MASTER DE QUÍMICA DE MATERIALS APLICADA

Trabajo Final de Máster

Estado Sólido y Materiales

- *Titulo*: Mechanosynthesis of Luminescent and magnetic 2D MOFS
  Tutor: E. Carolina Sañudo (esanudo@ub.edu, QI)
  Lanthanoid 2D MOFS are very interesting materials for sensing, luminescent thermometers, magnetocaloric effect or proton conductors for hydrogen fuel cells. The student will work on synthesis of 2D MOFs using green chemistry (mechanosynthesis, microwave assisted synthesis) and will characterize the prepared materials.

- *Titulo*: Ionic 2D Materials: Synthesis and Characterization
  Tutor: Eliseo Ruiz (eliseo.ruiz@qi.ub.edu, QI)
  2D materials are a hot topic because they provide a rational method reduce the size of optoelectronic devices and to provide new materials with appealing properties. The goal in this project is to obtain 2D materials from ionic 3D bulk structures. The exfoliation processes are based on the intercalation of molecules between the layers. The characterisation of the 2D flakes is performed by using different microscopies (AFM, SEM, TEM, ...), XPS, ICP and Raman.

- *Titulo*: Synthesis of single-crystals of quasi-2D perovskites for light-absorbing applications
  Tutora: Roc Matheu (roc.matheu@ub.edu, QI)
  As 3D halide perovskites (ABX3 formula, B = Pb, X = Br, I) are developed for light-absorbing applications (e.g., solar cells), concerns about their instability against moisture still hinder commercialization. A promising synthetic strategy to address the instability involves preparing 2D perovskites containing multiple layers of metal-halide sheets (n) partitioned by organic cations. Layered perovskites with several layers' inorganic sheets (n > 5) are called quasi 2-D perovskites because they benefit from the stability given by the hydrophobic organic cation while displaying the ideal optoelectronic properties for solar cells. However, their synthesis is restricted to a few examples because low-n 2D perovskites tend to be favored during crystallization. In this project, the student will attempt the preparation of the target compounds using several methodologies, including solid-state synthesis, microfluidic devices, and standard solution-based synthesis. The synthesis will involve the characterization of the mixtures by powder and single-crystal X-ray diffraction. The student will also visit the ALBA synchrotron, which will be used to characterize single crystals by X-ray diffraction.

- *Titulo*: Single-molecule spin-filtering in molecular rectifier devices
  Tutora: Albert Cortijos (acortijos@ub.edu, QF)
  Miniaturisation of electronic devices is one of the main challenges to further scaling down our electronic devices beyond the Moore limit. Spintronic devices are one of the best candidates due to their ability to control the spin information of transmitted charge carriers. In this project, single-molecule current measurements will be performed to study new devices, based on metal complexes, with a dual capability: current rectification and spin-filtering.

- *Titulo*: Desenvolupament de ciments de fosfat de magnesi sostenibles amb cendres riques en Si
  Tutor: Jessica Giró y Joan Formosa (jessicagiro@ub.edu, joanformosa@ub.edu, CEM)
  En l'àmbit industrial, una quarta part de les emissions de CO2 mundialment i una sisena part del consum d'energia industrial provenen de la indústria del ciment Portland (OPC). De fet, el 8% de les emissions globals de CO_2 són originades en la indústria del ciment. Això és degut a la gran quantitat de ciment que es produeix i als processos tèrmics utilitzats en la seva fabricació. Per això, s'han de buscar materials alternatius més

sostenibles per tal de reduir l'ús de l'OPC. Una alternativa viable i sostenible són els ciments de fosfat de magnesi (MPC), on s'usen residus i subproductes industrials com a matèries primeres, seguint models d'economia circular. El MPC de la present investigació utilitza, com a matèria primera, un residu refractari provinent de la indústria de l'acer, que actualment va directament a l'abocador i cendres de fibres vegetals com a font de Si, per tal de fer una xarxa d'estructura tridimensional estable i consolidada. La Directiva 2018/850 sobre l'abocador de residus especifica que tots els estats membres implementaran estratègies per garantir que els residus que es puguin reciclar o valoritzar no acabin als abocadors l'any 2030. Aquest TFM pretén desenvolupar un material de construcció alternatiu a l'OPC, de ràpid enduriment i certa resistència mecànica.

- *Titulo*: Compositionally-controlled multinary Quantum Dots for energy conversion technologies
  Tutores: Albert Figuerola (albert.figuerola@ub.edu, QI)

  The use of semiconductor nanocrystals with quantum properties in energy conversion technologies has attracted a great interest in the recent years. The use of ternary or quaternary semiconductors offers a new way to control physical properties by means of chemical composition tuning. This Master thesis is dedicated to the development of new colloidal bottom-up synthetic strategies for the preparation of size and shape-controlled semiconductor nanocrystals made by at least three different elements in an attempt to improve the performance of future optoelectronic and thermoelectric devices.

- *Titulo*: Nanostructured materials for microplastics removal
  Tutor: Núria Llorca y Oriol Rius (nullorca@ub.edu, oriolriusayra@ub.edu, CEM)

  L'objectiu d'aquest TFM serà desenvolupar nous materials nanoestructurats amb la possibilitat d'emprar diferents mètodes de síntesi (coprecipitació, deformació plàstica severa, tractaments electroquímics...) per tal d'estudiar la potencialitat d'aquests en l'eliminació de contaminants (olis, colorants o bé microplastics). A la vegada, s'empraran diferents tècniques de caracterització (FESEM, DRX, UV-Vis, HR-XPS, ATR-FTIR entre d'altres) per relacionar l'estructura i composició amb les seves potencials aplicacions ambientals.

- *Titulo*: Development of new High Entropy Alloy coatings by thermal spraying using low-cost materials
  Tutor: Vicente Albaladejo y Alessio Silvello (vicente.albaladejo@ub.edu, alessiosilvello@ub.edu, CEM)

  High Entropy Alloys (HEAs) are a new class of materials containing equimolar quantities of multiple metallic elements unlike traditional alloys. This combination of elements confers HEAs extraordinary properties, i.e. high hardness, thermal stability, ductility and wear and corrosion resistance. Bulk HEAs components are mostly produced from a liquid solution and perfectly controlling phase transitions during solidification. Thermal spraying has aroused as an interesting technology capable of generating HEAs coatings from powder feedstocks, however, there exist some drawbacks for the production of HEAs with this morphology. Thus, this project aims to study the possibility of depositing HEAs coatings by conventional thermal spraying techniques (HVOF & APS) using blends of low-cost as feedstock materials.

- *Titulo*: Curcuminoid-functionalized carbon nanotubes (CCMoid-CNTs) as sensors
  Tutor: Núria Aliaga y Arántzazu González (naliaga@icmab.es, agonzalez@icmab.es, ICMAB-CSIC)

  Curcuminoids encompass a family of small conjugated molecules with multiple applications in different fields of nanoscience and nanotechnology (bulk-heterojunction organic sollar cells (BHJ-OSCs), metallo-organic frameworks (MOFs), colorimetric/luminescent sensors, etc.). These molecular platforms can be designed with multiple functions for coordination to active substrates and metal/metalloid identification. This is the basis of the master's proposal, where the synthesis of a group of asymmetric curcuminoids and their subsequent coordination with functionalized CNTs is required, giving rise to systems that promote fluorescence and electronic changes in contact with certain analytes. The master work includes a part of organic synthesis/characterization and another part of deposition and measurement of CNT-CCMoid on substrates.

- *Titulo*: Pulse plating of ternary alloys
  Tutor: Teresa Andreu y Maria Sarret (tandreu@ub.edu, m.sarret@ub.edu, QF)
  Electroplating of thin film gold alloys in widely used in the jewellery industry. Electrolytes usually requires the the use of additives, a broad selection of chemical substances that affect the surface deposition-characteristics, which is a non-convenient at the environmental level, and it is necessary to rethink this manufacturing process. In this project, the research will be focused on pulsed DC working conditions for Au-Cu-In coating fabrication, which is currently at very early stage, as an strategy to avoid the use of additives. The student will adquire knowledge in nanomaterials synthesis, electrochemistry, statistical design of experiments and materials characterization (XRD, SEM, optical microscopy).

- *Titulo*: Strategies for the synthesis of MXenes: characterization and applications as catalysts for CO_2 conversion
  Tutor: Xavier Vendrell y Lourdes Mestres (xavier.vendrell@qi.ub.edu, lourdes.mestres@qi.ub.edu, QI)
  In this work different routes using diverse methods and techniques (ultrasounds, mecanochemical, microwave, hydrothermal, …) will be explored for the synthesis of materials based on 2D metallic carbides. The characterization will be accomplished using different available techniques and the catalysts tested in different reactions for CO_2 reduction.

- *Titulo*: Development of photocatalysts based on MXenes and diverse semiconductors for renewable H_2 production
  Tutor: Narcís Homs y Jaroslaw Serafin (narcis.homs@qi.ub.edu, QI)
  In this work different specific MXenes will be used as co-catalysts of known semiconductors (TiO_2, C_3N_4, …) for the photocatalytic H_2 production from bioethanol.

- *Titulo*: Metal organic framework nanosheets for chemical sensing
  Tutores: Daniel Sainz (daniel.sainz@ub.edu, QI) y Sachin T. Navale (stnavale2@ub.edu, EEBM)
  Sensors based on high conductivity nanostructured metal-organic frameworks (MOFs) materials, which present high porosity and specific surface area, are very interesting candidates for low cost and low power consuming gas sensing devices. The aim of this work is use different triphenylene derivatives and metals to obtain conductive MOFs suitable for gas sensing and to check their selectivity and sensibility with CO_2, H_2 and volatile organic compounds (VOCs).

Sistemas Moleculares

- *Titulo*: Halogen-bonded Metal Catalysts: Design and Application
  Tutor: Anton Vidal (anton.vidal@ub.edu, QI)
  This project aims to construct bidentate metal catalysts employing halogen bonding interactions. The design principle resides in the generation of catalysts by using one building block containing a halogen-bond donor motif and another one incorporating a halogen-bond acceptor moiety. The preparation of an array of structurally diverse catalysts will be studied, once the basic concept is put to work. This project also aims at developing new catalytic methods for selective transformations that currently lack a satisfactory solution (earth-abundant-metal based C-O and C-C bond forming reactions) and applying the discovered catalysts to the stereoselective synthesis of compounds with interest in the life-science and fine-chemical sectors.

- *Titulo*: Luminescent supramolecular gold(I) materials
  Tutora: Laura Rodríguez (laurarodriguezr@ub.edu, QI)
  La línia de investigación propuesta incluye la síntesis ycaracterización de compuestos de Au(I) a partir de compuestos orgánicospreviamente sintetizados y con elevada conjugación. Se estudiarán laspropiedades

luminiscentes de los compuestos resultantes y se analizaráel efecto de desarrollar sistemas supramoleculares a partir de lasunidades sintetizadas para favorecer dichas propiedades luminiscentes. Finalmente se analizará el efecto del átomo pesado en laposibilidad de tener emision por fosforescencia, y en la posibilidad detener sistemas promisores en terapida fotodinámica.

- *Titulo*: Metal Organic Frameworks estables en agua para aplicaciones en Energía y Medio Ambient
  Tutor: José Giner (jginerplanas@icmab.es, ICMAB-CSIC)
  El estudiante contribuirá a la síntesis y caracterización de polímeros de coordinación y/o metal organic frameworks (MOF). Para ello sintetizará ligandos derivados del m-carborano, un cluster de boro altamente hidrofóbico. Una vez preparados los MOFs, el estudiante usará una amplia variedad de técnicas para caracterizar el nuevo material (diffracion de rayos X en polvo y cristal, analisis termogravimétrico, IR, RMN, BET, SEM, etc.). El estudiante trabajará bajo la supervisión diaria de un estudiante de doctorado.

- *Titulo*: Ru(II) and Rh(I) complexes with methylene-bridged *P*-stereogenic diphosphanes
  Tutor: Arnald Grabulosa (arnald.grabulosa@qi.ub.edu, QI)
  *In the Homogeneous Catalysis group, we have recently described methylene-bridged, diphosphanes bearing a single P-stereogenic phosphorus and their coordination to Pd(II) moieties (Organometallics, **2020**, 39, 2511). The present PROJECT aims to expand these study to Ru(II) and Rh(I) moieties, which will be used as catalytic precursors in reductions of ketones and olefins.*

- *Titulo*: Luminescent materials with gold organometallic complexes
  Tutor: Inmaculada Angurell (inmaculada.angurell@qi.ub.edu, QI)
  En este proyecto se pretende obtener complejos de Au(I) con buenas propiedades luminiscentes. Para ello se sintetizarán primero diversos cromóforos (derivados de cumarina, trifenileno o fenantreno, entre otros) con sustituyentes tiol o alquinilo para su posterior coordinación al centro metálico de oro. El diseño racional de estos ligandos permitirá modular las propiedades luminiscentes de los complejos resultantes. También se analizará la influencia del átomo de oro (efecto del átomo pesado) y de la formación de estructuras supramoleculares sobre dichas propiedades luminiscentes.

- *Titulo*: Synthesis of seven membered *endo* cyclopalladated imines
  Tutores: Joan Albert y Daniel Sainz (joan.albert@qi.ub.edu, daniel.sainz@ub.edu, QI)
  *The reaction of Ph-N=CH-C_6H_3-2,5-Ph_2 (imine **A**) with $Pd(OAc)_2$ could produce a seven membered endo cyclopalladated imine by intramolecular C-H activation. The synthesis of the 2,6-diphenylbenzaldehyde, the precursor aldehyde of imine **A**, will be attempted by C-H functionalization or C-C coupling reactions starting from 2-phenylbenzaldehyde or 2,6-dichlorobenzaldehyde, respectively.*

- *Titulo*: Cyclometallated complexes of 1-pyrenylphosphanes
  Tutor: Arnald Grabulosa (arnald.grabulosa@qi.ub.edu, QI)
  *In the recent years, we have been studying the synthesis of 1-pyrenylphosphanes, their coordination Ru(II)-arene moieties and the antitumoral activity of the obtained complexes (Inorg. Chem., **2018**, 57, 14786; Organometallics, **2020**, 39, 2959). It has been shown that the phosphanes have a strong tendency to form cycloruthenated complexes, which are very active as antitumoral metallodrugs (Inorg. Chem., **2021**, 60, 7974). The proposed PROJECT will study the coordination and cyclometallation of 1-pyrenylphosphanes with other metallic systems, in particular those based on Re(I), Rh(III) and Ir(III).*

- *Titulo*: Síntesis y estudio de la fluxionalidad en complejos organometálicos plano-cuadrados de Níquel(II) con ligandos nitrogenados
  Tutores: Daniel Sainz (daniel.sainz@ub.edu, QI) y Jordi Vinaixa (ESADE)
  Las moléculas fluxionales son moléculas que experimentan un comportamiento dinámico por el cual algunos o

todos sus átomos se intercambian entre posiciones simétricas equivalentes. La fluxionalidad es un fenómeno que siempre ha despertado un especial interés en el estudio de las estructuras de los compuestos químicos y de las propiedades a ella asociadas. Este proyecto propone la síntesis y estudio de la estructura y de la fluxionalidad de complejos organometálicos plano-cuadrados de Ni(II) con ligandos naftiridina y piridazina, mediante Multinuclear RMN a temperatura variable y difracción de Rayos X de monocristales.

- *Titulo*: Dispositivo electroquímico para el bio-diagnóstico
  Tutor: Adaris López y Marta Mas (alopez4@icmab.es, mmas@icmab.es, ICMAB-CSIC)
  La detección electroquímica ha impulsado el desarrollo de dispositivos de "point-of-care", tanto para el monitoreo in-situ de contaminantes químicos de interés ambiental como de biomarcadores de interés clínico para el diagnóstico de enfermedades. En este proyecto se desarrollará un biosensor electroquímico hacia un "point-of-care"ac para la detección de un analito de interés clínico.

- *Titulo*: Heptazine derivate metal-organic capsules
  Tutor: Silvia Gómez Coca (silvia.gomez.coca@ub.edu, QI)
  The s-heptazine, also called tri-s-triazine or cyamelurine, derivate ligands are of great interest because of their possible application as photocatalyst, flame retardant, OLEDs, gas storage, liquid crystals or sensors. This project focus in the synthesis of new s-heptazine derivates and their use as building block for the synthesis of new metalorganic cages and the characterization of their properties.

Modelización Molecular

- *Titulo*: Simulació de processos d'adsorció de contaminants en microplàstics en medis aquàtics naturals
  Tutor: Sergio Madurga (s.madurga@ub.edu, QF)
  Aquest projecte de màster abordarà i dissenyarà noves estratègies computacionals per a l'estudi de l'efecte de l'adsorció i el transport de micro i nanoplàstics en medis que simulen la contaminació en entorns aquàtics naturals. L'efecte d'adsorció/complexació entre microplàstics, ions metàl·lics i biopolímers es durà a terme mitjançant simulacions de dinàmica molecular de Langevin combinades amb processos reactius mitjançant el paquet EspessoMD. L'objectiu principal de la simulació és el disseny d'una metodologia adequada per predir el grau d'adsorció de contaminants orgànics a microplàstics.

- *Titulo*: Development of ab initio based force fields for the Cr-MIL101 Metal-Organic Framework
  Tutor: Jordi Cirera (jordi.cirera@qi.ub.es, QI)
  Metal-Organic Frameworks (MOFs) are tridimensional porous materials with potential applications in gas storage and separation, catalysis, or even drug delivery. Among them, the Cr-MIL101 MOF ($Cr_3O(OH)(H_2O)(bdc)_3$, where bdc = benzenedicarboxilic acid) is of particular interest due to its stability against water, a major concern in terms of practical implementations. In this work, the student will develope a fully ab initio based force field based on the ligand-field molecular mechanics scheme (LFMM) to study the breathing behavior and water adsorption properties of such material. The force field will be developed by parameterising the Cr-ligand interactions using high-level electronic structure calculations (DFT and NEVPT2). All Cr(III) dependent terms will be simultaneously fit using a genetic algoritm, and the resulting force field will be used to study the structural changes that the material experiences upon different amounts of water loading.

- *Titulo*: Theoretical Insights in 2D Magnetic Materials
  Tutor: Eliseo Ruiz (eliseo.ruiz@qi.ub.edu, QI)
  The search of new 2D magnetic materials with appealing physical properties have shown important breakthroughs during the last years. However, despite the large number of research groups working in this topic, there are still many aspects that can be improved. In this project, with the help of periodic DFT calculations the

goal is to rationalize the magnetic properties in such 2D materials and to elucidate how improve them.

- *Titulo*: Application of Machine Learning techniques towards the optimization of metal-catalyzed coupling reactions
  Tutor: Jesús Jover (jesus.jover@qi.ub.es, QI)
  Most transition metal-catalyzed coupling reactions use different reagents to produce a single product, often building new C-C or C-X bonds. This project plans to apply Machine Learning techniques for investigating whether the performance of nickel-catalyzed reactions, for instance Suzuki-Miyaura and Sonogashira cross-couplings, can be predicted and improved by in silico design of the coupling organic reagents.

- *Titulo*: Molecular engineering of 2D Covalent Organic Frameworks for optoelectronic applications
  Tutor: Maria Fumanal (mfumanal@ub.edu, QF)
  2D covalent organic frameworks (COFs) have attracted significant attention in the field of optoelectronics due to the possibility of fine-tuning the target properties at the molecular level. The aim of this project is to set up a computational workflow based on band structure DFT calculations to evaluate the optoelectronic properties of 2D-COFs and ultimately, identify the structural features (functional groups, symmetries etc.) that hold the best promise for optoelectronics.

- *Titulo*: Ligand relationships to predict the properties of transition metal complexes
  Tutores: Sergi Vela (sergi.vela@ub.edu, QF)
  Computational screening techniques combining density functional theory (DFT) and machine learning (ML) enable an efficientexploration of the chemical space aiming at the discovery of new molecules and materials. In this project, the student will work on the development of quantum-chemistry based ML methods to predict the magnetic and optical properties of transition metal complexes from their constituent ligands.

- *Titulo*: Inclusion of Spin-Crossover systems in Carbon nanostructures
  Tutor: Jordi Cirera (jordi.cirera@qi.ub.es, QI)
  Spin-Crossover (SCO) molecules are molecular systems in which the metal center can change its spin-state upon external stimulus, most commonly the temperature. This natural switching behavior makes such systems quite interesting for applications in nanotechnology. However, working with single-molecule systems is quite challenging, and it will be desirable to incorporate such molecules in a more robust structure. In this project, the student will model, using electronic structure methods, the SCO behavior of several molecules and design, using computational tools, ligand modifications on their molecular structure that will allow for the inclusion of such systems in carbon nanorings, nanotubes, fullerene-based systems and nanosheets, analyzing how such inclusion alters the SCO behavior of the original system.

- *Titulo*: Development of generic chemical electronic descriptors
  Tutor: Jesús Jover (jesus.jover@qi.ub.es, QI)
  Electronic and steric descriptors are useful tools that often allow the rationalization of the behavior of chemical compounds, including the species formed and their structure or reactivity. Many chemical descriptors have been developed and measured over the time but the generalization of such descriptors is usually hampered by the difficulties found when trying to obtain them from experimental sources. This research line proposes the computational development of new electronic parameters for a diverse range of chemical species such as phosphane, carbene and amine ligands and, possibly, for functional groups, which will give rise to novel descriptors paralleling those of Hammett and Taft.

- *Titulo*: Magnetic exchange coupling in radical containing complexes
  Tutor: Silvia Gómez (silvia.gomez.coca@ub.edu, QI)
  Magnetic molecular materials have been proposed for the new technologies such as quantum computing or

spintronics, and in particular Single Molecule Magnets (SMM), molecules that are able to behave as a magnets at single molecule level. However, they face several problems in their application (such as, working temperatures and the presence of unwanted spin relaxation processes). In the search of improved systems one approach was based on the use of the strong coupling existing between metal ions and organic radicals but due to their larger complexity, the search for better systems has mostly been serendipitous because there is a lack of predictive models in the field. This project focus on the theoretical study of the coupling existing between metal ions and organic radicals in the search of a new qualitative model for the prediction of the metal-radical anisotropic magnetic exchange.

Sistemas Biomoleculares

- *Titulo*: Protein nanoparticles for medicinal applications
  Tutor: Ana Belén Caballero (ana.caballero@ub.edu, QI)
  Protein nanoparticles can be suitable candidates for drug delivery and other medicinal applications since they are biodegradable, non-toxic and non antigenic. Because of their usually well-defined primary structure, and high content of charged amino acids, the protein-based nanoparticles could allow both the electrostatic adsorption of charged molecules and the covalent linkage of conveniently functionalized compounds. This project will consist in the preparation of protein-based nanoparticles with a controlled shape and monodisperse size. Next, these particles will be evaluated for drug delivery including genetic material and metal complexes. In cellulo studies to test the efficacy of this new class of nanoparticles are also planned.

- *Titulo*: Colloidal synthesis of lanthanide-based nanostructured materials as theranostic agents
  Tutores: Albert Figuerola (albert.figuerola@ub.edu, QI)
  The use of semiconductor nanocrystals with quantum properties in energy conversion and biomedical technologies has attracted a great interest in the recent years. The use of lanthanide ions in these structures might allow to combine both magnetic and luminescent properties in a single nanoparticle, enlarging the fields of potential application. This Master thesis is dedicated to the development of new colloidal bottom-up synthetic strategies for the preparation of size and shape-controlled lanthanide-based semiconductor nanocrystals with potential application as theranostic agents.

- *Titulo*: Synthesis of self assembling block copolymers as hexosome and cubosome precursors
  Tutor: Carlos Rodríguez-Abreu (cranqb@cid.csic.es, IQAC-CSIC)
  Hexosomes and cubosomes are soft nanoparticles with an internal liquid crystal structure that provides nanodomains for the encapsulation of both hydrophilic and hydrophophic substances and therefore have potential as drug nanocarriers for controlled release. They can be functionalized on the surface to add targeting properties. The aim of this project is the synthesis and characterization of amphiphilic block copolymers with self-assembling properties that can lead to the formation of hexosomes and cubosomes.

- *Titulo*: Photoactive ruthenium(II) complexes for anticancer applications
  Tutores: Patrick Gámez (patrick.gamez@qi.ub.edu, QI)
  One of the main issues in cancer chemotherapy is to selectively treat a tumour, that is without affecting healthy tissues. One possible way to address this problem is to use coordination compounds which can be activated through light irradiation. The proposed TFM will aim at preparing new Ru(II) polypyridyl complexes, studying their photophysical properties and evaluating their photocytotoxic behaviour.

- *Titulo*: Colloidal synthesis of hybrid inorganic nanoparticles as bimodal therapeutic agents
  Tutores: Albert Figuerola y Marta Estrader (albert.figuerola@ub.edu y martaestrader@ub.edu, QI)
  Nanotechnology is gaining an increasing role in the therapy and diagnosis fields. In this Master thesis the

synthesis and characterization of new nanostructured bimodal therapeutic agents is pursued through the design of appropriate inorganic hybrid nanoparticles. This goal will be achieved by the presence of both a magnetic and a semiconductor domain sharing an interface within the nanoparticle. Each of the domains would accomplish its therapeutic role under the effect of a specific external stimulus such as light or magnetic field.

Materia Blanda

- *Titulo*: Formacion y estabilizacion de nuevas emulsiones de tipo agua-en-agua (W/W) basados en líquidos iónicos
  Tutor: Jordi Esquena (jordi.esquena@iqac.csic.es, IQAC-CSIC)
  Las emulsiones de tipo agua-en-agua (W/W) son dispersiones de una solución acuosa en forma de gotas que se encuentran en el interior de otra solución acuosa, en ausencia de aceite y de tensioactivo. Se forman en sistemas bifásicos por incompatibilidad termodinamica entre solutos. Son sistemas que existen en la naturaleza y que todavía están poco estudiados. Por ejemplo, los componentes intracelulares de las células eucariotas se almacenan dentro de gotas de emulsiones W/W, denominados orgánulos sin membrana ("membraneless organelles"). La presente propuesta desea continuar en el descubrimiento y estudio de nuevas emulsiones de tipo agua-en-agua basados en líquidos iónicos. En trabajos anteriores, hemos obtenidos nuevas emulsiones W/W en presencia de líquidos iónicos y el objetivo de la presente propuesta es avanzar en estas investigaciones.

- *Titulo*: Estudi polimòrfic de noves formulacions lipídiques amb aplicacions a la indústria alimentària
  Tutor: Laura Bayés (laurabayes@ub.edu, CR)
  Breu descripció: Els triacilglicerols, components majoritaris d'olis i greixos presents tant a la indústria alimentària, com a la farmacèutica o cosmètica, presenten un comportament polimòrfic complex, l'estudi del qual permet el disseny i desenvolupament de productes finals amb propietats fisicoquímiques concretes. Mitjançant tècniques calorimètriques i la difracció de raigs X, es pretén caracteritzar la cristal·lització i el polimorfisme de sistemes mixtes de triacilglicerols, amb l'objectiu de dissenyar formulacions aplicables a la industria alimentària amb propietats nutricionals saludables.

- *Titulo*: Preparació de polímers supramoleculars basats en curcuminoids
  Tutor: Arántzazu González-Campo y Núria Aliaga (agonzalez@icmab.es, naliaga@icmab.es, ICMAB-CSIC)
  El curcuminoids son derivats de la curcumina, considerada un anticancer natural, i que degut a les seves propietats hi ha un gran interès per la seva utilització en la síntesi de nous materials per la seva posterior aplicació tant en el camp de la biomedicina com per electrònica molecular. L'estudiant estudiarà la preparació de materials supramoleculars basats en interaccions host-guest de derivats de curcuminoids per controlar les seves propietats y la seva resposta a estimuls externs. L'estudiant es centrarà en la seva caracterització per tal de veure com afecta diferents paràmetres com la concentració, temps, entre altres a l'estructura final del material. Així mateix, s'estudiará la coordinacio amb metalls per la seva utilització en el camp del sensors i trasportadors de metalls.