Name of Supervisor: Prof. Paolo Melchiorre
Nº of Projects: 4

Ref. 2017/01-MEL: 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. 2017/02-MEL: New Catalytic Strategies for Enantioselective Photochemistry

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 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).

Ref. 2017/03-MEL: 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. 2017/04-MEL: 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. Pau Ballester
Nº of Projects: 2

Ref. 2017/05-BAL: Synthetic receptors and sensors for the supramolecular detection of low molecular weight molecules related to human health

Ref. 2017/06-BAL: Synthetic receptors and sensors for the supramolecular detection of low molecular weight molecules related to human health

Description of the projects: The group of Prof. Ballester is looking for two highly talented and motivated national or international students who wish to do their PhD under optimum conditions in a modern and stimulating environment, equipped with high-level instruments and technological resources. In partnership with the Universitat Rovira i Virgili (URV), ICIQ offers the PhD programmes "Chemical Science and Technology" and "Technologies for Nanosystems, Bioengineering and Energy". The PhD candidates will be working on the supramolecular detection field using molecular and supramolecular synthetic receptors for their application in the development of molecular sensors and sensor devices for molecules related to the human health.

Preferred skills or background:

- Master's degree in Chemistry.
- Good communication skills
- Good level of spoken and written English
- High motivation
- Excellent academic transcripts

Name of Supervisor: Prof. Kilian Muñiz
Nº of Projects: 2

Ref. 2017/07-MUN: C-H Amination Reactions for Alkaloid Total Synthesis

Ref. 2017/08-MUN: C-H Amination Reactions for Alkaloid Total Synthesis

Description of the projects: These projects will develop direct amination reactions of alkenes and alkanes in order to devise novel synthetic entries into alkaloid structures of higher complexity.

Selective aminations will constitute the key steps demonstrating that C-H to C-N bond formation can constitute a versatile alternative to common reductive amination. The final aim is to arrive at the total synthesis of molecules with biological or medicinal interest and with a significantly shorter number of steps than usually employed. Where

required throughout the course of the project, the candidate will also have the chance to work on methodology development and method improvement.

Preferred skills or background: The prospective candidate should have a solid background in synthetic organic chemistry including strong laboratory experience and knowledge on common analytics (NMR, IR, MS, HPLC). Basic knowledge on literature search and synthesis planning are expected and strong English language skills are required. Previous experience in biochemistry is a plus

Name of Supervisor: Prof. Antoni Llobet
Nº of Projects: 2

Ref. 2017/09-LLO: Catalysts for Artificial Photosynthesis – Oxidations

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 oxidative 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

Ref. 2017/10-LLO: Catalysts for Artificial Photosynthesis – Reductions

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 reductive 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 reduction of water to hydrogen, 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

Name of Supervisor: Prof. Arjan W. Kleij
Nº of Projects: 3

Ref. 2017/11-KLE: Functional cyclic organic carbonates as versatile precursors in selective fine chemical synthesis: a dual role of carbon dioxide

Description of the project: In previous years we have focused on the synthesis of highly substituted cyclic carbonates with wide functional group diversity. In this new project we will capitalize on their potential to act as versatile precursors in the catalytic synthesis of attractive synthetic targets using transition metal catalysis and challenging carbon nucleophiles. Mechanistic work will complement the experimental studies to ensure an appropriate understanding of the operative mode of the catalysts that allows for controlling the enantio-, stereo- and chemo-selectivity features.

Preferred skills or background: Suitable candidates should have profound knowledge of organic chemistry complemented with organometallic skills, interest in mechanistic work and a minimal level of English.

Ref. 2017/12-KLE: Stereoselective catalytic conversion of cyclic carbonates into high value fine chemicals

Description of the project: This project will take advantage over the use of easily accessible functional cyclic carbonates and their catalytic conversion into fine chemicals of high interest. Principally main group/transition metal catalysts will be used to activate the carbonate substrates in situ for nucleophilic attack, and a major focus will be on controlling the stereoselectivity of these transformations. Complementary to these studies mechanistic work is carried out both experimentally as well as computationally to elucidate the manifolds driving these conversions and iterative methods will allow for optimization of the process parameters and output.

Preferred skills or background: Suitable candidates should have profound knowledge of homogeneous catalysis/organic chemistry complemented with an interest in mechanistic studies. A minimal level of English is required.

Ref. 2017/13-KLE: Catalytic synthesis of bio-sourced polymers using terpenes as molecular scaffolds

Description of the project: Previously we have described an efficient new catalyst system for the copolymerization of limonene oxide and CO_2, and a detailed understanding of the polymerization mechanism. In this new project we will extend the use of other terpene-based monomers for the preparation of new polymers with high content of renewable components, and properties reminiscent of commercial though fossil fuel based polymers. Apart from this, the design of new thermal and mechanical properties for these polymers will be pursued in close collaboration with industrial partners.

Preferred skills or background: Suitable candidates should have profound knowledge of homogeneous catalysis complemented with interest in polymer chemistry and practical applications. A minimal level of English is required.

Name of Supervisor: Dr. Marcos García Suero
Nº of Projects: 1

Ref. 2017/14-SUE: New Reactivity Concepts for Small Molecule Asymmetric Activations

Description of the project: The goal of this project is to develop new asymmetric C=C and C–H bond activations and their application to simplify the synthesis of complex enantioenriched molecules, which are difficult to synthesized using current methodologies. This project will exploit the catalytic generation of unusual or unprecedented organic/organometallic reactive species able to provide new chemical reactivity and new disconnection approaches. It is envisaged that these concepts will have broad application in the synthesis of important natural products or therapeutic agents.

Preferred skills or background: Master Degree in Organic/Organometallic Chemistry, which must be completed by the time of enrolment in the PhD programme. Strong commitment to scientific research and good command of English

Name of Supervisor: Dr. Atsushi Urakawa
Nº of Projects: 1

Ref. 2017/15-URA: Continuous transformation of carbon dioxide to valuable chemicals and fuels by heterogeneous catalysis

Description of the project: The task of the project is to develop novel heterogeneous catalysts and processes for continuous catalytic transformation of carbon dioxide for the production of higher alcohols and organic carbonates among others. Besides novel catalyst syntheses and process optimisation, development of spectroscopic (e.g. IR, Raman and synchrotron spectroscopy) and visualization tools to monitor catalyst and catalytic reactors under working (high temperature and pressure) conditions is expected to facilitate rational catalyst design.

Preferred skills or background: Candidate should possess background in chemical engineering, chemistry, physics or material science with proven skills and/or convincing interests in synthesis and characterization of catalyst materials. Experience or strong interest in reaction engineering, spectroscopy and programming is highly valued.

Name of Supervisor: Prof. Anton Vidal
Nº of Projects: 1

Ref. 2017/16-VID: Discovery of supramolecularly regulated enantioselective catalysts for C-X bond forming reactions

Description of the project: This project is aimed at developing new synthetic catalytic methods for enantioselective transformations that currently lack a satisfactory solution, such as some types of intramolecular C-X bond forming reactions (X = N, O) leading to cyclic skeletons. The developed asymmetric catalytic tools will be applied to the stereoselective synthesis of compounds (or advanced synthetic intermediates of these products) with biological interest. From the methodological point of view, it should be mentioned that the design, preparation and optimization of the asymmetric catalytic systems will be based on the regulation of the geometry of the active site *via* supramolecular interactions.

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. Antonio M. Echavarren
Nº of projects: 3

Ref. 2017/17-ECH: Gold-Catalysis for the Synthesis of Biologically Active Molecules

Ref. 2017/18-ECH: Gold-Catalysis for the Synthesis of Biologically Active Molecules

Ref. 2017/19-ECH: Gold-Catalysis for the Synthesis of Biologically Active Molecules

Description of the projects: We propose to design new mono- and dinuclear gold or other metal catalysts with large ligands to induce the folding of the linear substrates (polyalkenes or polyenynes) in the manner required to achieve new cyclization types. New methods for the selective generation of reactive metal carbenes will be also studied to develop unconventional cyclopropanations, annulations, as well as metathesis processes.

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

Name of Supervisor: Prof. Núria López
Nº of projects: 3

Ref. 2017/20-LOP: Modelling and mapping pathways of electrochemical CO2 reduction

Description of the project: The work will consist on the detailed identification of the reaction routes able to convert CO2 into useful products. The simulations will encompass the study of the surface, the reaction networks and most likely reaction paths and the investigation of possible modifications to improve performance through the massive use of theoretical simulations based on Density Functional Theory. The work includes two secondments in other research groups of the ITN network.

Preferred skills or background: The candidates should have a B.Sc. or Master degree in Chemistry (Theoretical, Physical) or Physics and experience in computational/theoretical chemistry and the use of Unix-based operating systems is definitely a plus. English command is mandatory.

Ref. 2017/21-LOP: Molecular catalysts for CO2 reduction to CO and HCOOH

Description of the project: The work will be devoted to the study of molecular-based catalysts for the reduction of CO2 to suitable intermediates including CO and formic

acid. For this a close collaboration with experimental groups will be envisaged and two secondments are foreseen. The possibilities to implement the molecular properties to a heterogenous matrix will be investigated.

Preferred skills or background: The candidates should have a B.Sc. or Master degree in Chemistry (Theoretical, Physical) or Physics and experience in computational/theoretical chemistry and the use of Unix-based operating systems is definitely a plus. English command is mandatory.

Ref. 2017/22-LOP: Lignin valorization

Description of the project: Computational techniques based on Density Functional Theory to describe the reactivity of metals and bimetallic systems to describe the conversion of lignin derived compounds into platform chemicals will be explored in this project.

Preferred skills or background: The candidates should have a B.Sc. or Master degree in Chemistry (Theoretical, Physical) or Physics and experience in computational/theoretical chemistry and the use of Unix-based operating systems is definitely a plus. English command is mandatory.

Name of Supervisor: Prof. Feliu Maseras
Nº of Projects: 1

Ref. 2017/23-MAS: DFT characterization of single-electron processes in homogeneous catalysis

Description: The candidate will work on the application of DFT and DFT/MM methods in the characterization of reaction mechanisms of practical interest, probably in collaboration with experimental groups. The focus will be on single-electron transfer processes, with particular emphasis in cases where the reactant species are closed-shell.

Preferred skills : Master degree in chemistry of related field

Name of Supervisor: Prof. Emilio Palomares
Nº of Projects: 1

Ref. 2017/24-PAL: Charge transfer on hybrid photovoltaic devices: semiconductor nanocrystals/organic semicondcutor molecule

Description: FotoTransfer aims to study, analyse and understand the charge transfer processes that take place at the heterojunctions (interfaces) between small organic molecules and semiconductor nanocrystals that are used in solar cells with efficiencies close to 20%. The project targets to rationalize the solar cell efficiency with the charge recombination (carrier losses) at the different solar cell interfaces. FotoTransfer will use solar cells based on hybrid perovskites as photoactive material, combining solution processing and high vacuum techniques. To complete our objectives, the project has enrolled a multidisciplinary research team with previous experience on the fabrication of photovoltaic devices based on small organic molecules, the measurements and analysis of charge transfer processes in solar cells and the synthesis and characterization of perovskites. This project represents a challenge with a great deal of fundamental research that implies: (a) synthesis of semiconductor materials, (b) fabrication and assessment of hybrid solar cells, and (c) the study of the charge transfer processes under illumination conditions. The reason, for the importance of the understanding of the charge transfer processes, focusses on the fact that these processes are the ones responsible for the final light to energy conversion efficiency in the solar cells. Thus, to analyse and to understand, which process is the bottle neck that hamper these solar cells to reach their maximum theoretical efficiency is paramount.

Preferred skills/ background: The applicant must have a degree either in chemistry, physics or engineering. Proficiency english level is mandatory. Skills on programming, Matlab, Mathematica or Igor Pro will be appreciated.

Name of the Supervisor: Prof. Ruben Martin
Nº of Projects: 1

Ref.2017/25-MAR: metal-catalyzed functionalization of strong sigma bonds

Description of the project: The candidate will work on the design of conceptually new approaches for the catalytic functionalization of strong sigma bonds en route to added-value chemicals from simple precursors. These concepts will be complemented with in depth mechanistic and kinetic studies to unravel the intricacies of these transformations.

Preferred skills or background: the candidate must have a strong background in organometallic chemistry with good experience in Schlenk techniques when dealing with air- and moisture-sensitive species as well as considerable experience with the optimization of catalytic reactions.

Name of Supervisor: Prof. Miquel A. Pericàs
Nº of Projects: 1

Ref. 2017/26-PER: Development of Photoredox Catalysis and Tandem Processes in Flow with Immobilized Species

Description of the project: Visible-light photoredox catalysis has emerged as a powerful tool to control carbon radical reactions under mild conditions. The project involves the development of heterogeneous catalysts for their application in photoredox catalytic reactions in flow chemistry where photochemical reactions show an increased efficiency compared with batch reactions. At the same time, new catalytic tandem processes in flow will be studied, using different immobilized catalysts for the synthesis of high-complex structures compounds.

Preferred skills or background: we are looking for talented graduate students from any nationality, with an excellent academic record, enthusiastic interest in chemical research and solid working knowledge of English. Candidates must have a Master or an equivalent degree in the areas of Chemistry, Chemical Engineering or Biological Chemistry completed by the time of enrolment in the PhD programme.

Name of Supervisor: Dr. Julio Lloret Fillol
Nº of Projects: 4

Ref. 2017/27-FIL: Light-driven umpolung E+-E+ couplings

Description of the project: The project is focused on novel light-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. Steric and supramolecular interactions (including chiral pockets and artificial metallo-enzimes) will be studied to control the selectivity in umpolung E+-E+ couplings. This project aims to progress towards greener chemical transformations at the edge of the current methodologies.

Preferred skills or background: We are looking for students with strong skills (or affinity) in organic and organometallic chemistry, homogenous catalysis and mechanistic studies. The work will imply the use and the development of highly parallel synthetic methodologies. The candidates should be highly motivated, responsible, independent and creative with high level of English and an good academic record.

Ref. 2017/28-FIL: Reductive Chemistry – Towards Solar Chemicals

Description of the project: The PhD research program will be the development of new molecular catalysts for the photo- and electrocatalytic reduction of CO2 and organic compounds and to understand the basic mechanisms of action. The catalysts to develop will be based on 1st row transition metal complexes. organic substrates of technological interesting will be studied. The aim of the project is to utilize directly electrons extracted from water (water oxidation) avoiding the need of sacrificial redactors, which will contribute to cleaner and more sustainable reductive chemistry.

Preferred skills or background: We are looking for students with strong skills (or affinity) in organic and organometallic chemistry, electrocatalysis and experimental and and computational mechanistic studies. The candidates should be highly motivated, responsible, independent and creative with high level of English and an good academic record.

Ref. 2017/29-FIL: Photocatalytic C-H activations

Description of the project: The aim of the project will be discover new photoredox protocols to activate inactive C-H bonds by merging (photo-) redox catalysis with transition metal complexes. The aim of the project is to provide alternative C-H activation of large available raw materials such as methane to transform them in usefully building blocks.

Preferred skills or background: We are looking for students with strong skills (or affinity) in organic chemistry, light-driven catalysis 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 an good academic record.

Ref. 2017/30-FIL: 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: Prof. Carles Bo
Nº of Projects: 1

Ref.2017/31-CBO: Advanced computational methods for catalysts design

Description of the project: Modern catalytic transformations rely on elaborated recipes involving metal complexes, co-catalysts, additives, solvent mixtures. This project aims at developing computational protocols to advance in the multi-scale modelling of such complex systems. Workflows combining DFT based methods and molecular dynamics simulations will be developed and applied to environmentally relevant green processes.

Preferred skills or background: Chemistry, physics, materials science. Knowledge in high-level programming languages