Name of Supervisor: Prof Emilio Palomares
Number of Projects: 1

Ref. 2018/01: Perovskite Based Electronic Devices

Description of the project: The PhD researcher will work on the synthesis of novel semiconductor materials with perovskite structure. The new materials will be used for solar cells and light emitting diodes. Moreover, the interfacial charge transfer reactions in operando conditions will be also measured. Furthermore, the experimental data will be also used for advanced modelling to gain deeper understanding on the device performance.
Preferred skills or background: The applicant must have a background in physical chemistry or physics with knowledge in advanced programming (for example using Phyton, Matlab or similar). A high level of scientific English is required.

Name of Supervisor: Prof Anton Vidal
Number of Projects: 1

Ref. 2018/02: Discovery of Enantioselective Halogen-Bonded Catalysts for C-C and C-X Bond Forming Reactions

Description of the project: 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 enantioselective transformations that currently lack a satisfactory solution (earth-abundant-metal based C-B, C-O and C-C bond forming reactions) and applying the discovered catalysts to the stereoselective synthesis of compounds with biological interest.

Preferred skills or background: The position is ideal for eligible and talented candidates, who are highly motivated for pursuing the doctoral degree, are imaginative and willing to benefit from the breadth and depth of experience that the research group and host institution offer. A strong background in organic and inorganic synthesis would be advantageous.

Name of Supervisor: Prof Paolo Melchiorre
Number of Projects: 3

Ref 2018/03: Photochemical Enantioselective Organic Catalysis: Making Biologically Relevant Chiral Molecules with Light

Description of the project: Light-driven processes considerably enrich the modern synthetic repertoire, offering a potent way to build complex organic frameworks. In contrast, it is difficult to develop asymmetric catalytic photoreactions that can create chiral molecules with a well-defined three-dimensional arrangement. By developing innovative methodologies to effectively address this issue, we seek to provide a novel reactivity framework for conceiving photochemical enantioselective organocatalytic processes. We will proceed by translating the effective tools governing the success of ground state asymmetric organocatalysis into the realm of photochemical reactivity.

Preferred skills or background: The successful candidates will have a strong background in organic synthesis and asymmetric catalysis with an interest in medicinal chemistry and photochemistry. Excellent command of written and spoken English is required. Be familiar with common laboratory techniques and synthetic processes as well as with general analytical tools (NMR, GC, HPLC).

Ref 2018/04: Mechanistic Studies of Enantioselective Photo-Organocatalytic Processes

Description of the project: The development of effective light-driven enantioselective processes requires an intimate understanding of the photochemical and photophysical processes, which characterise the studied transformations. The main scientific aim of the PhD thesis is to combine experimental and mechanistic studies for conceiving photochemical enantioselective processes. This project will provide the PhD candidate with the unique opportunity of applying different mechanistic approaches, from conventional physical organic chemistry methods to classical experimental techniques most relevant to photophysical investigations, to guide the development of innovative photo-organocatalytic asymmetric strategies.

Preferred skills or background: The successful candidates will have a strong background in physical organic chemistry with an interest in radical reactivity, reaction mechanisms, kinetics, and photochemistry. Excellent command of written and spoken English is required. Be familiar with common laboratory techniques and general analytical tools (NMR, Time-Correlated Single Photon Counting, laser flash photolysis).

Ref. 2018/05: Light-driven Enantioselective Organic Catalysis

Description of the project: Photochemistry offers fascinating and unconventional ways for making molecules that are often complementary to traditional methods proceeding via thermal pathways. This is because the use of light excitation to bring a molecule to an electronically excited state can unlock unique reaction manifolds that are unavailable to conventional ground-state pathways. However, the involvement of high-energy excited states makes the development of enantioselective catalytic variants of photochemical reactions extremely difficult.
The proposed research seeks to develop novel strategies to control the stereochemical outcome of catalytic photochemical processes by translating the effective tools of organocatalysis into the realm of photochemical reactivity.

Preferred skills or background: The successful candidates will have a strong background in organic chemistry and asymmetric catalysis with an interest in radical reactivity and photochemistry. Excellent command of written and spoken English is required. Be familiar with common laboratory techniques and reaction screening conditions as well as with general analytical tools (NMR, GC, HPLC).

Name of Supervisor: Prof Núria López
Number of Projects: 1

Ref. 2018/06: Kinetic Monte Carlo for Heterogeneous Catalysis

Description of the project: The project will be devoted to the generation, maintenance and application of a Kinetic Monte Carlo code that can be employed in the chemical problems in heterogeneous catalysis.

Preferred skills or background: Physics, Chemistry, strong programming skills, English.

Name of Supervisor: Prof Ruben Martin
Number of Projects: 3

Ref 2018/07: Catalytic Remote Functionalization of Hydrocarbons

Description of the project: Metal-catalysed cross-coupling reactions have changed the landscape of organic synthesis. In these processes, bond-construction typically occur via functional group interconversion of pre-existing functionalities. This project will deal

with the development of earth-abundant catalysts for promoting a variety of C-C and C-heteroatom bond-forming reactions at remote and previously unfunctionalized positions within a hydrocarbon side-chain. The study of the mechanism by which these reactions operate will also be conducted, either by kinetic experiments or at the molecular level by the isolation of the putative reaction intermediates.

Preferred skills or background: The candidate should have a strong background and proven track record in organometallic chemistry with considerable experience with the optimization of catalytic reactions and excellent Schlenk techniques when dealing with air- and moisture-sensitive species. It is necessary to have a proven good knowledge of English.

Ref 2018/08: Visible Light Photochemical Functionalization of Unactivated sp3 C-H bonds

Description of the project: Recently, visible light photochemical technologies have provided a new technological push when building up molecular complexity. This project will face the challenge of designing new visible light photocatalysts for forging carbon-carbon bonds via the functionalization of unactivated sp3 C-H bonds, even in an asymmetric fashion.

Preferred skills or background: The candidate should have a strong background in photocatalysis and considerable experience with the optimization of catalytic reactions, particularly when dealing with air- and moisture-sensitive species. It is necessary to have a proven good knowledge of English.

Ref 2018/09: Unravelling the Mechanistic Intricacies of Catalytic Reductive Carboxylation Reactions

Description of the project: Although the development of nickel-catalysed carboxylation reactions of organic matter with CO_2 has gained considerable momentum, the mechanism by which these processes operate remain rather speculative and it is based on empirical evidences. This project aims at unravelling the mechanistic intricacies of nickel-catalysed reductive carboxylation reactions by physical organic methods as well as by the isolation of the putative nickel intermediates within the catalytic cycle.

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referred skills or background: The candidate should have a strong background and proven track record in organometallic chemistry with experience isolating and

characterizing exceptionally sensitive organometallic species, including paramagnetic intermediates. It is necessary to have a proven good knowledge of English.

Name of Supervisor: Prof Kilian Muñiz
Number of Projects: 2

Ref 2018/10: Development of C-H-Amination Reactions for Alkaloid Total Synthesis

Description of the project: This project aims to use direct C-H amination reactions of alkanes developed in our laboratory in order to devise novel entries into alkaloid structures of higher complexity. Throughout the course of the project, the candidate will also have the chance to work on ground-breaking new synthetic methodology development. The topic comprises both the development of such new synthetic methodology and the contribution to the total synthesis of molecules with biological or medicinal interest and with a significantly shorter number of steps than usually employed.

Preferred skills or background: The successful candidate should have broad knowledge on organic synthesis and methodology. A Master research project in this field will be valued positively, but is not a must. She/he should be highly motivated to contribute to solving challenging chemical questions, show a high degree of independent problem solving and enjoy laboratory research and team work. A high level of scientific English is required.

Ref 2018/11: Catalysis with Redox-Active Halide Reagents

Description of the project: The project aims to develop and explore new homogeneous halide catalysts in oxidation states -I, +I and +III. It includes the design of novel functionalisation processes of alkanes under environmentally benign catalytic conditions and the use of green oxidants such as peracids or hydrogen peroxide. Light-driven photoredox catalysis will also be considered.

Preferred skills or background: The successful candidate should have knowledge on organic synthesis and methodology. A Master research project in this field will be valued positively, but is not a must. She/he should be highly motivated to contribute to solving challenging chemical questions, show a high degree of independent problem solving and enjoy laboratory research and team work. A high level of scientific English is required.

Name of Supervisor: Prof Antonio Echavarren
Number of Projects: 2

Ref 2018/12: Gold-Catalysed Reactions for the Synthesis of Biologically Active Molecules

Description of the project: We propose to develop new cascade reactions for the synthesis of complex biologically relevant natural products.

Preferred skills or background: Bachelor and Master Degrees in chemistry with a background in organic and/or organometallic chemistry.

Ref 2018/13: Chiral Metal Catalysts Based on New Designs

Description of the project: We propose to design new gold or other metal catalysts with large ligands for the development of new cyclization types of polyunsaturated substrates.

Preferred skills or background: Bachelor and Master Degrees in chemistry with a background in organic and/or organometallic chemistry.

Name of Supervisor: Prof Feliu Maseras
Number of Projects: 1

Ref. 2018/14: Computational Treatment of Mechanochemistry

Description of the project: Mechanochemistry or mechanical chemistry is the coupling of mechanical and chemical phenomena on a molecular scale. The method of ball milling is widely used in this concern. The mechanisms of mechanochemical transformations are often complex and different from usual thermal or photochemical reactions. Computational chemistry can be helpful in their characterization, and this is the goal of this research project.

Preferred skills or background: Master in chemistry, chemical engineering or related matter. Experience in the use of Gaussian09 or related code using density functional theory.

Name of Supervisor: Dr Elisabet Romero
Number of Projects: 1

Ref. 2018/15: Design, Construction, and Investigation of Chromophore-Protein Systems to Achieve the Efficient Conversion of Solar Energy to Fuel

Description of the project: This multidisciplinary project involves biophysics, physical chemistry and synthetic biology. The objective is to design and construct bio-inspired chromophore-protein systems with the capacity to absorb and transfer sunlight energy and the ability to convert this energy into electrochemical energy (into a separation of charges). The energy and/or electron transfer dynamics will be investigated by ultrafast laser spectroscopy. Other systems' properties will be studied by steady-state spectroscopy, mass spectrometry, NMR, chromatography, and X-ray spectroscopy. These engineered systems will be utilized to construct solar cells, and ultimately, will be coupled to catalysts to achieve the efficient conversion of solar energy to fuel.

Preferred skills or background: The successful candidate's background should be physical chemistry or (bio)physics. Expertise in (ultrafast) spectroscopic techniques together with MatLab and Python programming skills will be preferred. Positive attitude, motivation to learn new methods and the ability to work in a team as well as individually are crucial for this position.

Name of Supervisor: Prof Carles Bo
Number of Projects: 1

Ref. 2018/16: Computational Chemistry to Tackle Complex Reactivity

Description of the project: Although Computational Chemistry has reached a high degree of maturity, still many issues remain to be solved. New chemical reactions that seem simple hide complex mechanisms and subtle effects that challenge theoretical models. The amount of data generated by current computational studies starts to be intractable so new protocols are needed. This project aims at developing computational models to fully understand homogeneous catalysis reaction mechanisms with varying levels of complexity. It includes both the development and use of new ioChem-BD pluggins, the platform developed by our research group, and the use of multiscale atomistic models combining DFT and molecular simulations.

Preferred skills or background: Master Degree in Chemistry, Chemical Engineering, Materials Science, or related areas, with demonstrable knowledge and practical skills of modern Computational Chemistry methods. Computer programing skills are highly desirable.

Name of Supervisors: Prof Anton Vidal and Prof José Ramón Galán-Mascarós
Number of Projects: 1

Ref. 2018/17: Separation of Stereoisomers Employing Highly Advanced Functional Materials

Description of the project: The separation of mixtures of enantiomers into the individual components represents the most challenging process in the field of separation of organic compounds. The present PhD project aims at designing and synthesizing new metal-organic frameworks (MOFs) that incorporate new functionalities in the pores. The separation properties of the developed materials, at the analytical and preparative scales, will be assessed in structurally diverse mixtures of enantiomers. The focus of this project will also be on developing sustainable separation methodologies that encompass the re-usability of the chiral phase and the use of benign solvents, amongst other variables.

Preferred skills or background: The position is ideal for eligible and talented candidates, who are highly motivated for pursuing the doctoral degree, are imaginative and willing to benefit from the breadth and depth of experience that the research group and host institution offer. A strong background in organic, inorganic and analytical chemistry (chromatographic methods) would be advantageous.

Name of Supervisor: Dr. Julio Lloret-Fillol
Nº of Projects: 1

Ref.2018/18: Electrocatalytic Organic Transformations

Description of the project: The goal is to develop 1st row coordination complexes active as electrocatalysts for reduction of C=O and C=C double bonds. Electrocatalysis presents an extraordinary opportunity to develop cleaner organic transformations since there is no need for elaborate sacrificial agents. However, (enantio) selective synthetic strategies have been rarely developed. In this regard, the project will provide greener methodologic solutions.
Little has been developed driven (enantio) selective reductive chemistry by merging (photo-) redox catalysis with transition metal mediated transformations for the synthesis of high-value chemicals using light as a source of energy.

Preferred skills or background: We are looking for students with strong skills (or affinity) in organic chemistry and mechanistic studies. The work will imply the use and

development of highly parallel synthetic methodologies. The candidates should be highly motivated, responsible, independent and creative with high level of English and a good academic record.

Name of Supervisor: Antoni Llobet
Number of Projects: 1

Ref. 2018/19: Catalysts for Artificial Photosynthesis

Description of the project: The research work to be developed is framed within the field of redox catalysis with transition metal complexes with a special focus on redox processes. The overall objective is to understand the various factors that affect catalyst's efficiency and selectivity with special focus to the transition metal electronic structure and space disposition. Particular attention is being paid to the catalytic oxidation of water to molecular dioxygen, given the implications of this reaction for new energy conversion schemes based on artificial photosynthesis. The final objective of the PhD thesis is the photo-production of hydrogen from water and sunlight.

Preferred skills or background: We are looking for a highly motivated, responsible and creative student in the Chemistry domain. The candidates must have an outstanding academic record and good command of English. Skills in the fields of coordination chemistry, spectroscopy, electrochemistry, catalysis, electrocatalysis and photocatalysis will be appreciated