrógeno .
- * Los catalizadores preparados se caracterizarán mediante las técnicas habituales para este tipo de materiales (PDRX, análisis elemental, SEM, TG, etc.) así como técnicas más específicas (espectroscopía UV-Vis, IES, etc.).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- * Diseñar y sintetizar sistemas LDH combinando diferentes metales divalentes, trivalentes y tetravalentes, utilizando un molino planetario y aplicando técnicas mecanoquímicas. El uso de estas estrategias sintéticas permiten reducir, incluso prescindir del uso de disolventes, dando lugar a procesos más respetuosos con el medio ambiente.
- * Como paso previo se establecerán las condiciones de uso del molino planetario necesarias para obtener sistemas LDH.
- * La caracterización de los sistemas LDH preparados se llevará a cabo combinando técnicas básicas como Difracción de Rayos X (DRX), Microscopia Electrónica de Barrido (SEM), Análisis Termogravimétrico (TGA), Análisis Elemental, etc. con técnicas más específicas como UV-Vis por Reflectancia Difusa y Espectroscopía de Impedancia Electroquímica (EIS).
- * Los resultados derivados de la caracterización serán utilizados para mejorar los procesos de síntesis.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

BEGOÑA VERDEJO VIU

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): INORGANIC CHEMISTRY

TITLE (Mandatory in English)

Evaluation of the Biological Activity of Metal Complexes with Heterocyclic Diamines

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Synthesis and characterisation of the acid-base behaviour and coordination chemistry of heterocyclic diamines.
- Study of the redox behaviour and antioxidant capacity of metal complexes against reactive oxygen species (ROS), using specific in vitro assays.
- Evaluation of carbonic anhydrase activity

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Using synthetic routes developed and optimised by the Supramolecular Chemistry group at the University of Valencia, new metal complexes with polyamine ligands will be synthesised, selected for their potential antioxidant activity. The study of the acid-base properties, as well as the stability and redox behaviour of metal complexes complexes, will be carried out using potentiometry and electrochemistry techniques in aqueous or hydroalcoholic media. To complement these studies, spectroscopic techniques such as UV-Vis, fluorescence and NMR will be used to characterise both the complexes and their interaction with reactive oxygen species (ROS). Their antioxidant efficacy will also be evaluated using specific radical scavenging assays and in vitro tests. Finally, attempts will be made to obtain suitable crystals for structural analysis by X-ray diffraction.

**DEGREE FINAL PROJECT
 CHEMISTRY DEGREE**

ACADEMIC TUTOR 1

Carlos Giménez Saiz

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Chromium-substituted polyoxomolybdates: synthetic strategies, structural diversity and applications

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Objective 1: To compile the different syntheses, strategies for modification, characterizations as well as diverse applications of Cr-containing polyoxomolybdates.

Objective 2: To catalogue the available literature on the synthesis and applications of Cr-polyoxomolybdates, modified via functionalization as well as supporting.

Objective 3. To provide in-depth insights, and a fundamental, representative and comprehensive overview of the work done so far in this field, emphasizing on industrially viable catalytic systems.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

This is a BIBLIOGRAPHIC research work. The main working tools will be: the Web of Science database, the programs Conquest and Mercury from the Cambridge Structural Database, and the Inorganic Crystal Structure Database. The scientific articles published to date on the proposed topic will be compiled and classified according to the different synthetic strategies, parent structures of the compounds involved, their ligand modifications, and their applications. The written report will include a description of the methods and tools used for the bibliographic survey, as well as a reference compilation and classification.

The possibility of submitting a review article on this topic for publication in a scientific journal will be considered, depending on the depth of the bibliographic work undertaken by the student.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Chromium-substituted polyoxotungstates: synthetic strategies, structural diversity and applications

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Objective 1: To compile the different syntheses, strategies for modification, characterizations as well as diverse applications of Cr-containing polyoxotungstates.

Objective 2: To catalogue the available literature on the synthesis and applications of Cr-polyoxotungstates, modified via functionalization as well as supporting.

Objective 3. To provide in-depth insights, and a fundamental, representative and comprehensive overview of the work done so far in this field, emphasizing on industrially viable catalytic systems.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

This is a BIBLIOGRAPHIC research work. The main working tools will be: the Web of Science database, the programs Conquest and Mercury from the Cambridge Structural Database, and the Inorganic Crystal Structure Database. The scientific articles published to date on the proposed topic will be compiled and classified according to the different synthetic strategies, parent structures of the compounds involved, their ligand modifications, and their applications. The written report will include a description of the methods and tools used for the bibliographic survey, as well as a reference compilation and classification.

The possibility of submitting a review article on this topic for publication in a scientific journal will be considered, depending on the depth of the bibliographic work undertaken by the student.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Carlos J. Gómez García

ACADEMIC TUTOR 2 Sam Benmansour Souilamas

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Systematic study of the gas-solid phase reactivity of transition metal-containing Metal Organic Frameworks (MOFs)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Sintetizar MOFs con estructuras porosas y metales de transición con posiciones de coordinación vacantes o lábiles
- Realizar un estudio sistemático de la reactividad de los MOFs preparados en presencia de distintos gases reactivos y vapores de disolventes
- Obtención de monocristales de los MOFs precursores y de los MOFs formados en las reacciones con gases y vapores de disolventes
- Caracterización de la estructura de los MOFs obtenidos
- Caracterización de las propiedades magnéticas de los MOFs obtenidos

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se empezará por una búsqueda bibliográfica de aquellos MOFs sencillos de sintetizar que posean porosidad y centros metálicos fácilmente accesibles. Se realizará la síntesis de dichos MOFs o bien de sus derivados con distintos metales de transición. Se estudiará la reactividad, en cámara cerrada, de estos MOFs frente a distintos reactivos gases y vapores de disolventes. Se realizará la caracterización estructural por difracción de rayos-X en monocristal, tanto de los MOFs precursores como de los obtenidos por reacción gas-sólido. Se procederá a la caracterización de las propiedades magnéticas de los nuevos MOFs obtenidos.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Carlos Martí Gastaldo

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Cobalt(II) pyrazolate MOFs with coordination vacancies: dynamics and stability of monovalent species

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El trabajo será de carácter experimental y se centrará en la síntesis de frameworks metal-orgánicos de cobalto(II) y pirazolato mediante química de disolución y síntesis solvotermal de cristales. Se estudiará el control de vacantes de coordinación y su ocupación por especies monovalentes (protones, cloruros) mediante técnicas in operando de difracción de rayos X e infrarrojo, con temperatura variable y atmósferas controladas de gases y disolventes. Además, se realizarán experimentos de valoración para analizar el consumo de protones en presencia de bases. Se evaluará la estabilidad estructural de los materiales frente a condiciones de pH extremo y durante el envejecimiento en cámaras de atmósfera controlada.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Diseñar y sintetizar frameworks metal-orgánicos de cobalto(II) y pirazolato mediante química de disolución y síntesis solvotermal.
- Generar materiales con vacantes de coordinación controladas y accesibles a especies monovalentes como protones o aniones cloruro.
- Caracterizar la estructura y la ocupación de las vacantes mediante técnicas in operando de difracción de rayos X e infrarrojo con temperatura variable y atmósfera controlada.
- Estudiar la dinámica de intercambio de especies monovalentes en las vacantes y su comportamiento frente a bases mediante experimentos de valoración.
- Analizar la estabilidad estructural de los materiales en condiciones extremas de pH (ácidas y básicas) y tras ensayos de envejecimiento en atmósfera controlada.
- Explorar preliminarmente el potencial de estos materiales como modelos para catálisis heterogénea en procesos de transferencia acoplada de electrones y protones (PCET).

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Carlos Martí Gastaldo

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Porous chiral frameworks built from helical Fe(II)-pyrazolate chains

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El trabajo será de carácter experimental. El estudiante llevará a cabo la síntesis de materiales de tipo Metal-Organic Framework (MOF) mediante técnicas de química de coordinación en disolución, utilizando sales de hierro(II) y ligandos derivados de aminoácidos sintéticos como agentes estructurantes quirales. Las síntesis se realizarán en atmósfera inerte mediante el uso de cajas secas o equipos de Schlenk, con el fin de evitar la oxidación del hierro(II). Se optimizarán las condiciones para obtener redes cristalinas y porosas de tipo MOF. Los materiales obtenidos se caracterizarán mediante difracción de rayos X de monocristal y de polvo, microscopia SEM, análisis termogravimétrico y mediciones de porosidad (adsorción de gases).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Diseñar y sintetizar frameworks metal-orgánicos microporosos basados en cadenas helicoidales de hierro(II) y ligandos quirales derivados de aminoácidos sintéticos.
- Desarrollar procedimientos sintéticos que permitan obtener redes cristalinas estables en atmósfera inerte, preservando el estado de oxidación del hierro(II).
- Determinar la estructura cristalina de los materiales y correlacionarla con la helicidad de las cadenas y la quiralidad global del framework.
- Evaluar las propiedades porosas mediante técnicas de adsorción de gases y establecer su relación con la disposición helicoidal de las cadenas metálicas.
- Estudiar la actividad óptica de los materiales mediante técnicas de dicroísmo circular, analizando el efecto de la organización helicoidal y de la quiralidad del framework.
- Explorar las propiedades eléctricas de los materiales mediante medidas de conductividad, con especial atención al posible comportamiento de valencia mixta inducido por la presencia de Fe(II/III).

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Efrén Navarro Moratalla

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Crystal growth of layered selenides for new atomically thin ferroelectric materials

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Estudio de la técnica de crecimiento de cristales por flujo.
2. Empleo de esta técnica para la obtención de monocristales de alta calidad y gran tamaño de seleniuros de indio laminares.
3. Aislamiento de un cristal de una sola capa atómica de un seleniuro metálico ferroelectrico.
4. Caracterización química y física del sistema.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se sintetizarán cristales de seleniuro de indio mediante crecimiento por transporte en un fundido (flujo), centrándose en el sistema de fosfoseleniuro de cobre e indio. Para ellos primero se estudiará el proceso de crecimiento cristalino por flujo y se ajustarán las estequiometrías y condiciones de reacción para optimizar la cristalinidad y tamaño de los cristales, que se cultivarán en ampollas de sílice durante varios días. Las muestras se caracterizarán mediante técnicas físico-químicas (como microscopía electrónica, la dispersioón Raman y difracción de rayos X).

Una vez obtenidos cristales de alta calidad, se aislarán monocapas mediante exfoliación mecánica, manipulándolos en atmósfera inerte para evitar su oxidación. Las monocapas se encapsularán para su posterior caracterización física.

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Efrén Navarro Moratalla

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Synthesis of layered hydroxides as new candidates for quantum spin liquids

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Estudio de procesos solvotermales para el crecimiento cristalino.
2. Empleo de estos métodos para el crecimiento de cristales de hidróxidos simples e hidróxidos dobles laminares (LDHs) con espín neto (magnéticos)
3. Familiarización con los métodos de caracterización de monocristales, aplicando estas técnicas a los cristales crecidos.
4. Caracterización magnética preliminar de los cristales obtenidos para identificar posibles rasgos de topografías magnéticas exóticas, como ahora son los líquidos de espín cuánticos.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Para sintetizar materiales tipo hidróxido se emplearán métodos modernos heterogéneos de crecimiento cristalino, como por ejemplo los que controlan el pH mediante compuestos que liberan amoníaco por descomposición térmica a altas presiones, controlando bien las condiciones de crecimiento. La cristalización se llevará a cabo en autoclaves para alcanzar las altas presiones necesarias.

Se trabajará con hidróxidos simples como introducción a estas técnicas de crecimiento, para luego avanzar hacia composiciones más complejas con distintos metales (como cobre o manganeso), ajustando sus proporciones para favorecer estados magnéticos exóticos como líquidos de espín cuánticos, aplicación final de interés de estos compuestos.

Finalmente, se realizará la caracterización de los materiales obtenidos (difracción de rayos-X, análisis de metales, Raman,...) en incluso se podrá llegar a estudiar su magnetismo por medidas de SQUID para estudiar la posible consecución del estado de líquido de espín buscado.

VNIVERSITAT
E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Emilio Pardo Marín

ACADEMIC TUTOR (if needed):

EXTERNAL TUTOR (if needed):

Department: Química Inorgánica

TITLE (Mandatory in English)

Design and synthesis of bioMOFs and their application in environmental remediation

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Preparación de nuevos polímeros de coordinación porosos (en inglés MOFs) a partir de biomoléculas orgánicas, que presenten gran estabilidad en agua y con la funcionalización adecuada para la captura de contaminantes del agua.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

- Preparación de ligandos orgánicos a partir de biomoléculas mediante técnicas de síntesis orgánica.
- Preparación de bioMOFs utilizando métodos racionales de autoensamblaje.
- Caracterización de los materiales sintetizados por difracción en rayos X, ATG, IR, isothermas de adsorción etc.
- Evaluación de la actividad descontaminante mediante técnicas analíticas.

(Department stamp)

VNIVERSITAT
E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Emilio Pardo Marín

ACADEMIC TUTOR (if needed):

EXTERNAL TUTOR (if needed):

Department: Química Inorgánica

TITLE (Mandatory in English)

Encapsulation of quantum dots in hybrid matrices and study of the optical properties.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Preparación de nuevos polímeros de coordinación porosos (en inglés MOFs) a partir de biomoléculas orgánicas, espumas y pellets que permitan la encapsulación de moléculas fotoactivas.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

- Preparación de ligandos orgánicos a partir de biomoléculas mediante técnicas de síntesis orgánica.
- Preparación de bioMOFs utilizando métodos racionales de autoensamblaje.
- Encapsulación de QD en MOFs, pellets y espumas.
- Caracterización de los materiales sintetizados por difracción en rayos X, ATG, IR, isothermas de adsorción etc.
- Evaluación de la actividad óptica..

(Department stamp)

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR: Emilio Pardo Marín

ACADEMIC TUTOR (if needed):

EXTERNAL TUTOR (if needed):

Department: Química Inorgánica

TITLE (Mandatory in English)

Host-guest chemistry of metal-organic frameworks (MOFs) and their use in water remediation.

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

- Preparación de nuevos polímeros de coordinación porosos (en inglés MOFs) con gran robustez, estabilidad en agua, cristalinidad y con la funcionalización adecuada para su uso en descontaminación ambiental.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

- Preparación de ligandos orgánicos mediante técnicas de síntesis orgánica.
- Preparación de MOFs utilizando métodos racionales de autoensamblaje racionales.
- Caracterización de los materiales sintetizados por difracción en rayos X, ATG, IR, isothermas de adsorción etc.
- Evaluación de la actividad descontaminante mediante técnicas analíticas.

(Department stamp)

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1 ENRIQUE GARCÍA-ESPAÑA MONSONÍS

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): INORGANIC CHEMISTRY

TITLE (Mandatory in English)

Catalytic applications of self-assembled hydrolytic metallocages

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Design and synthesis of polyamine ligands that enable the formation of catalytically active metallocages.
- Structural and spectroscopic characterisation of the metallocages obtained.
- Evaluation of the stability of metallocages in aqueous media, analysing their catalytic activity in model reactions and monitoring their efficiency and selectivity.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

New self-assembled hydrolytic metallocages will be synthesised using synthetic routes designed and optimised within the Supramolecular Chemistry group at the University of Valencia for use in catalysis. These structures will be obtained through the controlled self-assembly of organic ligands with suitable metal centres to favour the formation of defined cavities capable of hosting reactive substrates.

The study of the acid-base properties, as well as the stability and catalytic behaviour of these metallocages in aqueous or hydroalcoholic media, will be carried out using potentiometric and kinetic monitoring techniques. Spectroscopic techniques such as UV-Vis, fluorescence and NMR will also be used to characterise both the formation of the metallocages and their interaction with the model substrates.

Particular focus will be given to obtaining crystals suitable for X-ray diffraction analysis, to confirm the assembly geometry and the arrangement of the catalytic site inside the cavity.

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Enrique García-España Monsonís

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Department of Inorganic Chemistry

TITLE (Mandatory in English)

Luminescent nanoparticles without the inclusion of fluorophores

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this literature review is to analyze the current state of the art regarding water-soluble, non-conjugated polymer nanoparticles (PNPs) that exhibit strong fluorescence without the incorporation of conventional organic fluorophores. The review aims to identify the mechanisms behind their luminescence, synthesis methods, potential applications, and the main challenges in this emerging field.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The methodology will involve a systematic literature search using major scientific databases such as Web of Science (WOS) and Scopus. Specific inclusion and exclusion criteria will be applied to filter relevant peer-reviewed articles, including publication date range, language, relevance to the topic, and citation impact. Keywords and Boolean operators will be optimized to ensure comprehensive coverage. The selected studies will then be analyzed and classified according to themes such as synthesis strategies, photophysical properties, and applications.

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Antioxidant applications of liposome encapsulated polyamine metal complexes

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Synthesis and characterisation of the acid-base behaviour and coordination chemistry of polyamine ligands.
- Encapsulation of the complexes obtained in liposomes, as well as optimisation of loading conditions, stability and dispersion in aqueous media.
- Study of the redox behaviour and antioxidant capacity of free and encapsulated complexes against reactive oxygen species (ROS), using specific in vitro assays.
- Evaluation of the influence of encapsulation on the stability, solubility and antioxidant efficacy of the complexes.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Using synthetic routes developed and optimised by the Supramolecular Chemistry group at the University of Valencia, new metal complexes with polyamine ligands will be synthesised, selected for their potential antioxidant activity. These complexes will then be encapsulated in liposomes using passive or active incorporation methods, optimising loading and stability conditions. The study of the acid-base properties, as well as the stability and redox behaviour of both free and encapsulated complexes, will be carried out using potentiometry and electrochemistry techniques in aqueous or hydroalcoholic media. To complement these studies, spectroscopic techniques such as UV-Vis, fluorescence and NMR will be used to characterise both the complexes and their interaction with reactive oxygen species (ROS). Their antioxidant efficacy will also be evaluated using specific radical scavenging assays and in vitro tests. Finally, attempts will be made to obtain suitable crystals of the free complexes for structural analysis by X-ray diffraction.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jose Miguel Llinares Belenguer

ACADEMIC TUTOR 2 Estefanía Delgado Pinar

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Organic Chemistry and Inorganic Chemistry Department

TITLE (Mandatory in English)

Synthesis of Novel Fluorescent Polyamine Ligands and Evaluation of the Antioxidant Activity of Their Metal Complexes

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This work aims to synthesize new fluorescent polyamine ligands and to investigate their coordination behavior with biologically relevant metal ions. Special emphasis will be placed on the study of their acid-base properties, by determining protonation constants, and on the thermodynamic stability of the resulting metal complexes. Additionally, the antioxidant potential of both the free ligands and their metal complexes will be evaluated, with the goal of assessing their possible applications in biomedical or environmental contexts.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The research will begin with the synthesis of the fluorescent polyamine ligands using standard organic synthesis protocols. The resulting compounds will be purified and structurally confirmed through spectroscopic methods. Potentiometric titrations will be carried out to determine the acid-base properties and to calculate the protonation constants of the ligands. The formation of metal complexes will be studied by potentiometric methods, and their stability constants will be determined. Complementary spectroscopic techniques, such as UV-Vis and fluorescence spectroscopy, will be employed. Finally, the antioxidant activity of the synthesized compounds will be evaluated using established radical scavenging assays, such as DPPH or ABTS, to quantify their potential antioxidant capacity.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Francisco José Martínez Lillo

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUÍMICA INORGÁNICA

TITLE (Mandatory in English)

Current status and perspectives of iridium complexes as possible anti-cancer agents

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Llevar a cabo una búsqueda bibliográfica que permita establecer el estado actual del tema, junto con las principales líneas de investigación en las que se basa.
2. Estudio del efecto del estado de oxidación del ion metálico en las propiedades a estudiar.
3. Realizar una comparativa basada en los datos recabados que pueda aportar información adicional y generar ideas de síntesis para el desarrollo de nuevos sistemas que puedan presentar una mayor actividad.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se llevará a cabo una primera fase de indagación sistemática en diferentes bases de datos especializadas (PubMed, WoS, SciFinder, Google Scholar, CSD, etc.), que permita la obtención y estructuración de la información necesaria, teniendo en cuenta los criterios iniciales de la investigación.

A partir de las fuentes seleccionadas se realizará un análisis cuantitativo en el que se estudien diferentes aspectos, tales como documentos e investigaciones realizadas por país, número de documentos por año, métodos de síntesis, ligandos empleados, estados de oxidación y otros.

Finalmente, se interpretarán los resultados obtenidos y se extraerán las correspondientes conclusiones que se recogerán en el informe final.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Gonzalo Abellán

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

High entropy layered double hydroxides for green hydrogen production

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Synthesis of Iron-Based Layered Double Hydroxides (LDHs)

Advanced Characterization of the Materials

Catalytic Performance for Green Hydrogen Production in Alkaline Media

Degradation Behavior and Metal Leaching Under Operating Conditions

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Synthesis of LDHs: Iron-based layered double hydroxides will be synthesized using established methods reported in the literature, including our patented synthesis for LDH.
- Material Characterization: The obtained materials will be characterized using a suite of analytical techniques to assess their structural, morphological, and compositional features. These will include X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), scanning and transmission electron microscopy (SEM/TEM), and X-ray photoelectron spectroscopy (XPS).
- Catalytic Evaluation: The electrocatalytic performance of the materials for green hydrogen production in alkaline media will be evaluated using standard electrochemical techniques such as linear sweep voltammetry (LSV), cyclic voltametry and polarization curves.
- Degradation and Leaching Studies: Stability tests under continuous operation will be performed to assess the long-term durability of the catalysts. Metal leaching will be monitored. Structural changes post-operation will also be analyzed.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Gonzalo Abellán

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Meta-Layered Hydroxides for Energy Storage

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Synthesis of Meta-Layered Hydroxide (mLH) Heterostructures for Supercapacitor Applications
- Advanced Characterization of the Hybrid Layered Materials
- Electrochemical Performance Evaluation as Active Materials in Supercapacitors
- In-Depth Electrochemical Studies to Elucidate Battery-Like vs. Capacitive Behavior

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Synthesis of meta LDHs: Meta-layered hydroxides will be synthesized via a modified epoxide-assisted co-precipitation method, enabling controlled integration of LDH and α -LH phases by adjusting metal ratios and pH kinetics.
- Structural, morphological, and compositional features will be analyzed using XRD, FTIR, SEM/TEM, and XPS.
- Electrochemical Evaluation: Performance as supercapacitor materials will be assessed through cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS) in alkaline media. CV at varying scan rates and Dunn's analysis will be used to differentiate capacitive versus battery-like behavior.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Gonzalo Abellán

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): Edurne Nuin

DEPARTMENT(S): Quimica inorganica - Instituto de Ciencia Molecular (ICMol)

TITLE (Mandatory in English)

Preparation of Electrode Materials Based on Two-Dimensional Materials for Green Hydrogen Production.

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo de este trabajo es desarrollar electrodos activos y estables para la producción de hidrógeno verde mediante electrólisis del agua en condiciones alcalinas. Se pretende preparar materiales bidimensionales electrocatalíticos basados en elementos abundantes y de bajo coste (como Ni, Fe o Co), evitando el uso de metales nobles. Se busca optimizar tanto la actividad como la estabilidad de los electrodos frente a las reacciones de evolución de oxígeno (OER) y de evolución de hidrógeno (HER), con vistas a su posible aplicación en dispositivos de electrólisis sostenibles y escalables.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

La metodología consistirá en la síntesis y depósito de materiales catalíticos sobre sustratos conductores mediante técnicas como ultrasonic spray-coating, electrodeposición, crecimiento hidrotermal o serigrafía. Un aspecto clave será la optimización de la composición de las tintas (ionómeros, catalizador, disolvente, etc.). Los electrodos obtenidos se caracterizarán estructural y morfológicamente mediante DRX, SEM, EDX y espectroscopía Raman. La actividad electrocatalítica se evaluará en celdas de tres electrodos mediante voltametría cíclica, curvas de polarización y espectros de impedancia electroquímica, determinando parámetros clave como la sobrepotencial, la densidad de corriente y la estabilidad operativa a largo plazo.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Gonzalo Abellán

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): Edurne Nuin

DEPARTMENT(S): Química inorganica - Instituto de Ciencia Molecular (ICMol)

TITLE (Mandatory in English)

Synthesis of Perilenebisimides for Functionalization of Two-Dimensional Materials.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo principal de este trabajo es diseñar y sintetizar derivados de perilenbisimidas (PBI) con grupos funcionales específicos que permitan su interacción y anclaje con materiales bidimensionales (2D) como el grafeno, el antimoneno o el bismuteno. Se busca aprovechar las propiedades electrónicas, fotónicas y estructurales de las PBIs para modificar superficialmente estos materiales, mejorando su dispersabilidad, funcionalidad y posibles aplicaciones en dispositivos optoelectrónicos, sensores o almacenamiento de energía. Asimismo, se pretende establecer una correlación entre la estructura química de las PBIs sintetizadas y su afinidad con superficies 2D.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

El proyecto se dividirá en dos etapas paralelas. En la primera, el/la estudiante se centrará en el desarrollo y la optimización de la síntesis de PBI con diversas estructuras optimizadas para la funcionalización de grafeno, Sb y Bi (estos últimos preparados mediante una ruta coloidal). La segunda etapa estará dedicada a la caracterización de los nanomateriales obtenidos, con el objetivo de confirmar su morfología, estructura y pureza superficial. Se utilizarán diversas técnicas analíticas, entre ellas: RMN, MS, XPS y FTIR para identificar grupos funcionales; TEM y HRTEM para estudiar la morfología y la estructura; SEM para observaciones superficiales; y TGA-GC-MS para evaluar la estabilidad térmica y la presencia de residuos orgánicos. Estas herramientas permitirán validar la calidad del material y su idoneidad para futuras funcionalizaciones.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Gonzalo Abellán Sáez

ACADEMIC TUTOR 2 Rebeca Martínez Haya

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Exploring the Ti-based synthesis of Layered Double Hydroxides

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

To compare the use of different reagents and conditions over the synthesis of Layered Double Hydroxides (LDH) based on Ti (IV) in order to optimize the material synthesis. Ti-based LDHs are one of the most promising photocatalysts for water splitting.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Two different reagents will be used as starting materials for the synthesis of Layered Double Hydroxides (LDH). Besides, several reaction conditions will be explored. After that, LDH will be characterized through different techniques such as X-Ray diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) or X-ray Photoelectron Spectroscopy (XPS), among others. On the light of the characterization results, the best synthetic protocol will be selected. Finally, the material will be also electrochemically characterized.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Gonzalo Abellán Sáez

ACADEMIC TUTOR (if needed): Rebeca Martínez Haya

EXTERNAL TUTOR (if needed):

Department: Química Inorgánica

TITLE (Mandatory in English)

Two-dimensional Phosphorene: discharge agents for intercalated black phosphorous compounds

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

To compare the influence of different discharge agents in the discharge of black phosphorous intercalated compounds with alkali metals in order to obtain few layers of black phosphorous, one of the most exciting 2D materials reported to date.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

First, the black phosphorous intercalated compound (bPIC) will be synthesized in solid phase according to literature using an alkali metal. Then the removal of the metal will take place using different benzonitrile derivatives through electron trapping and mass transport. This removal will be monitored using UV-Vis spectroscopy. Finally, the obtained bP layered materials will be analyzed and compared through AFM, Raman spectroscopy and X-Ray diffraction in order to compare which agent provides the thinnest layered material.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The preparation of mesoporous materials, with pore sizes greater than 2 nm, allows for the inclusion of different types of large functional molecules within the pores through appropriate chemical design, enabling modification of the pore's chemical characteristics.

In this regard, we propose to study the encapsulation of different molecules into a mesoporous MOF developed in our laboratory, called MUV-2, which is based on trimetallic clusters and the molecule tetrathiafulvalene (TTF).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The following tasks will be performed:

- Synthesis and characterization of TTF derivatives
- Synthesis and characterization of MUV-2
- Preparation of polyoxometallates and other large molecules
- Inclusion of large molecules into MUV-2

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The objective of this project consists on the incorporation of active Pd(II) centres into porous crystalline structures.

In this regard, we propose to use of different palladium-based metalloligands in combination with inorganic clusters of different geometry to obtain a uniform distribution of the Pd centres along the material with no blockage of the pores.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The following tasks will be performed:

- Synthesis and characterization of Pd metalloligands
- Synthesis and characterization of inorganic clusters
- Preparation of MOFs
- Study of the physical properties of the bimetallic MOFs

VNIVERSITAT
E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Hendrik Jan, Bolink

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorganica

TITLE (Mandatory in English)

Optimizing the properties of metal halide perovskites for photovoltaic applications.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This project aims to improve the efficiency of perovskite based solar cells by reducing the imperfections in the metal halide perovskites prepared by vacuum based deposition methods.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Using co-sublimation of the perovskite precursors, PbI_2 , PbBr_2 , methylammonium iodide and other alkylammonium cations, 3D or quasi 2D perovskites will be grown as thin films on flat substrates. The effect of the composition of the precursors on the photoluminescence and crystallinity of the films will be studied using spectroscopic techniques and x-ray diffraction. Films will be grown on glass, substrates but also on thin films of organic conjugated molecules and lewis acid and basis to see if the growth condition of the perovskite can affect the photoluminescence efficiency. the effect of passivating molecules on the top of the perovskite layer will also be evaluated. Once a suitable perovskite composition and layer stack has been identified this will be integrated into a solar cells by applying two electrodes, one above and one below the stack, at least one of them semitransparent. The finished solar cells will be evaluated on efficiency using current voltage characteristics.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Isabel Abánades Lázaro

ACADEMIC TUTOR 2 Joaquín Soriano López

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Development of MOF-Based Electrocatalysts for Nitrate Reduction

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

-Síntesis y Caracterización estructural de MOFs mediante técnicas como XRD, SEM, BET, FTIR y TGA, entre otras.
 -Modificar electrodos con los MOFs sintetizados para su uso como electrocatalizadores en celdas electroquímicas.
 -Electrosíntesis de MOFs para deposición in situ en el electrodo de trabajo
 -Evaluar la actividad electrocatalítica de los MOFs en la reducción de nitratos.
 -Analizar la selectividad y eficiencia de conversión hacia productos deseados.
 -Correlacionar el rendimiento de los MOFs con sus propiedades estructurales con su comportamiento electrocatalítico.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Metodologías sintéticas para el control químico de MOFs en síntesis solvotermal y electrosíntesis.
 Caracterización estructural de las propiedades de los MOFs:
 Cristalinidad, composición, defectividad, porosidad, tamaño de partícula, hidrofobicidad/hidrofilicidad, carga, estabilidad coloidal, térmica, química y mecánica.
 Modificación de electrodos: Se prepararán electrodos de trabajo modificados con los MOFs mediante dos estrategias: drop-casting y electrosíntesis directa (in situ) del MOF sobre el electrodo.
 Evaluación de la actividad electrocatalítica de los MOFs hacia la reducción de nitrato:
 Voltametría cíclica para estudiar los procesos redox y la actividad catalítica, voltametría de barrido lineal para determinar el potencial de inicio de reducción y la corriente máxima, espectroscopía de impedancia electroquímica para analizar la resistencia de transferencia de carga y cronoamperometría para evaluar la estabilidad del MOF a largo plazo.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 JAMAL EL HASKOURI BENNAGI

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): QUIMICA INORGÁNICA

TITLE (Mandatory in English)

Sustainable synthesis of mesoporous fertilizers from rice production waste

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Este trabajo tiene como objetivo desarrollar un proceso sostenible para la producción de fertilizantes a partir de materiales mesoporosos obtenidos mediante la reutilización de residuos generados en la industria del arroz, principalmente la cáscara. Se busca transformar estos subproductos agroindustriales en materiales mesoporosos con propiedades fertilizantes. Se pretende evaluar sus características fisicoquímicas, capacidad de retención de nutrientes y potencial agronómico. Así, se contribuye a la economía circular, reduciendo residuos y generando productos de valor añadido para una agricultura más sostenible.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se recolectarán y prepararán residuos de cáscara de arroz para transformarlos en materiales mesoporosos mediante procesos térmicos y químicos. A continuación, se formularán fertilizantes incorporando nutrientes en estos materiales. Finalmente, se caracterizarán sus propiedades fisicoquímicas y se realizarán ensayos preliminares para evaluar su capacidad de liberación controlada y potencial agronómico.

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1 Jamal El Haskouri Bennagi

ACADEMIC TUTOR 2 Miriam Benitez Serra

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Rice Revaluation: New Materials for a Sustainable Future

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Emplear los deshechos de la cascarilla del arroz como producto de partida para la síntesis de materiales mesoporosos de sílice, con el fin de promover su revalorización dentro de una economía circular.

Analizar las propiedades físico-químicas de los materiales obtenidos y compararlas con los materiales ya existentes.

Evaluar el impacto ambiental y económico del uso de subproductos del arroz frente a materiales convencionales, en el marco del desarrollo sostenible.

Analizar posibles aplicaciones para estos materiales, destacando su viabilidad y beneficios.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Se realizará un primer paso que consta de un tratamiento térmico o calcinación para eliminar toda la materia orgánica y obtener la ceniza rica en sílice, en un horno mufla a 600°C durante 6h.

Posteriormente se extrae la sílice con un tratamiento con NaOH a 90°C 2h, obteniendo silicato sódico que será el precursor de partida empleado para la síntesis de materiales.

Obtención de materiales mesoporosos de sílice con distinta morfología y tamaño preferiblemente como UVM7, MCM41, SBA15 o Stöber empleando el silicato sódico obtenido de la cascara de arroz

Tras la obtención de estos materiales se requiere su caracterización a través de distintas técnicas como FTIR, SEM, TEM, DRX, Porosimetría entre otros

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Synthesis and characterization of metal-organic frameworks
Structurate metal-organic frameworks into organic (bio)-polymers
Elucidate the removal properties of emergent organic contaminants of metal-organic framework composites

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Introduction to the synthesis and characterization of metal-organic frameworks and metal-organic frameworks composites
Interpretation of physico-chemical properties of metal-organic frameworks and metal-organic frameworks composites

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Synthesis and characterization of metal-organic frameworks
Structurate metal-organic frameworks into organic (bio)-polymers
Elucidate the removal properties of emergent organic contaminants of metal-organic framework composites

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Introduction to the synthesis and characterization of metal-organic frameworks and metal-organic frameworks composites
Interpretation of physico-chemical properties of metal-organic frameworks and metal-organic frameworks composites

VNIVERSITAT
ID VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Joan Cano Boquera

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgànica

TITLE (Mandatory in English)

Evaluation of intermolecular interactions in the formation of molecular crystals

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- 1) Compile a selection of theoretical methods for estimating the magnitude of intermolecular interactions.
- 2) Compare the advantages and disadvantages of some of the compiled methods.
- 3) Establish the most appropriate conditions for using each method.
- 4) Propose the best alternatives for studying the formation of molecular crystals.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

This is a purely bibliographical study. Therefore, the methodology is simple:

- 1) Conduct publication searches via the ISI web platform or another equivalent database. Appropriate keywords will be used.
- 2) Download, read, and discuss the publications.
- 3) Conduct a comparative analysis based on the selected information.
- 4) If time permits and it is deemed feasible, artificial intelligence tools will be used to accomplish this task.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Joan Cano Boquera

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgànica

TITLE (Mandatory in English)

Theoretical Reflections on the Spin Crossover Phenomenon

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- 1) Estimate electronic parameters at the molecular level.
- 2) Establish a molecular-level model.
- 3) Determine the importance of cooperative phenomena in solids.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The methodology developed will vary depending on the objective to be achieved. These include:

- 1) Density-Functional (DF) calculations to optimize geometries and determine molecular vibrations. Perform a temperature-dependent thermochemical study based on previous results.
- 2) Discuss different molecular behaviors based on theoretical models, including electronic energies, entropies, vibrational wave functions, spin-orbit coupling, and potential curve crossings. Use of MC simulations in the application of these models.
- 3) Evaluation of intermolecular interactions between fragments that make up a crystal lattice using specific DF calculation methods and approximations.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 JORGE GONZÁLEZ GARCÍA

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): CRISTINA GALIANA ROSELLO

DEPARTMENT(S): DEPARTAMENTO DE QUÍMICA INORGÁNICA

TITLE (Mandatory in English)

DEVELOPING LIGANDS TO TARGET G-QUADRUPLEXES

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Preparation of ligands, evaluation of the interaction with G-quadruplex and duplex DNAs with molecules, data analysis and presentation of results.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- Synthesis and purification of small organic molecules and metal complexes and their characterization using standard techniques (chromatography, Nuclear Magnetic Resonance, mass spectrometry...).
- Evaluation of the interaction with DNA/RNA using biophysical techniques (UV-Vis, fluorescence, electrophoresis and thermal curves).
- Analysis and plot of results using data sheets (Microsoft Excel, Origin...).
- Presentation of the research results (Microsoft Word and Powerpoint).

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1

JORGE GONZÁLEZ GARCÍA

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

CRISTINA GALIANA ROSELLO

DEPARTMENT(S):

DEPARTAMENTO DE QUÍMICA INORGÁNICA

TITLE (Mandatory in English)

IDENTIFICATION OF PUTATIVE G-QUADRUPLEX FORMING SEQUENCES
INVOLVED IN CANDIDA

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Application of bioinformatic softwares for identifying sequences containing putative G4-forming sequences and validation of the G4 folding using biophysical assays.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- *Use of different bioinformatic tools (G4Hunter, G4Boost, Qqrs Mapper...) to identify and evaluate the propensity of forming G-quadruplex and other non-canonical nucleic acid structures.
- *Evaluation of the G4 folding using short oligonucleotide sequences and biophysical assays (UV melting, circular dichroism spectroscopy, UV-Vis spectra difference and thiazole orange light-up effect).
- *Analysis and plot of results using data sheets (Microsoft Excel, Origin...).
- *Presentation of the research results (Microsoft Word and Powerpoint).

VNIVERSITAT DE VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT CHEMISTRY DEGREE

ACADEMIC TUTOR 1 JORGE GONZÁLEZ GARCÍA

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed): ARIADNA BARGIELA SCHONBRUNN

DEPARTMENT(S): DEPARTAMENTO DE QUÍMICA INORGÁNICA

TITLE (Mandatory in English)

STRATEGIES FOR DEGRADING RNAs

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Bibliographic research of strategies to degrade RNA and application of novel drug-like molecules for degrading RNA in vitro

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

*Bibliographic research of the approaches to degrade and cleave RNA in cells using RNase mechanisms.

*Evaluation of the RNA cleave using biophysical techniques (EMSA, fluorescence spectroscopy, MST, circular dichroism...)

*Analysis and plot of results using data sheets (Microsoft Excel, Origin...).

*Presentation of the research results (Microsoft Word and Powerpoint).

DEGREE FINAL PROJECT**CHEMISTRY DEGREE**

ACADEMIC TUTOR 1 José Antonio Real Cabezos (Dpto. Química Inorgánica)

ACADEMIC TUTOR 2 Carlos Bartual Murgui (Dpto. Química Física)

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

The Spin Crossover Phenomenon in Iron(II) Complexes

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo de este TFG es introducir los conceptos fundamentales del fenómeno de transición de espín (Spin Crossover) en compuestos de hierro(II) y realizar la síntesis y caracterización de algunos de los compuestos más significativos de diferente dimensionalidad (0-, 1-, 3-D).

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- i) Introducir los conceptos fundamentales de campo de ligandos y la termodinámica del fenómeno de transición de espín (Spin Crossover) en compuestos de hierro(II).
- ii) Realización de un trabajo bibliográfico que refleje de forma razonable los avances más importantes del campo.
- iii) Preparación y caracterización de los complejos $\text{Fe(phen)}_2(\text{NCX})_2$ ($\text{X} = \text{S}, \text{Se}, \text{BH}_3$), $\text{Fe(triazol)(triazolato)}_2(\text{BF}_4)$ y $\text{Fe(piracina)}[\text{Pt}(\text{CN})_4]$.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jose Vicente Ros Lis

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Development of materials for agricultural applications.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El desarrollo de nuevos materiales puede ser una estrategia interesante para avanzar hacia una agricultura más sostenible. En el TFG se trabajará en las líneas de trabajo de nuevos fertilizantes, bioestimulantes y pesticidas.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Síntesis de nanomateriales
Caracterización de materiales
Cargado con sustancias activas
Ensayos de actividad

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Jose Vicente Ros Lis

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Development of sustainable strategies for chemical synthesis

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

El objetivo es el desarrollo de nuevos procesos de síntesis de menor impacto ambiental para la preparación de moléculas y materiales mediante el uso de materias primas alternativas, y procesos con menor consumo de energía y/o disolventes orgánicos

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Uso de materias primas de fuentes naturales
Síntesis asistida por microondas
Mecanoquímica
Preparación de colorantes
Preparación de nanomateriales
Caracterización de moléculas y materiales.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Development of Semiconductor Thin Films via Physical Vapor Deposition
Methods for Application in Optoelectronic Devices

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

1. Desarrollar películas delgadas semiconductoras mediante técnicas de deposición física de vapor (PVD).
2. Optimizar sus propiedades estructurales y ópticas para aplicaciones optoelectrónicas.
3. Evaluar su desempeño en dispositivos como celdas solares y LEDs.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

1. Material Selection: Choose suitable semiconductor materials for optoelectronic applications.
2. Thin Film Deposition: Fabricate thin films using Physical Vapor Deposition (PVD) techniques such as thermal evaporation, pulsed laser deposition or sputtering.
3. Characterization: Analyze structural, optical, and electrical properties using XRD, UV-Vis, SEM, and Hall effect measurements.
4. Device Integration: Incorporate optimized films into prototype optoelectronic devices.
5. Performance Evaluation: Test and compare device efficiency and stability under controlled conditions.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

M. Ángeles Úbeda Picot

ACADEMIC TUTOR 2

Francisco F. Pérez Pla

EXTERNAL TUTOR (if needed):

--

DEPARTMENT(S):

Química Inorgánica y Química Física

TITLE (Mandatory in English)

Preparation and evaluation of the catalytic activity of sustainable iron 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.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Matteo Andrea Lucherelli

ACADEMIC TUTOR 2 Gonzalo Abellán

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química inorganica - Instituto de Ciencia Molecular (ICMol)

TITLE (Mandatory in English)

Colloidal synthesis of 2D materials based on pnictogens elements

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Este trabajo de fin de grado tiene como objetivo el desarrollo de síntesis coloidal para obtener nanopartículas bidimensionales basadas en los elementos pnictógenos (Sb, Bi). El/la estudiante involucrado/a en el proyecto se encargará de modificar las condiciones de síntesis, como la temperatura, el disolvente, el tiempo de reacción y el agente reductor, con el fin de obtener nanomateriales bidimensionales sin grupos funcionales en la superficie, adecuados para posteriores funcionalizaciones mediante química orgánica

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

El proyecto se dividirá en dos etapas paralelas. En la primera, el/la estudiante se centrará en el desarrollo y la optimización de una síntesis coloidal en el laboratorio para obtener nanopartículas bidimensionales de Sb y Bi, estudiando el efecto de los distintos parámetros sobre la morfología y las propiedades del material. La segunda etapa estará dedicada a la caracterización de los nanomateriales obtenidos, con el objetivo de confirmar su morfología, estructura y pureza superficial. Se utilizarán diversas técnicas analíticas, entre ellas: FTIR para identificar grupos funcionales; TEM y HRTEM para estudiar la morfología y la estructura; SEM para observaciones superficiales; y TGA para evaluar la estabilidad térmica y la presencia de residuos orgánicos. Estas herramientas permitirán validar la calidad del material y su idoneidad para futuras funcionalizaciones.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Matteo Andrea Lucherelli

ACADEMIC TUTOR 2 Gonzalo Abellán

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química inorganica - Instituto de Ciencia Molecular (ICMol)

TITLE (Mandatory in English)

Production of metal-doped carbon nano onions (CNOs) for energy applications

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Este trabajo tiene como objetivo desarrollar y optimizar un método para la producción de carbon nano onions (CNOs), un nanomaterial de carbono con propiedades similares al grafeno y los nanotubos, y con dimensiones nanométricas. La meta final será optimizar el procedimiento sintético de este nanomaterial e investigar el dopaje de las CNOs utilizando diferentes metales para mejorar sus propiedades magnéticas y catalíticas. Además, se explorarán las aplicaciones electroquímicas de las CNOs dopadas.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

El trabajo se dividirá en tres partes principales que se desarrollarán de forma paralela.

La primera parte se centrará en la optimización de la síntesis de CNOs utilizando un horno especial en condiciones controladas.

La segunda parte abarcará la caracterización de las propiedades de los materiales mediante diferentes instrumentos, tales como espectroscopía FT-IR, UV-Vis, Raman, microscopía electrónica de transmisión (TEM) y TEM de alta resolución, así como técnicas para estudiar las propiedades magnéticas y la investigación electroquímica.

Por último, la tercera parte se enfocará en investigar las aplicaciones del material sintetizado en catálisis.

VNIVERSITAT
E VALÈNCIA [Q*] Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR: Michele Sessolo

ACADEMIC TUTOR (if needed):

EXTERNAL TUTOR (if needed):

Department: Departamento de Química Inorgánica

TITLE (Mandatory in English)

Thin-film photodetectors based on unconventional semiconductors

OBJECTIVES / OBJECTIUS / OBJETIVOS (Choose the language)

This project aims to develop materials and devices for novel light detection technologies. The objective is to investigate thin layers of materials with mixed electronic-ionic conductivity to be used as active materials in photodetectors.

METHODOLOGY / METODOLOGIA / METODOLOGÍA (Choose the language)

- 1) Deposition of thin film semiconductors, optical and electrical characterization
- 2) Incorporation of semiconductors into photodetectors
- 3) Optoelectronic characterization of devices and subsequent optimization

(Department stamp)

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Miguel Clemente León

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Multifunctional spin crossover compounds

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Preparation and characterization of multifunctional spin-crossover complexes that combine the switching properties of the spin-crossover property with the new functionalities afforded by the chirality (piezoelectricity, pyroelectricity or ferroelectricity), magnetic ordering or others in the form of crystalline materials, nanoparticles or deposited as thin films or monolayers.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Growth of single crystals of the complexes
Structural characterization by single crystals and powder X-ray diffraction
Magnetic characterization of the bulk samples
Deposition on surfaces
Characterization of the deposited complexes by AFM, X-ray photoelectron spectroscopy, Raman and IR spectroscopy

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Pedro José Amorós del Toro

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Mechanochemically functionalised porous silicas: a sustainable strategy.

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Introducir al estudiante en procesos de síntesis clásicos, como la química sol-gel, para la preparación de materiales.

Explorar las oportunidades de la mecanoquímica para funcionalizar las sílices porosas como una alternativa de bajo coste, eficiente, rápida y sostenible.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

- 1.- Preparación de sílices mesoporosas mediante el uso de micelas de surfactante como agentes plantilla.
- 2.- Modificación mecanoquímica de las sílices puras mediante el uso de especies orgánicas e inorgánicas.
- 3.- Adecuación y optimización del proceso.
- 4.- Control del grado de funcionalización.
- 5.- Caracterización de los materiales obtenidos mediante difracción de rayos-X, microscopia electrónica, absorción de gases etc.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

-

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Abargues López

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Inorganic Chemistry

TITLE (Mandatory in English)

In-Situ Synthesis of NiO_x Films for Efficient Hole Transport Layer in Perovskite Solar Cells

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This Final Degree Project is focused on the in-situ low-temperature synthesis of mixed metal oxide thin films, specifically NiO:Li and NiO:Cs for hole transport. These transparent semiconducting oxides will be developed as alternative charge-selective layers in perovskite solar cells, aiming to replace conventional materials with more stable, earth-abundant, and scalable options. The goal is to investigate their structural, optical, and electronic properties, and to evaluate their impact on photovoltaic device performance and stability.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project will follow an in-situ solution-processing approach and include the following steps: 1. Formulation of precursor solutions combining nickel salts doped with lithium or cesium (NiO:Li/Cs), using solvents compatible with perovskite materials. 2 Deposition of thin films over large-area substrates via scalable techniques such as spin-coating or spray-coating. 3. Post-deposition annealing (thermal or solvent-assisted) to induce crystallization and optimize film morphology, transparency, and conductivity. 4. Multimodal characterization, including structural (XRD), morphological (SEM, AFM), optical (UV-Vis), and electrical (I-V curves) techniques. 5. Integration into perovskite solar cell architectures, evaluating the functionality of NiO:Li/Cs films as hole transport layers, and assessing their effect on power conversion efficiency, charge extraction, and device longevity.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Abargues López

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Inorganic Chemistry

TITLE (Mandatory in English)

In-Situ Synthesis of SnO₂ Films for Electron Transport Material in Perovskite Solar Cell

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This Final Degree Project is focused on the in-situ low-temperature synthesis of mixed metal oxide thin films, specifically SnO₂:Zn for electron transport. These transparent semiconducting oxides will be developed as alternative charge-selective layers in perovskite solar cells, aiming to replace conventional materials with more stable, earth-abundant, and scalable options. The goal is to investigate their structural, optical, and electronic properties, and to evaluate their impact on photovoltaic device performance and stability.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The project will follow an in-situ solution-processing approach and include the following steps: 1. Formulation of precursor solutions combining tin and zinc salts for SnO₂:Zn, using solvents compatible with perovskite materials. 2. Deposition of thin films over large-area substrates via scalable techniques such as spin-coating or spray-coating. 3. Post-deposition annealing (thermal or solvent-assisted) to induce crystallization and optimize film morphology, transparency, and conductivity. 3. Multimodal characterization: structural (XRD), morphological (SEM, AFM), optical (UV-Vis), and electrical (I-V curves). Integration into perovskite solar cell architectures, evaluating the functionality of each oxide as an electron or hole transport layer, and assessing their effect on power conversion efficiency, charge extraction, and device longevity

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Abargues López

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Inorganic Chemistry

TITLE (Mandatory in English)

In Situ synthesis of transparent electrically conducting polymers for Perovskite-based Photovoltaics and LEDs

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

In solar cell manufacturing, a broad range of materials is required to optimize photovoltaic performance. This project focuses on the in-situ synthesis of a transparent conducting polymer in apolar solvents, with the goal of integrating it into the fabrication processes of both perovskite-based solar cells and light-emitting diodes (LEDs) as a sustainable alternative to PEDOT:PSS. The study will explore and optimize the structural, electronic, and optical properties of the polymer, evaluating its effectiveness as a hole-selective layer in lead-free perovskite photovoltaic devices and as a hole injection layer in perovskite-based LEDs.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The methodology involves formulating solutions for in-situ synthesis in apolar solvents and the deposition of conducting polymers within various polymeric matrices, such as polymethacrylates and polystyrenes, directly onto lead halide perovskites (APbX_3). Key tasks include the development of solvent systems and the deposition of precursor solutions via spin-coating, ensuring full chemical compatibility with the perovskite layers. The deposition and curing processes will be optimized using advanced electrical, optical, morphological, and structural characterization techniques. Ultimately, the study will evaluate the performance of these materials as hole transport layers in the fabrication of both metal halide perovskite solar cells and perovskite-based LEDs, with the goal of significantly improving their efficiency and operational stability.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Abargues López

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Inorganic Chemistry

TITLE (Mandatory in English)

Lead-Free Double Perovskites Nanocomposite for Photodetectors,
 Photocatalysis and Memristors.

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The main objective of this Final Degree Project is the in-situ synthesis and integration of lead-free double perovskites ($A_2BB'X_6$, with $B/B' = Bi^{3+}$, Ag^+ , Sb^{3+} , etc.) into functional organometallic matrices to produce hybrid materials for large-area applications in photodetectors photocatalysis and memristors. The project aims to develop scalable and environmentally friendly solution-processable materials with enhanced stability, optical performance, and light-induced charge separation efficiency.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The methodology will be based on an in-situ synthesis approach, enabling the direct crystallization of perovskite domains within organometallic matrices over large-area substrates. The key steps include: 1. Formulation of precursor solutions containing halide salts and metalorganic matrixes in compatible solvents. 2. Deposition over large areas using scalable techniques such as spin-coating, doctor-blading, or spray-coating. 3. Thermal or solvent-assisted annealing to induce in-situ crystallization of the perovskite phase within the host matrix. 4. Characterization of the resulting films by structural (XRD, SEM), optical (UV-Vis, PL), and electrical (I-V, photocurrent) techniques. 5. Evaluation of functional properties, including photoconductive behavior, photocatalytic activity, and resistive switching performance, in order to assess their suitability for integration in memristive devices. The ultimate goal is to correlate the nanoscale structure and composition of these hybrid materials with their macroscopic electronic and optoelectronic behavior.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Current commercial LED lighting systems are based on blue-emitting diodes combined with phosphors composed of rare-earth-doped aluminum oxides. However, these materials suffer from limited spectral conversion efficiency, constraining overall device performance. In addition, the reliance on rare-earth elements raises sustainability and supply concerns. This project aims to develop advanced nanocomposites incorporating highly luminescent lead halide perovskite nanocrystals, enabling next-generation high-efficiency large area LEDs with enhanced spectral performance and reduced dependence on critical raw materials for down-conversion and electrically injected LED.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Over the past year, we have developed an innovative method for synthesizing highly luminescent perovskite nanocrystals through a simple and efficient solution-based approach. This strategy involves the incorporation of lead halide perovskites into various metal-organic matrices, yielding nanocomposites capable of efficiently converting blue LED emission into broadband visible light. The methodology will include the formulation of precursor solutions in solvents that ensure chemical compatibility with the perovskite phase, followed by their deposition using advanced techniques such as spin-coating and large-area coating methods such as slot die coating and spray coating. Optimization of both the deposition and curing steps will be carried out through comprehensive optical, morphological, and structural characterization. Ultimately, the project will evaluate the photophysical performance of the resulting materials, aiming to validate their applicability in high-efficiency light-converting and potentially electrically driven LED devices.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Rafael Abargues López

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Synthesis of 0D perovskite nanocrystals for optoelectronic devices

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Las perovskitas 0D se presentan con aniones octaédricos de haluro metálico aislados rodeados de cationes orgánicos o inorgánicos, donde los excitones están fuertemente confinados a cada octaedro. El principal objetivo de este TFG es la síntesis y caracterización de la perovskita compuesta por TEA4SnBr6 en el interior de matrices metalorgánicas como estrategia para formar una estructura 0D.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Este trabajo de TFG se llevará a cabo dentro de una caja seca con condiciones atmosféricas controladas. La síntesis de la perovskita TEA4SnBr6 se realizará en disolución dentro de una matriz metalorgánica. La optimización de la síntesis tendrá en cuenta diversos factores, entre ellos, el porcentaje de TEA óptimo para conseguir una estructura 0D. Para comprobar su estabilidad, se realizará un estudio en diferentes concentraciones de humedad para ver el efecto de ésta sobre la óptica, electrónica y morfología de la perovskita sintetizada.

VNIVERSITAT
E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Structural and Anti-oxidant properties of Metal Complexes with small azamacrocycles

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Study the formation of the metal complexes by means of several analytical techniques.
- Study of the redox behaviour and antioxidant capacity of metal complexes against reactive oxygen species (ROS), using specific in vitro assays.
- Relate the activity with the structural features.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Starting with metal ions of the first transition series, new complexes will be formed with polyamine ligands available in our lab.

The formation of the complex will be assessed with several analytical techniques, namely potentiometry, electrochemistry and spectroscopic techniques.

Their antioxidant efficacy will also be evaluated using specific radical scavenging assays and in vitro tests.

Also, attempts will be made to obtain suitable crystals for structural analysis by X-ray diffraction.

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S):

TITLE (Mandatory in English)

Exploring the performance of known MOFs based on copper for diverse vapour capture

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The aim of the Degree Final Project is to immerse the student in the field of scientific research through exposure to various methods of synthesis, material characterisation, and critical analysis of potential results—or even the absence of them.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The synthesis will follow multiple established pathways to obtain the target compounds, allowing comparison of reaction conditions, yields, and purity. Emphasis will be placed on evaluating efficiency and reproducibility across different synthetic strategies. The reactivity of the prepared MOFs will be studied for different gases and solvent vapours.

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1 Sam Benmansour Souilamas

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Investigating the reactivity of known zinc MOFs towards different vapour and gases

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

This project is designed to provide students with hands-on experience in the research environment, exploring different synthesis techniques, characterization tools, and reflecting on the significance of both the findings and possible lack of results.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

This methodology explores alternative synthetic routes to known compounds, including greener or less conventional approaches when possible. Variations in precursors, solvents, or catalysts will be tested to optimize conditions and assess scalability. The student will also check the solid-gas reactivity/stability of the prepared MOFs with different gases and solvent vapours

VNIVERSITAT
E VALÈNCIA Facultat de Química

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1

Sam Benmansour Souilamas

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Synthesis and characterisation of new metal complexes using anilato organic ligands and transition metals

OBJECTIVES / OBJECTIUS / OBJETIVOS: (Choose the language)

The main goal of the Degree Final Project is to introduce the student to the world of investigation, engaging with diverse synthesis and characterisation methods, and fostering critical thinking about any obtained outcomes—or the implications of obtaining none.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

The synthesis of a novel compound will involve designing and testing original or adapted procedures based on related structures. The approach includes iterative modification of reaction parameters, with close monitoring to identify promising reaction pathways or intermediates. The student will use an anilato-type ligand with transition metals.

DEGREE FINAL PROJECT
CHEMISTRY DEGREE

ACADEMIC TUTOR 1 Sergio Tatay Aguilar

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgánica

TITLE (Mandatory in English)

Synthesis of Ultrastable Metal–Organic Frameworks Based on azolate-Type Ligands

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

Azolate-based metal–organic frameworks (MOFs) exhibit exceptional thermal and chemical stability due to strong metal–nitrogen coordination. Their robust architectures make them ideal candidates for harsh environments.

This TFG aims to familiarize the student with all stages involved in the synthesis of MOFs: ligand design and synthesis, selection of the target network, assembly, and characterization, with a particular focus on applications as demanding as CO₂ electroreduction.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

Ligand design and synthesis.

The student will have the opportunity to become familiar with basic synthetic and characterization techniques for azole-type compounds. Alternatively, pre-synthesized or commercially available ligands may be used.

Selection of the target framework.

Depending on the ligand chosen, the most suitable MOF topology will be selected.

Assembly.

Hydrothermal synthesis methods, commonly used in MOF preparation, will be employed. The parameters to be studied include temperature, ligand-to-metal ratio, solvent, and modulator, among others.

Characterization.

At minimum, the following techniques will be used: powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and gas sorption analysis (porosimetry).

**DEGREE FINAL PROJECT
CHEMISTRY DEGREE**

ACADEMIC TUTOR 1 Víctor Rubio Giménez

ACADEMIC TUTOR 2

EXTERNAL TUTOR (if needed):

DEPARTMENT(S): Química Inorgànica

TITLE (Mandatory in English)

Solvent-free synthesis of stable azolate metal-organic frameworks

OBJECTVES / OBJECTIUS / OBJETIVOS: (Choose the language)

- Design and synthesis of volatile azolate MOF linkers.
- Fabrication and characterization of azolate metal-organic frameworks (MOFs) by solvent-free vapor-phase synthesis.
- Study of their stability under relevant conditions for electrocatalysis.

METHODOLOGY / METODOLOGIA / METODOLOGÍA: (Choose the language)

First, we will synthesize new azolate linkers and study their volatility of solvent free MOF synthesis. Next, we will test the vapor-phase reactivity with two types of metal precursors to synthesize azolato-based MOFs: 1) solid metal and metal oxide layers and 2) sublimable metal-organic complexes (metal alkoxides and β -diketones). In the first case, the MOF would be formed by a solid vapor reaction between the previously deposited metal precursor and the organic ligand, since the former will be converted by the latter.

Then the prepared MOFs will be fully characterized using powder X-ray diffraction (XRD), Infrared spectroscopy, scanning electron microscopy (SEM) and gas physisorption to evaluate the intrinsic porosity.

Finally, their stability will be studied under electrocatalytic conditions.