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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

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**Título:**

RATIONAL DESIGN OF POROUS SOLIDS WITH APPLICATION IN RELEVANT CHEMICAL PROCESSES

**Resumen de la Memoria:**

The design of porous solids with specific textural and chemical properties is important for their application in interesting technological and industrial processes. In this project, a rational design of microporous inorganic materials (such as zeolites) and porous hybrid materials (organic-inorganic), with appropriate physical and chemical properties for relevant chemical processes is proposed. First, new concepts in the design of organic structure directing agents (OSDA) in zeolite synthesis will be introduced. Amines and quaternary ammonium cations are often used as OSDAs. Despite the interaction of the OSDA with the inorganic host are still heavily studied in order to rationalize the OSDAs properties with the framework topology, the design of OSDAs based on transition state mimics of relevant industrial reactions is proposed as a new potential approach. Then, new zeolitic structures synthesized by using a mimic of a transition state would show suitable cavities or channels to admit the desired transition state, while the distribution of the active sites in known zeolite frameworks would be modified allowing a unique reactivity for this process. Other important challenge is the synthesis of chiral zeolites. They are very interesting for the pharmaceutical industry because enantioselective separations and syntheses can be achieved. To synthesize a chiral zeolite, specific chiral templates must be found. However, the chirality of the OSDA has still not been transferred to the inorganic host due to the rotation about axes of symmetry of the organic molecules, avoiding the desired  $\zeta$ template $\zeta$  effect. Thus, the design of new chiral OSDAs with an alkoxysilane group in their structures is proposed. The absence of free rotation of the guest molecules due to their grafting to the inorganic matrix, will allow the introduction of rigidity in the  $\zeta$ template $\zeta$  molecule avoiding the chirality loss. Second, the design of porous hybrid (organic-inorganic) catalysts with distinctive functional groups in their structure is considered. This multi-functionality permits the combination of different sequential reactions in the same reactor ( $\zeta$ one-pot $\zeta$ ). The rational distribution of isolated Lewis acid sites (Sn, Ti, Nb, Ta) together with organic acid/base groups in siliceous supports (crystalline lamellars, or ordered mesoporous) will allow an ideal combination for  $\zeta$ one-pot $\zeta$  reactions, avoiding the problems of homogeneous catalysts (such as corrosiveness, or difficulties in separation). Those hybrid materials are the proper catalysts for various important biomass conversion schemes towards valuable chemical intermediates.

**Resumen del Curriculum Vitae:**

Manuel Moliner received his B.Sc. in Chemical Engineering at the  $\zeta$ Universidad de Valencia $\zeta$  (UV) (1997-2003). Then, he started his Ph.D. studies at the  $\zeta$ Instituto de Tecnología Química-ITQ $\zeta$  (UPV-CSIC) under the supervision of Prof. Avelino Corma and Dr. Maria J. Díaz-Cabañas with an I3P-CSIC pre-doctoral scholarship. His thesis involved the synthesis of microporous materials by means of high-throughput techniques, creating a new accelerated methodology for the discovery of model zeolitic structures. He obtained his Ph.D. in Chemistry from the  $\zeta$ Universidad Politécnica de Valencia $\zeta$  (UPV) in February 2008, receiving the Cum Laude qualification. The scientific quality of his Ph.D. was recognized by three awards: the  $\zeta$ UPV-Extraordinary Award $\zeta$  for the best thesis defended at the UPV (2007-2008), the  $\zeta$ SUSCHEM-RSEQ $\zeta$  for the best thesis in any area of chemistry in Spain (2008), and the  $\zeta$ EFCATS-2009 $\zeta$  for the best thesis in the field of catalysis in Europe (2007-2009). He performed his post-doctoral research with Prof. Mark Davis at the California Institute of Technology (Caltech), frequently ranked among the top three technological universities in the world. There, the applicant focused his research on the design and synthesis of multifunctional materials with applications in industrially-relevant processes, mainly in biomass transformations. Since December 2010, he is performing research at the ITQ, focusing on new scientific projects for the rational design of novel heterogeneous catalysts. He is co-author of 21 high-profile publications, some in multidisciplinary journals (2 Nature, 1 PNAS), in general chemistry journals (2 Angewandte, 1 JACS, 1 Chem. Commun., 2 Chem-Eur.J), and in specialized journals (4 J. Catal., 2 Chem. Mater., 2 J. Phys. Chem. C, 2 Microp. Mesop. Mat.); these publications were well-distributed throughout his Ph.D. and postdoctoral research. The applicant has 7 international patents and 1 patent application, 5 of them transferred to industry (ExxonMobil and Albemarle Netherlands). He has attended several international congresses, presenting five oral communications. He has been invited to write a general text for the  $\zeta$ Spanish Technologic Platform of Sustainable Chemistry $\zeta$ , and he is also a reviewer of the journal  $\zeta$ MatChemPhys $\zeta$  from Elsevier.



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**Título:**

Peptide and protein chemistry for the conjugation of biomolecules to nanoparticles.

**Resumen de la Memoria:**

The world of nanotechnology promises to change our vision of science and spread the advances in numerous fields, being particularly interesting the possible applications that could have in medicine. Semiconductor nanocrystals or quantum dots (QDs) made of a CdSe-ZnS core-shell have gained special attention in recent years due to their excellent photophysical properties: wide absorption bands, high extinction coefficients, narrow and symmetrical emission bands, large Stokes shifts, long luminescent bands and large cross-section absorptions. These properties make the QDs the ideal candidates in biotechnological research, spanning from live cell imaging to proteolytic sensors designed to detect toxins. To accomplish those objectives a very important issue is the chemistry associated to the interface between material science and biology: it is required good and reliable chemistries to form stable and defined QD-biomolecule hybrids. Such chemical tools will enable an efficient and controlled ligation of macromolecules to nanoparticles making easier to control the macromolecular properties of the conjugates. A part of my research line is addressed to the development of new approaches to attach biomolecules (peptides, proteins, nucleic acids) to QDs or other nanoparticles. One of these approaches that came up in the last years and has been shown very successfully is the polyhistidine tag (His6) appended in the C- or N-terminal position of peptides and proteins. The His6 tag binds the ZnS shell of the QDs similarly as His6 proteins bind nitrilotriacetic columns, allowing the conjugation up to 60 peptides and ~12 medium size (~50 KDa) proteins like the Maltose Binding Protein. Equally interesting is the possibility of performing chemical reactions on the QDs, which represents a more convergent approach and spans the array of molecules that can be assembled. For example, by functionalization of the His6 tag with an aldehyde and the biomolecule desired to attach with a hydrazine derivative it is possible to synthesize different types of QDs conjugates with different properties and functions: QD-peptide sensors to monitor proteolytic activity, QDs-DNA dye labeled hybrids for energy harvesting complexes and QD-peptide conjugates for cell imaging that target different cellular compartments. The design in the majority of this biosensing systems relies in the assembling of the multiple copies of a dye labeled peptide able to accept the fluorescence signal emitted from the QDs. Upon addition of the sensed biomolecule, the QDs suffer a change in their fluorescence signal that can be quantified and directly associated to the concentration of the analyte measured. In summary, the continuous research in peptide and protein chemistry in aqueous phase is fundamental to bring out new nano-bioconjugates for biotechnological applications.

**Resumen del Curriculum Vitae:**

On September 2000, I graduated in Chemistry at the University of Santiago de Compostela and started off my research career under supervision of Professor José Luis Mascareñas working on DNA catalyzed cycloaddition and peptide bond formation reactions for what I got my MS degree in Organic Chemistry in 2002. Then, I went on to the PhD continuing the research line that was established in the group about DNA binding peptides. The aim of this project was the design and synthesis of new DNA binding peptides that could interfere in the cellular transcription process to be able of controlling the aberrant expression of certain types of genes that could induce tumor processes. These peptides comprise two different modules, either covalently or non-covalently linked: a peptidic fragment from the basic region of the transcription factor (TF) GCN4 and a polyamide or tripyrrol. The peptidic moiety binds the DNA major groove, while the polyamide simultaneously inserts in the adjacent minor groove. Those constructs have a much higher affinity and specificity than every component isolated and can bind their target sequence with an association constant around  $3.3 \times 10^8 \text{ M}^{-1}$  at room temperature, similar to the natural TFs. For this work, I obtained my PhD degree in 2006 in Organic Chemistry. In the meantime, I had the opportunity to spend 4 months on 2003 in the laboratory of Professor Barbara Imperiali at the Massachusetts Institute of Technology where I learnt about peptide combinatorial chemistry and new fluorophores that are environment sensitive. After that, on October 2006 I moved to San Diego (California, USA) to begin a postdoctoral period at the The Scripps Research Institute under supervision of Professor Philip E. Dawson, first with a Fulbright fellowship and then with a Marie Curie International Outgoing Fellowship. My research interests are centered on new methodologies for solid phase peptide synthesis, peptide and protein modification in aqueous solution using chemoselective reactions (hydrazones, cycloadditions, Wittig) and nanotechnology applied to biology, i.e., new biosensors to monitor proteolytic activity, energy harvesting complexes and cell delivery and imaging approaches of hybrids made of gold or quantum dot nanoparticles and biomolecules (peptides, proteins and nucleic acids). I am coauthor of 24 articles in different journals: J. Am. Chem. Soc. (5), ACS Nano (4), Angew. Chemie (3), Small (2), ChemBiochem (2), Bioconjugate Chemistry (1), Chemistry-An European Journal (1), Organic Letters (1), Integrative Biology (1), Nature Materials (1), Chemistry & Biology (1), Journal of Medicinal Chemistry (1), Biopolymers (1) receiving a total of 188 citations with a h-index = 7. In addition, I am the coauthor of 2 patents internationally extended.



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CONVOCATORIA 2011**

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**Título:**

The interplay between environment and light-harvesting in photosynthetic pigment-protein complexes

**Resumen de la Memoria:**

In photosynthesis, special antennae proteins that contain multiple light-absorbing chromophores (mostly chlorophylls) are able to capture sunlight and transfer the excitation energy to reaction centres with almost 100% quantum efficiencies. Recent work has discovered that a contribution to the dynamics of energy transfer within some photosynthetic proteins involves quantum coherence. (Collini et al., Nature, 2010, 463, 644). Those reports have inspired many theoretical studies, where the critical role played by the environment has been highlighted. Mimicking these systems to develop optimized artificial light-harvesting devices, however, is difficult because a detailed understanding of the role played by the environment on resonance electronic energy transfer (RET) processes is still missing. This is due to the complex interplay between the nuclear modes of the protein and the excited-state dynamics of the participating chromophores. For example, decoherence and energy transfer are caused by coupling of electronic transitions to the stochastic fluctuations of the environment. The frequency spectrum of the environment (spectral density) is therefore an important quantity, but equally important is the way the electronic coupling between molecules is influenced by the environment. The proposed research line aims at elucidating such interrelations, based on the development and application of atomistic quantum mechanics/molecular mechanics (QM/MM) methodologies coupled to Molecular Dynamics techniques for the simulation of energy transfer in biological environments. This methodology will combine time-dependent density functional theory (TD-DFT) for the description of chromophore excited states, while the protein and surrounding solvent will be accounted for through polarizable force fields. The key objective of the research line is the development of accurate first principles approaches able to describe the RET parameters (transition energies and electronic couplings) and their time-evolution (spectral densities), needed to develop quantitative models of light harvesting. The research will be initially focused on RET dynamics in phycobiliproteins (PBPs), a family of antenna proteins present in marine algae that contain special pigment molecules called bilins. The active collaboration of the candidate with the group of professor Gregory D. Scholes (University of Toronto, Canada), who leads a research line on RET dynamics in PBPs using state-of-the-art ultrafast two-dimensional electronic spectroscopy techniques, assures a fruitful synergy between theory and experiment of great added value to the research proposed.

**Resumen del Curriculum Vitae:**

Carles Curutchet received his B.Sc. degree in Chemistry from the University of Barcelona (1999). There, he began his research career at the group of Prof. F. J. Luque and M. Orozco working on the development of quantum-mechanical continuum solvation models, the most remarkable achievement being the development of a methodology aimed at predicting molecular 3D hydrophobic/hydrophilic profiles from fractional contributions to the octanol-water partition coefficient, with application to drug design studies. This methodology has been recently included in the commercial Gaussian 09 package. In 2005, he obtained his Ph.D. degree and started a postdoctoral stay at the Universities of Pisa (2005) and Parma (2006-2007), joining the PCM group led by Prof. J. Tomasi, B. Mennucci and R. Cammi. During these years, he worked in the development and implementation of solvation models aimed at the study of excited state dynamics in the Gaussian package, being the above mentioned professors co-authors of this code. From this period, it is worth remarking a series of pioneering studies on solvent screening effects on electronic energy transfer processes, which revealed a previously unidentified contribution to the distance dependence of the transfer rate. In 2008, he moved to the prestigious group of Prof. G. D. Scholes at the University of Toronto (Canada), with the objective of achieving a solid background in the study of excited state dynamics of biological and nanoscale systems combining theory with advanced ultrafast nonlinear spectroscopy. There, he collaborated with other leading groups in the study of photosynthetic systems (R.J. Silbey, Massachusetts Institute of Technology), semiconductor nanocrystals (A. Zunger, National Renewable Energy Laboratory), carbon nanotubes (S. Tretiak, Los Alamos National Laboratory) or organic conjugated polymers (D. Beljonne, Université de Mons-Hainaut). Product of these fruitful collaborations it is worth remarking a high-impact Feature Article published in J. Phys. Chem. B in 2009, which is included in the Top 20 most cited articles for the journal that have been published within the last 3 years. In November 2009 he moved to the group of Prof. Miquel Solà (University of Girona) where he won a Beatriu de Pinós postdoctoral position. Overall, the trajectory of the candidate includes 35 articles, with more than 500 citations (h-index 14), published in high impact journals (16 as first author, 7 as corresponding author): Angew. Chem. Int. Ed. (1), J. Am. Chem. Soc. (2), Acc. Chem. Res. (1), Laser Photonics Rev. (1), J. Med. Chem. (1), Biophys. J. (2), J. Chem. Theory and Comput. (3), Phys. Chem. Chem. Phys. (2), J. Phys. Chem. B (7), J. Comput. Chem. (5), J. Chem. Phys. (4), J. Phys. Chem. A (1), J. Phys. Chem. C (1), Photochem. Photobiol. Sci. (1), Chem. Phys. Lett. (1), Tetrahedron (1), J. Mol. Struct. (1), 3 book chapters (one as single author), and 16 communications in conferences (9 oral). He has also performed reviewer tasks for several leading journals, including J. Am. Chem. Soc. This trajectory has been recently recognized by the ANECA, that gave the candidate the accreditations necessary to become Profesor Contratado Doctor, Profesor Ayudante Doctor and Profesor de Universidad Privada in Spanish universities.



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**Título:**

Sustainable organic chemistry: C-H- and C-C-bond functionalization and cycloisomerization reactions

**Resumen de la Memoria:**

Society's demands for energy and materials are continuously growing. Seeing the limited availability of our natural resources and their consequences, new solutions are required to overcome this situation. Chemistry, particularly organic chemistry and catalysis, plays a significant role in science and society, influencing essential areas such as agriculture, medicine or material sciences. Sustainable chemistry appears as a key tool to tackle this worrisome state. Thus, the research proposal consists of the development of new catalytic processes to achieve sustainable chemical transformations. Traditionally, teaching of organic chemistry has revolved around transformations of functional groups. Any fundamental text-book about organic chemistry contrasts the reactivity of functional groups and the inertness of C-H-bonds. Thus, despite the ubiquitous occurrence in organic molecules, the C-H-bond was far from being considered as a functional group. However, selective functionalization of C-H-bonds constitutes an economically and ecologically attractive strategy in synthesis. Through insertion of new moieties into C-H-bonds the need for additional functional groups that are directly involved as reactive partners is removed. As a result, this strategy significantly shortens a synthesis and diminishes the generation of unwanted byproducts. In last years, a huge growth in the field of C-H-bond functionalization occurred, nevertheless, novel challenging transformations can still be envisioned. The main research line will focus on selective C-H-bond functionalization, stressing on more challenging C(sp<sup>3</sup>)-H-bonds. An interesting aim concerns the use of removable and reusable covalent or non-covalent linkers in order to control regioselectivity. Particular attention will be made on exploiting renewable/simple feedstock such as O<sub>2</sub>, N<sub>2</sub> or CO<sub>2</sub> as coupling partners. Mechanistic studies will be performed to establish user- and environmental friendly reaction conditions, the use of cheap/reusable catalysts or solvents, and alternative energy sources such as visible light. Alternatively, C-C-bonds compose the scaffold in organic molecules. Selective cleavage of C-C-bonds, mainly in cyclic compounds, might enable a double functionalization, allowing an increase of the molecular complexity in one-pot. Therefore, efforts to develop selective functionalizations of C-C-bonds will be made. Conversely, cycloisomerization reactions constitute a sustainable synthetic strategy due to their atom-economic nature. Thus, search for new pathways in cycloisomerization reactions, mainly catalyzed by inexpensive catalyst like copper or iron, will be performed. Additionally, metal-catalyzed cascade reactions can considerably enhance structural complexity by multiple iterations of well-known organometallic steps. Merging cycloisomerizations with C-H- or C-C-bond functionalizations in cascade reactions might allow a straightforward preparation of molecules with structural complexity minimizing handling and waste generation. Consequently, combination of these types of transformations into cascade reactions will be pursued. In summary, this proposal focuses on the development of sustainable methodologies for the preparation of organic molecules through new disconnection strategies, which could be applied to the rapid synthesis of chemicals with relevance to academia and industry.

**Resumen del Curriculum Vitae:**

I was educated at the Complutense University of Madrid (UCM), where I gained a degree in Chemistry (June 2000). Then, I joined for one year the group of Prof. M. A. Sierra (UCM), working on beta-lactam chemistry. After one year working in programming, I was awarded with a fellowship (Spanish Ministry of Education and Science) to carry out Ph. D. studies at the University of Oviedo, under the guidance of Prof. José Barluenga (July 2002-June 2006). At this stage, I worked in organometallic chemistry and its applications to organic synthesis, particularly, on the modification of the well-known reactivity of group 6 Fischer-carbenes by using rhodium catalysts. I completed my scientific formation with two short-term research stays at the University of Bonn (Prof. K. Muñiz) and at Boston College (Prof. M. L. Snapper) working on alkene oxidation and ruthenium-catalyzed cascade reactions, respectively. I obtained my Ph.D. (Summa Cum Laude) in June 2006. The quality of the research performed during the Ph.D. was recognized by several publications (four in J. Am. Chem. Soc., among others). Subsequently, I worked as a researcher at the University of Oviedo (September 2006-December 2006), developing new copper-catalyzed cascade reactions (two publications in J. Am. Chem. Soc.). In 2007 I joined the group of Prof. Lutz Ackermann at the University of Munich (LMU) and later at the University of Göttingen (January 2007-December 2009) as a post-doctoral researcher, funded by fellowships from the Spanish Ministry of Education and Science and Alexander von Humboldt Foundation. The main topic of my research at this stage was the study of mechanism and synthetic applications of metal-catalyzed C-H-bond functionalizations. We found that inexpensive carboxylates can be used as additives in direct arylations (four publications in 4 Org. Lett. and one in Adv. Synth. Catal.) and alkylations (in Angew. Chem. Int. Ed.) into C-H-bonds or that polyethyleneglycol allowed for the first time to reuse the catalyst in a process involving C-H-bond functionalization (in Org. Lett.). Next, I moved to the University of Oviedo as a Juan de la Cierva fellow (January 2010-now) to join the group of Prof. José Barluenga. Along with teaching duties at the Faculty of Chemistry, I am investigating new reactivity patterns in electrophilic catalysis (one publication in Angew. Chem. Int. Ed. and in Chem. Eur. J.). In addition, I am collaborating with the industry in a project concerning catalytic transformations through C-H-bond functionalization. From the work I developed in my career, I am co-author of 27 research publications (most of them in journals with high impact factor: 6 J. Am. Chem. Soc., 2 Angew. Chem. Int. Ed., 5 Org. Lett., 2 Chem. Eur. J., 1 Chem. Commun., 1 Adv. Synth. Catal., 1 J. Org. Chem.), 2 reviews (1 Angew. Chem. Int. Ed., with already more than 110 citations) and 2 book chapters. Moreover, I have presented my results at several congresses (Burgstock Conference 2007, by invitation).



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**Título:**

Deep Eutectic Solvents (DES) as environmentally-friendly media in selective processes

**Resumen de la Memoria:**

Deep Eutectic solvents (DES), also called *Advanced Ionic Liquids*, are defined as a mixture of an ammonium salt (usually choline chloride (2-hydroxy-N,N,N-trimethylethanammoniumchloride) with a H-bond donor molecule (amines, carboxylic acids, glycerol or urea) which are liquids at room temperature at the eutectic ratio (typically 1-4 molecules of hydrogen donor per molecule of salt are needed). As traditional ionic liquids (IL), DES are non flammable, non volatile and can be applied as environmentally friendly solvents. In addition, they present some advantages compared with classical ILs: - Their physical properties (viscosity, conductivity, polarity) and phase behaviour can be simply modelled by changing the molar ratio of their components - Their components are obtained from biodegradable resources and are readily available and inexpensive. DES don't require purification (elimination of NaCl in IL) and can be used under basic conditions - DES are less toxic than traditional IL and in some cases biodegradable. Although DES have been used as solvent in biologic transformations or as electrolytes for dye-sensitized cells, the ability of DES solvents to serve as an eco-friendly solvents in the field of selective organic transformations has been neglected. With this idea in mind, the central research line that I pretend to develop in the present Ramón y Cajal Program is based on the synthesis of new DES and the search of organometallic catalyst active and selective in different organic processes using DES as environmentally-friendly solvents. In this sense, I will study the catalytic activity of different electron-rich organometallic complexes (Re, Rh, Fe, Ir, Pd, Cu, etc.) using DES as environmentally-friendly solvent in: - Atom economy processes (cycloisomerizations of alkynes or enynols and intramolecular hydroamination of alkynes). - Tandem processes, which constitute simple and competitive alternative routes to already known multi-component approaches, allowing us to perform these transformations in a one-pot manner. - The catalytic activation and subsequent functionalization of C-H bonds, like the alkene and alkyne hydroacylation reactions, which are atom-economic processes - Formation of C-C bonds by transition metals catalyzed direct functionalization of C-H bonds for the preparation, transformation and functionalization of aryl derivatives, without precedent in the area of metal-catalyzed organic reactions in ionic liquids as solvents. - Cycloaddition reaction fulfilling the requirements of the so called *Click-Chemistry*, like: i) cycloaddition of azides and alkynes to generate 1,4-triazoles; ii) cycloaddition reactions of azides and nitriles to generate tetrazoles, and iii) cycloaddition of internal alkynes and nitrile-oxide to afford oxazoles. Thus, with this project, I pretend to take advantage of the huge experience obtained during the different stages of my scientific formation in the fields of organometallic chemistry, catalysis and the use of environmentally friendly solvents (Water and IL) with the final target of design a new generation of efficient, eco-friendly, economically profitable and highly selective catalytic systems active in DES as solvents. At this point, is important to note that, there are not researchers or groups working in the field of DES in Spain (only A. P. Abbott in Europe (Leicester, UK)).

**Resumen del Curriculum Vitae:**

From the end of 2000, when I started my research tasks, until now, it has been various fields of the chemistry where I was implicated through different research projects. Concerning to the organometallic chemistry of transition metal elements, I performed the synthesis and characterization of a huge variety of complexes. I worked with different metals like Ru, Pd and Ag, combining them with different ligands. Thus, I have a solid formation in Coordination Chemistry of transition metals. The application of some of these complexes as catalyst precursors in different organic processes, such as hydrogen transfer from alcohols to ketones and the cycloisomerization of (Z)-enynols into furans, allowed me to obtain an extensive experience in catalysis. During my postdoctoral stay, I gained experience in another field completely different from the Organometallic Chemistry of the late transition metals, the Chemistry of the elements from Main Group. In this sense, I have performed the synthesis and characterization of a large variety of organometallic mixed-metal synergic compounds (lithium- and sodium-aluminates, magnesiates, zincates or manganates) and their use as selective metallation reagents of different organic molecules, which required strictly air-sensitive techniques. In September of 2007, I returned to the University of Oviedo where I developed my own and independent line of investigation based in: i) my experience in the study of organic processes catalyzed by transition metals obtained during my Ph. D.; and ii) my knowledge in Main Group Chemistry obtained during my postdoctoral stay which allowed me to use these reagents in an efficient way in the synthesis of new organic compounds as interesting substrates for metal-catalyzed organic transformations. This new and independent research activity has been awarded with a project from the National Plan of the MICIIN of Spain (CTQ2008-00506), from which I am Principal Investigator. In this new and independent line of research I developed the synthesis of new Re(I) complexes as highly active and efficient catalysis for the isomerisation of propargylic alcohols into unsaturated carbonyl compounds using the ionic liquid [BMIM][PF<sub>6</sub>] (BMIM = 1-butyl-3-methylimidazolium) as reaction media. By using this solvent I was able to recycle the catalytic system up to ten times. Also, I have studied the synthesis of new water soluble and stable Cu(I) complexes as highly active and efficient catalysis for the [3+2] cycloaddition of azides and alkynes in water and under aerobic conditions. In this sense, I have acquired a huge experience in metal-catalyzed organic transformations in non-conventional solvents (water and ionic liquids), necessary to perform organic transformation catalyzed by organometallic complexes in Deep Eutectic Solvents (DES), the main goal of this Ramón y Cajal project. To conclude, along all these years of scientific path, the work I done has been published in 26 research articles (2 more manuscripts have been already submitted this year) in addition of one review and one book chapter (h (Hirsch) index 13; 315 citations; average impact factor 4.5). I obtained two postdoctoral reincorporation grants from the Principado de Asturias and Spanish Government (Juan de la Cierva), a *Royal Society Travel Grant*, from the RSC, and a national project in which I am principal investigator.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

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**Título:**

Electrochemical Colorimetric and Fluorescent Halogen-Bonding Receptor for Anion

**Resumen de la Memoria:**

With a view to increasing the understanding of molecular recognition processes in biological systems and producing new molecular sensors, switches and devices, my research is focused on the synthesis of novel host molecules that contain redox- or photo-active reporter groups. These systems have been designed to complex and sense cationic, anionic or neutral inorganic or organic guest species via electrochemical and optical methods. Selective binding of a particular guest species is of paramount importance for commercial applications such as potential prototypes of new molecular sensory devices, molecular switches and extraction agents for cleansing the environment of toxic materials. Recently I have been exploring the use of the halogen bonding in solution as a receptor of anions. Halogen bonding is largely underexploited, with the majority of reported cases in the solid state. However, I have recently reported the first example of a receptor for anions in aqueous media through halogen bonding. Integrating halogen atoms into molecular host frameworks influences greatly the host's recognition behaviour. Especially interesting is the area of surface and nanoparticle chemistry, due to the singular optical and electrochemical properties of nanoparticles and their applications in catalysis, biomedical imaging and materials. My research in this area focuses on exploiting the remarkable surface enhancement of anion recognition to fabricate highly sensitive and selective anion detection devices.

**Resumen del Curriculum Vitae:**

Antonio Caballero studied chemistry in the University of Murcia (1996-2001). Then he joined the Pedro Molina group in the Organic Chemistry Department at the same university. In 2003 he obtained his M.Sc and was granted a  $\zeta$ Formación de Personal Investigador (FPI) $\zeta$  fellowship. In 2007 he finished his Ph.D. thesis, under the supervision of Profs. Pedro Molina and Alberto Tárraga, focussing on the synthesis of new mono- bi- and tri-ferrocenyl  $\pi$ -conjugated compounds and study of the electronic properties, intramolecular electron transfer phenomena, and sensing properties of molecules containing nitrogen-functionalities, in particular, new acyclic and cyclic structural motifs, in which the ferrocene unit is linked by unsaturated aza-bridges to a chromogenic or fluorescent signalling unit. Attention is drawn to the electrochemical and optical properties of these aza-substituted ferrocene derivatives as well as their use in multichannel molecular recognition processes towards metal cations and anions, obtaining the best qualification ( $\zeta$ Sobresaliente Cum Laude). Furthermore, he was awarded the extraordinary prize to the best thesis in chemistry in 2007 at the University of Murcia and was a finalist for the Lilly Research award in 2006, awarded to the best Ph. D. chemistry student in Spain. Having finished his thesis he continued in the Molina group carry out postdoctoral research. At the end of 2008 he gained a Marie Curie Intra European Fellowship of the 7th EU Framework and in 2009 he moved to the University of Oxford (U. K.) to work in the Chemical Research Laboratory, ones of the internationally leading laboratories in the field, working in the Paul Beer group researching in many areas of coordination and supramolecular chemistry, in particular in the field of design and synthesis of novel redox- and photo-active macrocyclic ligand and new rotaxanes and catenanes systems which can selectively bind, recognise and sense cationic, anionic and neutral guest species. He is currently author of 28 publications at the highest level, most highlighted include: 2 *Angewandte Chemie int. ed.* (2005, 1977; and recently published in the web page on 14th January of 2011 (DOI: 10.1002/anie.201006916)); 1 *Journal of the American Chemical Society* (2005, 15666); 6 *Organic Letters* (2004, 4599; 2005, 3171, 2006, 3235, 2007, 2386; 2008, 41; 2009, 3466); 6 *Journal of Organic Chemistry* (2006, 1161; 2007, 6924, 2008, 4034, 2008, 5489; 2009, 4747; 2010, 162); 5 *Dalton Trans.* (2006, 390; 2009, 2121; 2009, 3900; 2009, 9653; 2010, 5429); 2 *Inorg. Chem.* (2007, 1161; 2009, 11566); 3 *Eur. J. Inorg. Chem.* (2005, 2436; 2008, 3401; 2010, 697). Antonio Caballero is the first or the second author in more than the 86% of his papers, has received 567 citations. He has an impact factor average of 4.762 and a citation index (h) of 14. Additionally, he is author of 1 European patent (WO 2008077985). He has also participated in 5 research projects and 20 national and international meeting. The applicant has co-directed 1 Ph. D thesis titled, 2 M. Sc. theses and is currently supervising the research work of an mChem student at the University of Oxford. During the academic year 2007-08 and 2008-09 he has dedicated 110 hours in teaching Experimental Organic Chemistry to the undergraduate registered within the Chemistry and Chemical Engineering studies at the University of Murcia.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

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**Título:**

Super-resolution fluorescence microscopy of DNA

**Resumen de la Memoria:**

Fluorescence microscopy is one of the most convenient and widespread tools to study key issues in the life sciences. An important challenge, however, is to improve its spatial resolution, which is limited by light diffraction to about 200 nm. Recently developed  $\zeta$ super-resolution $\zeta$  techniques such as stochastic optical reconstruction microscopy (STORM) can provide images with a spatial resolution of tens of nanometres. STORM and related techniques rely on the fact that a single emitter can be localized with nm precision by fitting its emission pattern to a 2D Gaussian function. To separate in time the emission of the fluorophores in a sample, cycles of stochastic switching, detection and localization of single photoswitchable molecules on a widefield microscope are performed. After a few thousands cycles, a map containing the precise localization of all the switchable fluorophores in the sample can be reconstructed. Most studies performed so far with super-resolution techniques have imaged the nanoscale distribution of proteins, since appropriate methodology exists to label proteins with photoswitchable fluorophores in high density. However, little progress has been seen on DNA super-resolution imaging due to challenges in labelling. My main research is thus aimed at exploring new ways to label DNA in high density with photoswitchable fluorophores and improving spatial resolution in fluorescence microscopy. This will allow opening up new opportunities to study a broad range of problems in Biology and Nanoscience. My recent research has shown that it is possible to perform STORM-like imaging of DNA with a spatial resolution below 40 nm by using intercalating cyanine dyes in combination with a special buffer. The buffer promotes the photoinduced formation of dark states (photoblinking) in the appropriate timescale for STORM-like imaging. This proposal aims at optimizing this approach, as well as at finding new alternatives for DNA super-resolution imaging. I propose two research lines: 1) Use correlative atomic force microscopy and super-resolution fluorescence imaging to optimize the methodology for super-resolution imaging of DNA. As targets, DNA-based nano-objects of controllable shapes such as DNA origami will be used. Conversely, super-resolution fluorescence imaging will be used as a new way to characterize DNA-based materials by adding advantages such as multicolour detection; 2) Study the photophysical properties at the ensemble and single-molecule level of a new material, CyDNA (DNA highly substituted with cyanine dyes in a controllable way). Bringing together Cy3 and Cy5 dyes in the same CyDNA with high density results in a controllable photoswitch with new properties. CyDNA photoswitching will then be used to perform super-resolution imaging in combination with fluorescence in situ hybridization experiments to study chromosome structure. Further opportunities to apply the developed methodology will also be identified throughout the fellowship.

**Resumen del Curriculum Vitae:**

Following my degree in Chemistry, I completed my PhD at the Institut Químic de Sarrià in Barcelona, funded through a pre-doctoral fellowship from the Catalan Government (2000-2004). I studied the photophysical properties of phenalenone derivatives using a range of spectroscopic techniques, under the supervision of Prof. Santi Nonell. During that period I also visited other research institutions in Denmark, Italy and the UK to acquire further skills in spectroscopy and imaging. My PhD work led to an invited review in a top chemistry journal (Flors and Nonell, Acc. Chem. Res. 2006). In 2005 I moved to the laboratory of Prof. Johan Hofkens at the Katholieke Universiteit Leuven, Belgium, to learn single-molecule spectroscopy and super-resolution microscopy. I investigated the photophysical properties of different molecules such as perylene diimide dendrimers and a range of fluorescent proteins (FPs). My most representative result from that period was the single-molecule characterization of the photoswitching properties of the FP Dronpa and its mutants. Importantly, we showed how the thorough understanding of photophysics can help optimize super-resolution imaging (Flors et al, J. Am Chem. Soc. 2007). Having gained expertise in a new technique with great potential, I moved to the University of Edinburgh in 2008 to start my independent research program. My expertise was recognized by the Engineering and Physical Sciences Research Council and I was funded to setup the first super-resolution microscope in the UK based on single-molecule photoswitching. I then started to develop methodology for super-resolution imaging of DNA (e.g. Flors et al, ChemPhysChem 2009, issue front cover). In collaboration with biologists in Edinburgh we have applied the technique to study the chromosome, leading to a new model for chromatin architecture (Ribeiro et al, Proc. Natl. Acad. Sci. 2010). In 2010 I was awarded further funding by The Royal Society to continue my work on this topic. In parallel to my super-resolution work, and together with Prof. Santi Nonell in Barcelona, we have established a new research program to study the singlet oxygen photosensitizing properties of FPs (Jiménez-Banzo et al, Biophys. J. 2008; Ragàs et al ChemPhysChem 2011, issue front cover). We have secured funding for this work through an International Joint Project of The Royal Society. My results so far as an independent researcher have been highly appreciated by the community, as judged by the more than 10 invitations to give talks in conferences and institutions across the UK and Europe, as well as to submit articles to high impact journals. In total, I have published 28 papers (11 as 1st author, 8 as corresponding), with an invited review and a book chapter in preparation. My h-index is 14, and my papers have been cited more than 450 times. I have also received the 2009 Young Investigator Award from the European Society for Photobiology. Importantly, so far I have been able to secure funding as a principal investigator for both the super-resolution microscopy and the singlet oxygen work. I have teaching experience in 3 countries and I have been guest lecturer in 2 international summer schools. My research and teaching activities have been accredited by the ANECA in 2008 (Prof. Contratado Doctor).



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**Título:**

Single-molecule junction approach to map electron and energy pathways in biomolecular architectures

**Resumen de la Memoria:**

Este proyecto propone explotar nuevas metodologías basadas en la formación de contactos unimoleculares para el estudio de mecanismos de transferencia electrónica (ET) y transferencia de energía (EnGT) en estructuras biomoleculares. Las nuevas metodologías provienen del campo de la Electrónica Molecular y consisten en fabricar contactos eléctricos entre dos electrodos metálicos (o semiconductores) con una sola molécula anclada covalentemente entre ambos. Dichos métodos se pueden instalar en un microscopio de Sonda Próxima (SPM) de manera que se pueden medir corrientes (pA) y fuerzas (pN) simultáneamente teniendo así acceso completo a la dinámica del proceso de transferencia de carga a través de la molécula. Durante la última década se han caracterizado una gran variedad de contactos unimoleculares con sistemas moleculares simples en medios líquidos (solventes orgánicos, disolución acuosa). Los parámetros a controlar en este tipo de medidas son: la interacción molécula-electrodo, la detección unívoca de contactos unimoleculares y la relación estructura-comportamiento eléctrico. En este último caso, se ha demostrado que la presencia de determinados grupos químicos en la molécula (p. ej. enlaces saturados, nivel de conjugación, presencia de heteroátomos, etc.) puede dar lugar a una gran variedad de comportamientos eléctricos. A pesar de lo aprendido en ET con moléculas simples, los contactos unimoleculares incorporando biomoléculas han sido mucho menos explorados, siendo prácticamente el único ejemplo las medidas de transporte en DNA. Esta investigación propone hacer uso de las metodologías descritas anteriormente para explorar ET y EnGT en metaloproteínas redox y en complejos fotosintéticos directamente relacionados con la regulación de dichos procesos en sistemas biológicos. En el primer caso, los mecanismos de ET se estudiarán empleando el modelo de metaloproteína Azurina. Procesos de mutagénesis dirigida serán llevados a cabo para modificar posiciones específicas en la superficie de la proteína de manera que podamos formar contactos mono-proteinicos con diferentes orientaciones y elaborar así un mapa con los diferentes caminos de ET a través de la misma. Una vez conseguido este objetivo, se añadirá la fuerza como parámetro adicional para elucidar como la estructura conformacional afecta los procesos de ET. En el segundo caso, los mecanismos de EnGT se estudiarán empleando membrana fotosintética purificada de bacteria purpura. Aprovechando la resolución nanométrica del SPM, podremos establecer contactos unimoleculares con complejos antena (LH2) en posiciones específicas del cristal fotosintético y cuantificar así la transferencia de energía desde distintas posiciones (LH2) hasta el centro de reacción (RC) donde la separación de carga tiene lugar. Este proyecto sin duda abrirá nuevos horizontes en el estudio de procesos ET y EnGT en biología. La información obtenida a nivel de molécula individual aportará nuevos detalles sobre los mecanismos fundamentales en dichos procesos. Además, este trabajo supondrá un paso directo para evaluar la implementación de sistemas biomoleculares en dispositivos optoelectrónicos a escala nanométrica.

**Resumen del Curriculum Vitae:**

Me licencié en Química en 1999. Ingresé en el departamento de Química Física de la Universidad de Barcelona (UB) para realizar un Máster Experimental en Electroquímica (1999-2000), donde me introduje en el mundo de las técnicas de Sonda Próxima (SPM). El trabajo de Máster produjo mi primera publicación (2001) con las primeras imágenes in situ a nivel nanométrico del proceso de oxidación electroquímica sobre un electrodo de Fe. Mi tesis doctoral (2001-2006) se centró en el desarrollo de nuevos métodos basados en técnicas SPM para caracterizar in situ las propiedades eléctricas durante el proceso de pasivación y corrosión sobre electrodos metálicos (resultados principales en dos Electrochem. Comm.). La nueva metodología desarrollada (descrita en dos Anal. Chem.) permite capturar espectros electrónicos de interfaces sólido-líquido con resolución nanométrica. Durante mi tesis realicé dos estancias; una en el laboratorio del Prof. Miquel Salmerón en Berkeley (experto en técnicas SPM) y otra con el Dr. Philippe Allongue en París (experto en Electroquímica de Semiconductores). Además realicé 2 estancias en las instalaciones de sincrotrón en Grenoble. El proyecto de tesis generó un total de 13 publicaciones, 8 de ellas como principal autor, más un capítulo de libro. Al final de mi tesis, fui premiado con varios seminarios y ponencias invitadas (p. ej. GRC Aqueous Corrosion en Boston) y con dos premios a joven investigador; el premio nacional CIDETEC y el premio internacional Hans-Jürgen-Engel (ISE). En el transcurso de mi tesis, pasé a ser líder de la unidad de Técnicas Nanométricas de la UB (PAS-1 2002-2007) donde desarrollé nuevos métodos para abordar sistemas bioquímicos desde la nanoescala, y cuyos resultados se recogen en 15 publicaciones. Mi estancia postdoctoral (2007-2011) se llevó a cabo en el laboratorio del Prof. Nongjian Tao en Arizona, pionero en el campo de la Electrónica Molecular. Durante mi primer año, usé mi bagaje técnico para incorporar nuevos métodos a las técnicas ya establecidas (publicado en Nano Letters) y elaboré un proyecto para medir transporte electrónico acoplado a procesos fotoquímicos en moléculas de interés biológico. El proyecto fue premiado por dos becas posdoctorales de prestigio internacional: International Outgoing Marie-Curie (ref. PIOF-GA-2008-220974) y Cross-disciplinary Human Frontier. Mi trabajo postdoctoral se resume en 6 publicaciones en revistas de alto impacto, 3 de las cuales corresponden a 3 efectos eléctricos descritos por primera vez en contactos unimoleculares y publicados en revistas del grupo Nature (Nat. Chem., Nat. Commun. y Nat. Nanotech.). Actualmente, trabajo en el Instituto de Bioingeniería de Cataluña (IBEC) donde superviso una tesis doctoral y dispongo de dos equipos SPM (fondos beca Marie-Curie) equipados con capacidad para caracterizar contactos unimoleculares. Se me ha concedido un proyecto europeo dentro del programa International Reintegration Grant (ref. FP7-277182) para continuar mi investigación en transporte eléctrico en sistemas biomoleculares. Mi carrera científica se resume con 50 publicaciones, la mayoría dentro de las 10% mejores de su campo. Tengo alrededor de 450 citas (h índice de 13) y he participado en 12 proyectos, dos de ellos en agencias americanas (NSF y DOE) y uno de desarrollo tecnológico en colaboración con la empresa Nanotec Electrónica.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

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**Título:**

Key insights into oxidation chemistry through synthetic systems: N<sub>2</sub>O activation with first-row transition metals and O<sub>2</sub> activation in heterobimetallic Fe-Ni systems

**Resumen de la Memoria:**

Nowadays oxidation reactions are one of the most important chemical transformations applied both in bulk and fine chemistry. In nature, this type of reactions is catalyzed by metalloenzymes which can perform highly selective transformations under mild conditions. For this reason, many research groups aim towards the development of model compounds that mimic biological systems. Despite these efforts, key issues remain to be successfully developed both from the catalysis point of view and also from the fundamental understanding of key reaction intermediates. In this project, we will tackle two of these topics. Activation of nitrous oxide (N<sub>2</sub>O) with first-row transition-metals: nitrous oxide is a potent greenhouse gas but it also constitutes an environmentally friendly alternative to the traditional oxidants used nowadays as it has a high active-oxygen content and only generates unproblematic N<sub>2</sub> as waste. Despite being thermodynamically a potent oxidant, N<sub>2</sub>O is kinetically very stable but a few selected works have shown that these kinetic barriers can be overcome through binding and activation by suitable metal centers. In the present proposal we will activate nitrous oxide with carefully chosen mononuclear first-row transition metal complexes. The prospective metal-oxo species derived from this process will be used as oxidants for the selective oxidation of organic substrates. Therefore, in the present project N<sub>2</sub>O will be consumed as an oxidation reagent in useful chemical syntheses, thus reaching two aims: decreasing the amount of this greenhouse gas in the atmosphere and performance of practical chemical reactions. Fe-Ni heterobimetallic systems involved in O<sub>2</sub> activation: heterobimetallic dioxygen intermediates are less common than homometallic species, yet they are of great interest due to the possible synergistic effect of two different metal ions acting together. In addition, O<sub>2</sub> activation at heterometallic complexes will result in novel chemical species fundamentally distinct from those resulting from homometallic O<sub>2</sub>-activation, and therefore they are envisioned to exhibit new reactivity patterns in their oxidation reactions that could eventually translate into novel selectivity. In this research proposal, we will pursue the synthesis of heterobimetallic complexes involved in O<sub>2</sub> activation combining iron and nickel. The applied synthetic strategy involves the reaction of a well-characterized and remarkably thermally stable nickel-dioxygen species with iron(II) metal complexes with known reactivity in oxygen-activation processes. Although the reactivity of both independent components is already known, their synergistic action is envisioned to lead to unprecedented reactivity in oxidation reactions.

**Resumen del Curriculum Vitae:**

The candidate studied Chemistry at the University of Girona (Spain, 2000 - 2004) obtaining a university award and a national award (Tercer Premio de Terminación de Estudios Universitarios) for her good academic record. In January 2005 she started her PhD studies in the Department of Chemistry at the University of Girona in the "Bioinorganic and Supramolecular Chemistry" group under the supervision of Dr. Miquel Costas. These studies were financed by a FPU fellowship from the Spanish Government. Her PhD work was focused on the development of model systems of O<sub>2</sub>-activating proteins containing copper and iron. Specifically, she developed dinuclear copper complexes as models of the enzyme tyrosinase, she prepared novel non-heme iron complexes as catalysts for the oxidation of alkanes and olefins and she synthesized a remarkably stable non-heme iron(IV)-oxo compound that behaves as a strong oxidizing reagent. During her PhD studies the candidate performed two short research stays in groups of recognized international prestige. In 2006 she spent 3 months in the University of Minnesota (Minneapolis, USA) under the supervision of Prof. Dr. L. Que Jr. and in 2007 she stayed 2.5 months in the laboratories of Prof. Dr. K. Wieghardt in the Max Planck Institut für Bioorganische Chemie (Germany). The candidate obtained her PhD in December 2008 with the maximum qualification "excellent cum laude" and her thesis was awarded with a PhD award from the University of Girona. Moreover, she was finalist in the VI Lilly awards for PhD students and in the European Young Chemist Award organized by the European Association for Chemical and Molecular Sciences (EuCheMS). Since April 2009 the applicant is working as a postdoctoral researcher in the group of Prof. Dr. M. Driess at the Technische Universität Berlin (Germany) with a Marie Curie Intra-European Fellowship (total duration: 2 years) and her current work is focused on the study of the mechanisms of O<sub>2</sub> activation at nickel centres. Four articles have already been published from the research performed during this postdoctoral stay. As a result of her scientific career, the candidate has been selected as the winner of the prestigious 2010 Dalton Young Researchers Award awarded by the Royal Society of Chemistry and she was selected to attend to the 60th Meeting of Nobel Laureates in Lindau 2010. The applicant is the first author of 12 of the articles she has published (21 in total) and she has been actively implicated in the others by supervising the younger students that appear as the first authors. Moreover, all of her works have been published in peer-reviewed journals with high impact factors: *Angewandte Chemie International Edition* (3), *Journal of the American Chemical Society* (1), *Chemistry - A European Journal* (5), *Chemical Communications* (1), *Organic Letters* (1), *Inorganic Chemistry* (7), *Dalton Transactions* (2) and *ChemCatChem* (1). The candidate is also the author of three book chapters. The average impact factor of her publications is 6.1, her papers have received more than 150 citations and her H-index is 9 (source: ISI Web of Knowledge, 3rd February 2011). Finally, the applicant's work has been presented in several conferences either as oral presentations (6 invited lectures, 13 oral communications) or as posters (22 contributions).



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

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**Título:**

New photoactive metal complexes as dual anticancer drugs

**Resumen de la Memoria:**

The discovery of cisplatin as a chemotherapeutic drug is a landmark of modern inorganic medicinal chemistry. Despite its widespread use, cisplatin has several disadvantages and side-effects. A multitude of strategies have been adopted in order to increase the effectiveness of platinum drugs and the search for new anticancer compounds has widened to several other transition metals and to new biological targets. In addition, the anticancer potential of photoactivable drugs is being explored. Light activation offers the advantage of time- and spatial-control of the active species in tissues, potentially reducing undesired secondary effects due to the toxicity of such species. PhotoDynamic Therapy (PDT) allows the effects of drugs to be localised to irradiated areas because the drug (a porphyrin) produces toxic species only upon irradiation with low-energy light. Unfortunately, PDT applications are currently limited to certain types of cancers. Also, PDT is dependent on the presence of dioxygen in tumor cells. The success of this approach is limited, since many tumour cells are in fact hypoxic. Therefore, new photoactivable compounds with different mechanisms of action are highly desirable. The application of metal complexes in photochemotherapy can be extended far beyond their use as photosensitizers.

Photoactivation of metal complexes can lead to new and more effective cytotoxicity mechanisms. Indeed, their rich photochemistry can result in redox transformation of the metal centre, in ligand release and substitution, in isomerisation reactions and in stoichiometric or catalytic chemical reactions with a biological substrate. Excited states determine absorption and emission properties in metal complexes as well as their light-induced reactivity. Hence, the mode of activation and the cytotoxic effect of photoactive metal anticancer agents are dependent on the nature of the excited states. A complete characterisation of the photophysical and photochemical properties of such systems is necessary to elucidate their mechanism of action in tumour cells, to discover novel mechanisms, but also to rationally improve the design and synthesis of new derivatives with superior features. An innovative objective in the field is to develop new photoactivable metal-based chemotherapeutic agents able of releasing biologically-active ligands inside cells and simultaneously forming a reactive metal-based species. The released ligands can interfere with the cell cycle at a number of specific targets, while the metal-containing species can inhibit mitosis by binding to DNA (like cisplatin). Such dual-action compounds increase the efficacy of metal complexes against tumour cells. The proposed strategy can lead to development of novel and target-specific compounds, which would decrease the negative side-effects of chemotherapy and prevent the development of resistance mechanisms. The specific objectives addressed in the research are summarised as follows: 1) design and synthesise a new active metal complexes with dual action; 2) investigate their photoreactivity and photodecomposition pathways (fate of the bioactive ligand) and optimise such properties for physiological conditions; 3) study the mechanism of action of the new compounds, in relation to their structure-activity relationships, in normal and tumour cells, and investigate their anticancer efficacy.

**Resumen del Curriculum Vitae:**

**Education** Scope: Synthesis of new photoactivable ruthenium complexes and study of their photochemical properties by spectroscopy and computational methods. Jan. 2007-Jun. 2007 University of Montana Visiting scholar (Prof. E. Rosenberg); Scope: Synthesis and characterization of ruthenium luminescent complex for spectroscopy studies on synthetic membranes. Feb. 2006-Dec. 2006 Novi-Elah-Dufour (Chocolate and Confectionery) Research and Development, Production Manager Assistant. University of Turin Part-time Collaboration; Scope: Study new metal complexes for selective photodelivery of neuroactive molecules. Insights in the photophysical properties of the synthesized compounds using DFT calculation. Jan. 2005-Dec. 2005 University of Montana Postdoctoral Fellowship (Prof. J. B. A. Ross); Scope: Investigate glutamate-transporter proteins and DNA-repairing enzymes labelled with luminescent metal probes. Nov. 2002-Mar. 2004 University of Turin Teaching Assistance in various Laboratory course spanning from General Chemistry to Inorganic Chemistry. Apr. 2001-Nov. 2001 University of Turin Fellowship (Prof. R. Gobetto); Scope: Develop new hydrogenation catalyst for optimizing magnetic polarization transfer from para-hydrogen to small organic molecules. Others: Dr. Salassa has published 38 articles (plus 2 recently submitted) on international peer-reviewed journals and co-authored 46 contributions to national and international conferences. Dr. Salassa presented his work at several conferences and workshops as poster communications and short talks (among these, the  $\mu$ EXAFS is back  $\mu$  workshop at Diamond). Furthermore, he was invited to present his work on photoactivable metal complexes at the chemistry departments of the University College London (October 2008), of the University of Utrecht (November 2008) and at the Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques of the Université Paris Descartes (January 2010). The applicant won the scholarship sponsored by the "Divisione di Chimica Inorganica della Società Chimica Italiana" to attend the 14th International Conference on X-ray Absorption Fine Structure in Camerino (Italy, 26-31 July 2009).



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**Título:**

Hierarchical Organization of Nanostructures from opto-electroactive building blocks

**Resumen de la Memoria:**

The hypothesis supporting this project is based on the unique properties of relatively simple suitably functionalized molecules, namely 2-[9-(1,3-dithiol-2-ylidene)anthracen-10(9H)-ylidene]-1,3-dithioles (exTTF), perylenes, fullerenes and carbon nanotubes (CNTs) for the preparation of sophisticated supramolecular ensembles able to carry out a function. For the development of this project, different electron donor systems derived from p-extended TTF (exTTF), will be appropriately functionalized. As a basic electron accepting unit, the fullerene (C60) - given its exceptional electrochemical and photophysical properties - will be used. Perylene and single wall carbon nanotubes (SWNTs) will also be tested. For the construction of these supramolecular ensembles, the presence of different chemically substituted tails based on p-conjugated systems, H-bond head groups and amino acid sequences are key issues to be addressed in the molecular design. Therefore, the final goal of the project is to develop a new methodology for ordering p-type and n-type organic compounds and new donor-acceptor supramolecular polymers exploiting the peculiar shape of both components, namely the concave surface of electron donor exTTF and the convex surface of electron acceptor fullerenes. In this sense, the controlled self-assembly of complex molecules into well defined hierarchical structures is a promising route for fabricating nanostructures. In particular, the self-assembly towards 1D, 2D and 3D ordered nanostructures is at the forefront in science for developing new smart materials within the bottom-up approach. In this sense, one important challenge involves the construction of ordered nanostructures with photonic and/or electroactive units because of their potential interest to enhance the performance of a variety of optoelectronic devices. Although most of nanostructured electronic materials are so far derived from inorganic components, the self-assembly of organic p-systems has recently emerged as a new promising field that allows to tune the properties of thin film materials and devices. The majority of these systems are p-type organic semiconductors in organic media and, consequently, the development of methods to build new n-type supramolecular materials in apolar and polar solvents remains barely exploited and only a few examples have previously been reported. With the exception of some fullerenes and a few concave polycyclic aromatic hydrocarbons (PAHs), the common feature for all the examples mentioned above is the use of planar aromatic cores in their components. Even though significant progress has been made in the design and study of such nanostructures the use of non planar electroactive units, such as fullerene and exTTF, rely on a topic barely exploited and from which important and unexpected properties should be expected. Furthermore, our goal is to find new methodologies for creating new supramolecular polymers in which the donor and acceptor components are able to form segregated stacks between them, thus favoring charges mobility generated upon light excitation in photovoltaic devices.

**Resumen del Curriculum Vitae:**

Carmen M<sup>a</sup> Atienza Castellanos obtained her BSc (1999) and DEA (2001) from the University of Autónoma of Madrid, working in the formation of benzo[b]fluorenes and the benzo[a]fluorene core of the fluostatins by cyclization of diaryldiynes under the supervision of Prof. Dr. Antonio M. Echavarren. Then she moved on to the University Complutense of Madrid (UCM) where she obtained her Ph.D. in 2005 with the thesis entitled Synthesis photo- and electroactive systems based on [60]fullerene and tetrathiafulvalene (TTF) under the supervision of Profs Nazario Martín and Carlos Seoane. During this period, she spent three months at the ETH Zurich joining the group of Prof. Dr. François Diederich and working on the synthesis of new TTF acetylenic-CEEs system for NLO. From 2005 to 2006 she worked as a postdoctoral researcher with Prof. Dirk M. Guldi at Lehrstuhl für Physikalische Chemie I in Friedrich-Alexander-Universität Erlangen-Nürnberg on photophysics study of electron transfer in electroactive organic systems. After, she joined the group of Prof. E. Díez Barra working on synthesis of dendrimeric structure for nanophotonic application worked at University of Castilla La Mancha. From 2007-2009, she enjoyed as a visiting professor contract at UCM. From October 2009, she joined the group of Prof. Nazario Martín's at University Complutense of Madrid as a Juan de la Cierva postdoctoral contract and she is currently working on the design and synthesis of ideal molecular wires and of active compounds for application in photovoltaic devices. Her main research interest concern the hierarchical organization of nanostructures from opto-electroactive building blocks. Selected publications: *Angew. Chem. Int. Ed.*, 2010, 49, 9876-9880; *J. Am. Chem. Soc.* 2010, 132, 16488-16500; *J. Am. Chem. Soc.* 2009, 131, 12218-12229; *Chem. Commun.*, 2009, 5374; *Chemical Society Review*, 2009, 38, 1587-1597; *Dalton Transactions and CrystEngComm*, 2009, 3955-3963; *Chemistry - A European Journal*, 2008, 14, 6369-6390; *J. Org. Chem.*, 2008, 73 (8), 3189-3196; *Chem. Commun.*, 2007, 48, 5164-5166; *Eur. J. Org. Chem.*, 2007, 30, 5027-5037; *J. Org. Chem.* 2007, 72, 6662-6671; *J. Am. Chem. Soc.* 2006, 128, 10680-10681; *J. Am. Chem. Soc.* 2006, 128, 14145-15154; *J. Org. Chem.* 2006, 71, 7603-761; *Chemical Communications*, 2006, 5, 514-516; *Chemical Communications*, 2006, 30, 3202-3204; *Eur. J. Org. Chem.* 2006, 1430; *J. Mater. Chem.*, 2005, 15(1), 124-132; *J. Org. Chem.*, 2004, 69 (21), 6986-6995; *Eur. J. Org. Chem.* 2001, 163-171; *Organic Letters* 2001, 3, 153-155.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

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**Título:**

Nanoplasmonics based on Colloid Chemistry for Lighting Applications

**Resumen de la Memoria:**

Nanoplasmonics develops upon the possibility of focusing and manipulating light through the resonant excitation of plasmon modes in metal nanoparticles. As a result, metal nanostructures have a strong ability to enhance as much as 50 fold the luminescence (fluorescence or phosphorescence) of dyes occurring within the local field generated close to the nanoparticle surface. Furthermore, the electromagnetic fields associated with the plasmon modes supported by complex metal nanostructures (in particular, the so-called hot-spots occurring at the junction of particle assemblies) amplify this enhanced optical response. Within this context, I intend to develop a research line at the frontier between Colloid Chemistry, Spectroscopy and Nanotechnology. The study will be focused on the self-assembly of colloid metal nanoparticles for hot-spot plasmonic enhancement of the luminescence of species with optoelectronic interest, such as organometallic complexes and semiconductor nanocrystals (quantum dots, QDs). Both molecular and nanocrystal systems are of wide interest for the design and preparation of light-emitting diodes (OLEDs and QD-LEDs, respectively) due to their high photo-stability and emission tunability. The main scientific goals of the project are: (i) The colloidal synthesis of plasmonic nanoparticles with different metallic nature (gold and silver), size (10-150 nm), shape (nanospheres, nanorods and nanostars) and surface functionalization (surfactants, polyelectrolytes and silica). (ii) The chemical coupling of complementary functionalized photoresponsive systems (iridium and ruthenium organometallic complexes, and CdSe and CdTe multishell QDs) at the metal nanoparticles surface; and the study of the effect of separation distance on the enhancement/quenching of the luminescence (excitation, emission, lifetime, quantum yield) both in solution and at the single particle level. (iii) The development of chemical and physical methods for modulating the extension and dimensionality of the assemblies of the optimized metal nanoparticles/photoresponsive systems on optical surfaces; and the determination of the luminescence enhancement capability of these ensembles. (iv) Finally, and once all these variables are controlled, these directed assemblies will be used for the design and construction of novel OLEDs and QD-LEDs using a simple sandwich architecture in which the device efficiencies are expected to be improved. This research work will provide the candidate the opportunity to collaborate with national and international recognized research groups with complementary expertise spanning nanoparticle synthesis and characterization, plasmonics, spectroscopy, and design and realization of electroluminescent devices, which will also be beneficial for the host research Institution.

**Resumen del Curriculum Vitae:**

Andrés Guerrero graduated in Chemistry from the Universidad Complutense de Madrid (UCM, 1995). Thanks to the funding provided by a UCM-Ph.D. fellowship, he received his Ph.D. (¿Premio Extraordinario de Doctorado¿) under the supervision of Prof. G. Tardajos at the Dpt. of Physical Chemistry I (UCM, 2006), working on the thermodynamics and spectroscopy of colloids. During this period, the candidate visited the group of Prof. S. Berger at the Universität Leipzig (Germany), where A. Guerrero investigated the diffusion of colloids by NMR (6 months, 2004). Then, A. Guerrero was appointed ¿Profesor Titular de Universidad Interino¿ in the Dpt. of Physical Chemistry I (UCM, 12 months, 2006-2007). Following this teaching period, the candidate was awarded with a MEC postdoctoral research fellowship to join Prof. L. De Cola group at the new Center for Nanotechnology of the Universität Münster (Germany, 26 months, 2007-2009), carrying out investigations on molecular energy transfer processes and their application in OLEDs. Additionally, A. Guerrero visited the group of Prof. N. Kotov at the University of Michigan (USA, 1 month, 2009), where he learned about nanoparticle assembly methodologies. After this postdoctoral stay, A. Guerrero joined the group of Prof. L. M. Liz Marzán at the Universidad de Vigo with a Juan de la Cierva postdoctoral research fellowship (24 months, 2009-to date), where his current research is focused on the development of metal nanoparticles with tailored plasmonic properties, work that has resulted in his first supervised Ph.D. thesis. Moreover, the candidate visited the group of Prof. H. Weller at the Universität Hamburg (Germany, 4 months, 2010), where he worked on surface enhanced spectroscopies with quantum dots. Throughout all the reported period, A. Guerrero's work has resulted in 32 peer-reviewed papers in high impact factor journals of the areas of Chemistry and Materials Science, among which the most outstanding publications are 1 NanoToday (submitted), 4 Angew. Chem. Int. Ed. (two highlighted as cover pictures and one as Hot Paper, and one submitted), 1 Adv. Mater. (cover picture, and among most accessed papers of the journal), 1 Curr. Opin. Colloid Interface Sci., 1 Chem. Eur. J., 1 J. Mater. Chem. (cover picture), 1 Phys. Chem. Chem. Phys., 6 J. Phys. Chem. B, 1 Inorg. Chem, 1 Langmuir, 2 ChemPhysChem, 1 Appl. Phys. Lett. (submitted), and 2 Chem. Phys. Lett. The candidate is the first and corresponding author of 14 and 9 of these publications, respectively, and part of these studies has been recently presented in an invited review in Anales de Química. During his research, A. Guerrero has participated in 6 International and European Projects (standing out PLASMAQUO-European Research Council and UNINANOCUPS- European Marie Curie Network), 6 National Projects, and more than 25 International and National Congresses (14 oral presentations). Regarding the overall impact of his publications, A. Guerrero has an h index of 10 and more than 180 citations. Additionally, the candidate currently acts as reviewer for high-impact journals of Chemistry and Materials Science such as Angew. Chem. Int. Ed., Chem. Eur. J., Phys. Chem. Chem. Phys., Langmuir, and J. Mater. Chem.. Furthermore, during all this period, A. Guerrero taught different subjects of the Bachelor of Chemistry (18.5 lecturing and 22.5 laboratory credits), and participated in the translation of the book Physical Chemistry (I. N. Levine, 5th Ed.) into Spanish.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

**Nombre:** MARTIN SOLANS, SANTIAGO

**Referencia:** RYC-2011-07869

**Area:** Química

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**Título:**

Hybrid Molecular Architectures for Molecular Devices

**Resumen de la Memoria:**

This proposal addresses the development of new molecular electronics paradigms by using metal-organic compounds (MOCs), which are hybrid organic-inorganic molecules with rich and exploitable molecular properties (redox activity, magnetism etc.), in novel metal-molecule-metal and semiconductor-molecule-metal nanoelectronic devices. MOCs represent an attractive family of molecular materials that have received far less attention for molecular electronics applications than other materials (e.g. carbon nano-tubes, -particles, -wires; graphitic systems; SAMs of organic thiols on gold, DNA and metal oxides). However, MOCs possess properties controllable through synthetic chemistry that make them particularly attractive candidates as emerging research materials for electronics. Therefore, devices with very small dimensions (less 20 nm) will be constructed from molecular MOCs assembled into metallic and semiconducting architectures using self-assembly, Langmuir-Blodgett technique, and novel hybrid methods of both molecule and metal deposition. Critically, these hybrid metal/semiconductor-MOC devices will offer functionality beyond the achievable limits of simpler organic molecule junctions based on the redox and magnetic properties of the MOC components due to the presence of valence electrons in d-orbitals, and because the population and depopulation of these high-lying electron sinks lead to variable spectroscopic, redox and magnetic properties. Thus, these MOC-based molecular components will be used to introduce more complex I-V response in hybrid devices than is possible with simple organic molecules, such as redox switching, spin and Coulomb blockade and Kondo resistance. This aim is a natural follow-up of my postdoctoral training research lines, mainly based on understanding mechanisms of charge transport by using a scanning tunnelling microscope (STM) in organic molecules (both single molecules and on molecular assemblies) and how the molecular, electronic structure, contacts and conformation of the molecular junction influence its electrical behaviour.

**Resumen del Curriculum Vitae:**

I obtained my B.Sc. in Chemistry in July 2000 from the University of Zaragoza (UZ). That year I joined to the Félix Royo's group at the same university, and I got my M.Sc. in 2002 working in the characterization, and physicochemical properties of several organic and biochemical compounds. Between 2002-03 I spent seven months in the laboratory of Prof. Dietmar Möbius at Max-Planck Institut für Biophysikalische Chemie in Göttingen working in characterization techniques to determine the order and architecture of Langmuir films. In 2005 I finished the Ph. D. thesis focused on the study of molecules having potential applications as modified electrodes and in non-linear optical devices arranged by means of the LB technique with the best qualification. In the academic years 2003-04 and 2004-05 I was also working as Associated Lecturer at the Physical Chemistry Department of UZ. From September 2005 to January 2006 I worked as a post-doc researcher with Prof. José Miñones at the Organic and Physical Chemistry Department of Santiago de Compostela working with Co magnetic nanoparticles which were assembled by the LB method and characterized using several techniques. In February 2006, I got a Local Government Grant to work at the Chemistry Department of Liverpool University under the supervision of Prof. Richard J. Nichols to determine charge transport of single molecules using scanning probed based methods (STM). In September 2006 I got an EU Marie Curie Early Stage Training Fellowship to continue working in the same research line as well as in two new projects to establish new expertise in (bio)-molecular electronics achieved through the development of electronic devices from new materials. In May 2007 I got a post-doctoral fellowship from Ministerio de Educación y Ciencia (MEC) which allowed me to continue my work at Liverpool University performing measurements on the single molecule electrical properties in collaboration with Colin Lambert from Lancaster University (UK), Martin Bryce from Durham University (UK), Fausto Sanz from Barcelona University and Ernesto Calvo from Buenos Aires University. From May 2009 until now, I am working under the group of Dr. Félix Royo in the Physical Chemistry Department at the UZ with a "Juan de la Cierva contract" and I was incorporated to the Instituto Universitario de Investigación en Nanociencia de Aragón (UZ) as a postdoc researcher. During this period the applicant has opened new research lines concerning to understanding fundamental charge transport mechanisms for molecular junctions, and to advance in the development of the nascent field of single molecular electronics and has also collaborated with 80 hours/year in teaching at UZ. I am co-author of 50 publications at the highest level and other are currently under revision or preparation. Most highlights include: Nano Letters; 3 J. Am. Chem. Soc. (one of them was selected as front-cover page, March 2010, vol. 132, number 32); Chem. Eur. J.; Chem. Mater.; Soft Matter; 2 Phys. Chem. Chem. Phys. (one of them has been highlighted as hot article, 2009, 11); 6 J. Phys. Chem.; Organometallics; Langmuir; Nanotechnology; etc. In addition, I have produced 24 communications in international and national conferences, presented in oral and poster sessions. Finally, the candidate is qualified as Profesor ayudante doctor and Profesor contratado doctor by ANECA.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

**Nombre:** GAWELDA , WOJCIECH

**Referencia:** RYC-2011-08584

**Area:** Química

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**Título:**

Probing the ultrafast solvation dynamics in real-time with atomic scale resolution

**Resumen de la Memoria:**

The proposed research line seeks to unravel the elementary dynamic processes involved in guest-host interactions during a chemical reaction in liquid media. For this purpose we will exploit complementary structural tools using advanced optical and x-ray spectroscopies with femtosecond (fs) to picosecond (ps) temporal resolution. Since internal relaxation processes of a molecular solute occur on similar time scale(s) as the solvation cage dynamics, and thus their interpretation so far has been severely hampered, this research line will focus on photogenerated nascent halogen atoms, which exhibit no internal degrees of freedom. As a starting point the research line proposes investigating aqueous halides, e.g. iodide and bromide, whose hydrophilic solvation shell turns hydrophobic after photodetachment of a valence p electron, thus generates a nascent halogen radical. The lack of further internal degrees of freedom allows probing the solvation dynamics in its purest form. In subsequent steps more complex aspects of solvation dynamics in larger systems will be investigated. One example of such systems are halogenated alkanes, which upon impulsive photoexcitation exhibit a complicated dynamics involving a sequence of reactions such as bond dissociation, vibrational relaxation, reaction fragment rearrangements and caging, isomerization, reaction fragment dissociation and recombination, reaction fragment reactions with solvent environment. The nature of solvent cage and its interaction with the reactive core is essential for the outcome of a chemical reaction. All the above mentioned reaction steps, in one way or another, are the constituents of many chemical reactions. To structurally characterize these events and understand how the interplay between intrinsic properties and solute- $\zeta$ solvent $\zeta$  interactions determine the outcome of reactions is of general interest for obtaining a molecular scale picture of chemical reactivity. In order to probe electronic and structural relaxation dynamics occurring during solvation dynamics ultrafast optical spectroscopies will be employed to recording, on the femtosecond (fs) time scale, the fluorescence, the excited state absorption, or the stimulated emission originating due to solute-solvent interactions. Yet, optical methods have their limitation, i.e. they cannot deliver the structure of the solvent shell before, during, and after solvent rearrangement, and therefore complementary and structure-sensitive techniques will be applied to deliver the molecular level description of solvation dynamics. The proposed research line will use picosecond- and femtosecond-resolved x-ray methods (x-ray emission/absorption spectroscopies and scattering techniques) to provide a direct access to the underlying structural dynamics information. The proposed approach will deliver i) a real-time motion picture of the expanding cage (via x-ray scattering) following photodetachment (observed via x-ray absorption and emission spectroscopies), ii) possibly including electronic details and dynamics of the interaction between the empty p orbital and the caging O<sub>2</sub>- (via x-ray emission spectroscopy), iii) the propagation of the expanding caging shells (via previously calibrated x-ray scattering), and iv) thermalization next to formation of bimolecular subsequent products I<sub>2</sub>-, I<sub>3</sub>-, on the sub-nanosecond time scale.

**Resumen del Curriculum Vitae:**

PREVIOUS SCIENTIFIC ACTIVITIES:1) 2010-up to date: Research Scientist, European XFEL, Hamburg, Germany2) 2007-2010: Postdoctoral Researcher I3P, Instituto de Óptica, CSIC, Madrid, Spain3) 2006-2007: Postdoctoral ResearcherLaboratoire de Spectroscopie Ultrarapide, EPFL, Lausanne, Switzerland4) 2002-2006: PhD studentLaboratoire de Spectroscopie Ultrarapide, EPFL, Lausanne, Switzerland5) 2001-2002: Post-graduate student, Instituto de Óptica, CSIC, Madrid, SpainEDUCATION:1) 2006: Doctor in Sciences (Ph.D)Grade: Cum Laude (3rd Prize for the Best PhD Thesis 2006)École Polytechnique Fédérale de Lausanne, Lausanne, SwitzerlandTitle: Time-Resolved X-ray Absorption Spectroscopy of Transition Metal Complexes2) 2001: Graduate in Physics (M. Sc.)Grade: Cum laude (Best Student Award)Adam Mickiewicz University, Poznan, PolandTitle: Noncollinear Optical Parametric AmplifierPARTICIPATION IN RESEARCH PROJECTS:Total number of projects (A+B+C): 38A: National and international projects (long-term): 15B: Postgraduate projects: 3C: Experimental beamtime proposals (short term): 20PUBLICATIONS:Número total de publicaciones (A+B+C+D): 53A: Publications in peer-reviewed international journals: 31 (3 invited)B: Book chapters: 4C: Conference Proceedings: 14D: Research projects: 4MOST RELEVANT PUBLICATIONS:1x Science1x Phys. Rev. Lett.3x J. Am. Chem. Soc1x Angew. Chem. Intl. Ed.1 x Coord. Chem. Rev.4 x Appl. Phys. Lett.TOTAL NUMBER OF CITATIONS: 406 AVERAGE CITATION PER PUBLICATION: 14.5H-INDEX: 11RESEARCH HIGHLIGHTS:1) Research Highlight of the European Journal of Chemical Physics and Physical Chemistry2) Research Highlights of the Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland3) Research Highlights of the Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland4) Scientific Highlights of the Advanced Light Source, Berkeley, USASCIENTIFIC VISITS AT RESERACH CENTERS:Total number of visits (A+B+C+D): 16A: Postdoctoral: 5B: Doctoral: 8 C: Postgraduate: 1D: Graduate: 2CONFERENCE CONTRIBUTIONS:Total number of contributions (A+B): 63A: Oral presentations: 42 (20 invited)B: Poster presentations: 21TEACHING EXPERIENCE:1) Lecture tutorials for 3rd year graduate students in PhysicsTitle: "Atomes et Rayonnement" (Atoms and Radiation)Lecturer: Prof. Dr. Christian BresslerFaculty of Physics, University of Lausanne, Lausanne, Switzerland (03/2003-07/ 2003)Faculty of Basic Sciences, EPFL, Lausanne, Switzerland (03/2004-07/2004)Faculty of Basic Sciences, EPFL, Lausanne, Switzerland(03/2005-07/2005)2) Invited Lectures for Master students  $\zeta$ Quimilaser: Laser Applications in Chemistry $\zeta$  Faculty of Sciences, University of Valladolid, Valladolid, Spain (01/2011)AWARDS:1) Best Poster Award, Physical Chemistry Section of the Swiss Chemical Society Meeting 20062) 3rd Prize for the Best PhD Thesis of École Polytechnique Federale de Lausanne 20063) Best Student Award 2001, Faculty of Physics, Adam Mickiewicz University, Poznan, PolandDOCTORAL THESIS SUPERVISION:1) PhD thesis co-director, (Francisco Javier Hernández Rueda, September 2008-January 2010)2) Master project director: (Francisco Javier Hernández Rueda, January 2009-July 2009)



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

**Nombre:** MIGANI , ANNAPAOLA

**Referencia:** RYC-2011-09582

**Area:** Química

**Correo electrónico:** annapaola\_migani@ehu.es

**Título:**

Fotocatálisis y fotoquímica de superficie a partir de primeros principios

**Resumen de la Memoria:**

Titanium oxide is a very important semiconductor due its use in photocatalysis - self-cleaning and sterilizing surfaces, air and water remediation, H<sub>2</sub> fuel production - and in dye sensitized solar cells. Developments in this field rely on the complementary knowledge coming from electrochemistry, inorganic and organic chemistry, physics, etc. Theoretical/computational studies are of fundamental importance in providing the basic understanding of these processes. Based on my knowledge in materials and molecular photochemistry, my aim is to explain and predict the behavior of a variety of complex TiO<sub>2</sub> systems upon light absorption. Using state-of-the-art theoretical methods I will address two subjects. The first one is the electronic and optical properties of TiO<sub>2</sub> nanoparticles and surfaces (neat and covered by small organic molecules such as methanol, acetic acetate, and ethylene glycol), which are the relevant aggregates in photocatalysis and photovoltaics. Their catalytic and spectral properties are intrinsically associated with their structure, but to date there is no systematic study of this subject. Therefore, I will construct a suitable set of nanoparticles and calculate the optical and electronic spectra of this set, together with those of the relevant surfaces, to obtain the relationship of interest. The second subject is a surface photochemical reaction, the photocatalytic dissociation of carboxylic acids at the rutile TiO<sub>2</sub>(110) surface (Kolbe reaction). This process is very important in the elimination of pollutants, and it involves the formation of a hole/electron pair between the adsorbate molecule and the surface. I will pay special attention to the de-excitation step and the competition between carboxylic acid degradation and hole/electron recombination. In addition to the Kolbe reaction, I will study a more complex case of photochemistry on surfaces, the ultrafast photoinduced proton electron coupled transfer (PECT) at the rutile TiO<sub>2</sub>(110) surface covered with methanol. This reaction is the first report of a not equilibrated process where the coupling of the electron to light atoms (protons) has been observed in the ultrafast dynamics of a heterogeneous system.

**Resumen del Curriculum Vitae:**

I have expertise in two computational fields: photochemistry and material science. I was a PhD student from 1997 to 2001 (4 years) at the  $\zeta$ Computational Photochemistry Group $\zeta$  of Prof. M. A. Robb FRS at King's College London (UK) and a post-doctoral fellow from 2001 to 2003 (2.5 years) at the  $\zeta$ Computational Photochemistry and Photobiology Laboratory $\zeta$  of Prof. M. Olivucci at the University of Siena (Italy). In 2004 I joined the  $\zeta$ Computational Material Science Laboratory $\zeta$  of Prof. F. Illas at the University of Barcelona (Spain) as a Marie Curie post-doctoral fellow for two years. I spent then two years (2006-2008) in the theoretical and computational photochemistry group of Prof. L. Blancafort at the University of Girona (Spain) as post-doctoral fellow and associate professor. In July 2008 I joined again the group of Prof. Illas as a Beatriu de Pinós post-doctoral fellow where I stayed until July 2010. I had two maternity leaves (32 weeks), in 2004 and in 2006. In theoretical photochemistry my most important contribution is the study of the extended nature of the conical intersection between two surfaces (intersection seam). I studied the intersection seam for the Z $\rightarrow$ E photoisomerization of retinal chromophore at the basis of the vision process (JACS 2003 with 60 citations; JPCA 2004 with 37 citations, JPCA 2004 with 40 citations, Farad. Discuss 2004 with 33 citations); and the intersection space and the connectivity of minimal energy conical intersections in the excited state intramolecular proton transfer in ortho-hydroxybenzaldehyde, a prototypical system of industrial photoprotectors (JACS Communication 2008, selected for JACS  $\square$  issue #3  $\zeta$ Molecular Modeling of Complex Chemical Systems $\zeta$ ). Another important contribution is the study of photochemical stability of commercial nitro-enamine pesticides (JACS 2007) and that of isolated DNA bases (thymine photodimerization) at the basis of the DNA photostability (JACS 2007). One important aspect of my research in photochemistry is that it received 4.5 years of industrial fundings. My work in material science includes two parts. One part is important in the context of catalysis by metal surfaces (Surf. Sci. 2006 with 28 citations, JPCB 2006 with 19 citations). The second part regards the study of CeO<sub>2</sub> nanoparticles (with Prof. K. Neyman, ICREA professor at the University of Barcelona). The nanoparticle models better mimic the complex features of real catalysts and explain the results of experiments that cannot be explained on the basis of calculations employing surface slab models (Chem. Comm. 2010, J. Mater. Chem 2010 J. Phys. Chem. C, under revision). My first publications (CPL 2008, PCCP 2009, JCP 2009) have already in total 40 citations. My most important paper is in press in Nat. Mater. In this paper it was demonstrated that of the Pt-O species that are the key catalytic sites in the combined Pt-CeO<sub>2</sub> catalyst form exclusively on nanostructured ceria supports. Since September 2010, I am a post-doctoral fellow in the  $\zeta$ Nano-Bio Spectroscopy Group $\zeta$  of Prof. A. Rubio at the Centro Mixto de Física de Materiales CSIC-EHU(UPV) (Spain). This group has a solid tradition in the use and development of methods to compute excited state in materials and molecules. My decision is motivated by the fact that I want to study excited state in materials, as excited states is my main area of interest.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

**Nombre:** GULIAS COSTA, MOISES

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**Area:** Química

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**Título:**

CHANGING THE RULES IN ORGANIC SYNTHESIS. THE C-H BONDS AS FUNCTIONAL GROUPS.

**Resumen de la Memoria:**

In recent years the area of C-H bond functionalization has experienced a rapid growth because it offers an exceptional opportunity to develop novel chemical transformations. Most of current C-H functionalization research is being focused to the activation of C-H bonds of aromatic compounds, while alkane functionalization have been much less explored, probably because the crucial catalyst-substrate interactions leading to C-H bond cleavage are less understood and defined. In general, C-H bond cleavage can be facilitated by pre-coordination of a metal complex to a carbon or heteroatom in the molecule. A careful design of reactants and catalysts should allow the use of pre-existing functionalities in the substrate to activate  $sp^3$  C-H bonds and create new functionalities. We will explore the reactivity of simple and commercial available materials as well as the chemo- and stereoselective functionalization of more complex molecules in presence of designed metal complexes. Importantly, we will try to couple the C-H activation processes with other transformations, particularly alkyne and alkene insertions, something that has been very scarcely explored. This research might be pivotal in the future of the chemical synthesis by providing new disconnection possibilities that would not be predicted by classical retrosynthetic analysis. Furthermore I also am interested in the development of procedures to carry out consecutive controlled C-H activation that coupled to the alkyne insertion can lead to the formation of complex aromatic heterocycles. The field of C-H bond functionalization is going to attract plenty of attention in forthcoming years, and therefore the Spanish chemical community should also be involved. The impact of this research is planned to be noticeable both from the academic and the industrial point of view. My current experience in C-H bond functionalization and my strong background in metal catalysis warrant a well focused, competitive work.

**Resumen del Curriculum Vitae:**

Me licencié por la Universidad de Santiago de Compostela en el año 2001. Entre los años 2001 y 2006 desarrollé mi tesis doctoral bajo la supervisión del profesor Jose Luis Mascareñas en nuevos métodos de ciclación y cicloadición basados en catálisis metálica calificada con Sobresaliente Cum Laude y por la que obtuve el premio extraordinario de doctorado de la universidad. Como resultado de este trabajo predoctoral los meses posteriores a la defensa de mi tesis se publicaron 8 artículos: Organic Letters (2003), 5, 1975-1977; Journal of Organometallic Chemistry (2005), 690 (24-25), 5609-5615; Organic Letters (2005), 7, 5693-5696; Advanced Synthesis Journal of the American Chemical Society (2006), 128, 384-385; Journal of the American Chemical Society (2007), 129, 11026-1102; Chemistry--A European Journal (2008), 14(1), 272-281 and Angewandte Chemie, International Edition (2008), 47(5), 951-954). Además, durante mis estudios de doctorado en 2004 hice una estancia predoctoral de 3 meses en los laboratorios del Professor Barry Trost, en la Stanford University (California, Estados Unidos) que resultaron en un trabajo publicado en Org. Lett., 2004, 6 (23), 4235-4238. En Abril del 2007, inicié mi estancia postdoctoral bajo la supervisión del Dr. Matthew J. Gaunt en la University of Cambridge (Reino Unido) con un contrato Postdoctoral del MEC donde investigué nuevos procesos de funcionalización de enlaces C-H mediante aminación, arilación y carbonilación. Con posterioridad se me concedió una beca Marie-Curie Intraeuropean Fellowship (IERG) entre febrero del 2008 y septiembre 2009. Como resultado de mi trabajo postdoctoral he publicado 3 artículos Journal of the American Chemical Society (2008), 130(48), 16184-16186; Chemical Science, 2011, 2, 312-315; Angewandte Chemie-International Edition 2011, 50 (5), 1076-1079. En octubre del 2009 regreso al grupo del Profesor José L. Mascareñas con un contrato Ángeles Alvariño de la Xunta de Galicia, para trabajar en el estudio de nuevas cicloadiciones con catalizadores de Ni y Ru. Durante este tiempo he publicado artículos en Angewandte Chemie-International Edition 2010, 49 (51), 9886-9890 (¿Hot paper¿); Pure and Applied Chemistry (en prensa) y un J. Am. Chem. Soc. ha sido enviado recientemente. Actualmente continúo en el mismo grupo de investigación a través de un contrato Parga Pondal de la Xunta de Galicia y se me concedió una beca Marie-Curie Reintegration Grant para la realización de un proyecto de C-H activación/cicloadición en tándem. Durante mi tiempo en la Universidad de Santiago de Compostela colaboré como profesor en la Licenciatura de Química (250h). El resultado de mi trayectoria investigadora queda reflejado en la publicación de 14 artículos en revistas de prestigio internacional (3 J. Am. Chem. Soc., 3 Angew. Chem. Int. Ed., 1 Chem. Eur. J., 1 Adv. Synth. Cat., 3 Org. Lett., 1 J. Organomet. Chem., 1 Pure App. Chem.) que han sido citados más de 200 veces. Tengo un coeficiente  $h=9$  a pesar de que varias de las publicaciones son muy recientes y un índice de impacto medio de 7.13.



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**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

**Nombre:** MAS MARZA, ELENA

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**Area:** Química

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**Título:**

Added value products from easily available unactivated substrates

**Resumen de la Memoria:**

This research project aims the preparation of transition metal-based complexes for environmentally benign and economically attractive catalytic procedures. For the preparation of efficient catalysts, sophisticated ligands are being designed that do far more than just fulfil their traditional spectator roles in homogeneous transition metal catalysis. Additional functional groups in ligands can change ligand-properties as a result of external stimulus, or undergo catalytically-relevant ligand-based reactivity. In this regard, a large number of functionalities (alcohols, amines, esters, etc..) can be easily added to common ligands, and eventually enhance the catalytic performances of transition metal catalysts. These improved catalysts will be tested for the activation of small molecules and their transformation into organic compounds with potential pharmaceutical applications. Taking these simple ideas into account, this research line will be developed in two steps: I) Development of catalysts. A series of catalysts with ligands carrying NH, OH and C=O functionalities will be prepared. The incorporation of these functionalities will have a dual purpose: to facilitate the in situ study of the mechanism of the catalytic process by monitoring the transformation of the ligand functionalities under catalytic conditions, and to improve the catalytic performances by multifunctional behaviour of the ligand, via proton responsive effect, hydrogen bonding or  $\zeta$ NH effect. We will initially design a series of Ir(III) and Ru(II)-based complexes which will be applied to the activation of C-H bonds and new borrowing-hydrogen type reactions. II) Evaluation of the catalytic activity. The activation of small molecules represents an alternative to traditional synthetic procedures and constitutes attractive industrial alternatives since high atom efficiency and reduction of waste and energy are feasible. In this regard, the direct synthesis of nitrogen-containing molecules from ammonia, or carbon-containing molecules from carbon dioxide is an important goal that is far from being accomplished. The catalysts prepared will be used in the formation of C-C, C-N and C-O bonds by borrowing-hydrogen mechanisms, using NH<sub>3</sub>, CO<sub>2</sub> and alcohols as starting materials. It is important to emphasize that the use of CO<sub>2</sub> has an important additional advantage because of the position of CO<sub>2</sub> as the primary greenhouse gas and its great potential to become an important feedstock and reagent for organic transformations.

**Resumen del Curriculum Vitae:**

I obtained my Chemistry at Jaume I University in 2002. In the year 2001-2002 I obtained a *beca de colaboración* (MEC) under the supervision of Prof. Eduardo Peris (Jaume I University). In 2002 I started my PhD in the same group with a FPU/MEC fellowship. My PhD Thesis (European mention, Premio extraordinario de doctorado) was focused on the design of N-Heterocyclic carbene ligands (NHC) with new topologies, their synthesis and coordination, along with study of the catalytic applications of the metal complexes obtained (14 articles). During my graduation period, I carried out three pre-doctoral stays: Universitat Rovira i Virgili (under the supervision of Dr. Elena Fernández and Prof. Carmen Claver, Tarragona, 1 month), Department of Chemistry and Biochemistry, UCSD (under the supervision of Prof. Karsten Meyer, San Diego, 4 months) and Instituto de Tecnologia Quimica e Biológica de la Universidade Nova de Lisboa (under the supervision of Dr. Beatriz Royo, Oeiras, 4 months). In 2007 I joined the group of Prof. Antoni Llobet at Institut Català d'Investigació Química (ICIQ). During this period I was involved in the synthesis of dinuclear ruthenium complexes and study of their application in the catalytic oxidation of water to molecular dioxygen (3 articles). In 2008, I was awarded with a two-years post-doctoral fellowship funded by MEC. This fellowship allow me to continue my research training at the Department of Chemistry at the University of Bath under the supervision of Prof. Michael K. Whittlesey. During this second post-doctoral stay my research interest was mainly focused on the coordination and activation of small molecules and C-H activation of N-Alkyl NHC ligands (4 articles, 1 microreview, 1 book chapter). In January 2010, I started to work with a Juan de la Cierva contract in the Group of Prof. Eduardo Peris. This contract has allowed me to follow with my research career and combine it with teaching tasks. My current research areas deals with the design and application of metallo-organocatalytic systems for tandem catalysis and catalytic activation of CO<sub>2</sub> and NH<sub>3</sub> for the synthesis of organic molecules with an added value (1 article, 1 submitted). Throughout my scientific formation as a researcher, I have acquired experience in experimental chemistry, mainly related to organometallic chemistry, homogeneous catalysis and organic synthesis, thus achieving a formation with a wide multidisciplinary character. The scientific quality of my research career is supported by the number of publications in high impact journals, 24 articles in international journals (22 published, 1 accepted, 1 submitted): *Angewandte Chemie International Edition* (3), *Journal of the American Chemical Society* (1), *Chemical Communications* (1), *Chemistry-A European Journal* (2), *Inorganic Chemistry* (4), *Organometallics* (6), *Tetrahedron Letters* (1), *European Journal of Inorganic Chemistry* (2), *Journal of Organometallic Chemistry* (2) and *Journal of Chemical Education* (1). All the publications derived from my work have received 610 citations, with an average citation per item of 27.73, and my *h<sub>i</sub>* index is 15 (source ISI Web of Science, 23/01/2011), which may provide an idea of the impact of the developed research. In addition to this I have also co-authored a chapter in a book and I am the corresponding author in two of my articles.



MINISTERIO  
DE CIENCIA  
E INNOVACIÓN

**SUBPROGRAMA RAMON Y CAJAL  
CONVOCATORIA 2011**

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Isonucleosidos: Synthesis using organocatalysis and applications

**Resumen de la Memoria:**

Nucleosides are an important family of molecules of life. From the chemical point of view, the syntheses of nucleoside analogues that mimic the natural molecules have been of great interest for the medicinal chemists. In this sense, one of the main applications of nucleoside analogs has been its ability for biological processes modulation. Furthermore, nucleoside analogs have also been applied for the synthesis of oligonucleotides with therapeutic or analytical purposes. Traditionally, the synthesis of nucleoside analogues has been carried out by either modification of the natural nucleoside, or by glycosidation between modified carbohydrates and the corresponding heterocyclic base. These main strategies for the synthesis of non-natural nucleosides require the design of new routes for each different kind of nucleoside (usually linear and with many steps), making these procedures quite hard and tedious. Therefore, the development of a short, modular and general method for the synthesis of new nucleoside analogs starting from non carbohydrates precursors is highly desirable. In the last years, organocatalysis  $\zeta$  the use of small chiral organic molecules as catalyst  $\zeta$  has been a valuable and attractive tool for the synthesis of enantiomerically enriched molecules. Despite of the huge number of organocatalysts and processes, the synthesis of nucleosides or nucleoside analogues using organocatalysis has been never explored yet. The general aim of the future research line is the synthesis of isonucleoside analogs using organocatalysis and their application as therapeutic agents. Isonucleosides are a nucleoside family chemically and metabolically more stable than other nucleosides, but they have been less studied due to their long-step synthesis. The specific aims of the project would be: (a) Design and synthesis of new families of isonucleoside analogues by an alternative and innovative route based on two organocatalytic steps. Thus, the desired isonucleosides will be synthesized via aldol reaction of two aldehydes containing the appropriated functionalization which will be previously prepared by alpha-functionalization. These two organocatalytic steps will determine the final stereochemistry of the objective nucleosides. Both enantiomers and all the possible diastereoisomers of the isonucleosides would be synthesized by choosing the appropriated enantiomer and/or type of catalyst for each organocatalytic step, making this approach very attractive. Three different families of nucleosides analogs: isonucleosides, and their tio- and aza-isonucleosides analogues will be prepared. Each family will contain pyrimidine or purine bases, i.e. adenine, thymine, cytosine, guanine and uracil, for having complete series of isonucleosides. (b) Their biological evaluation against a broad panel of DNA and RNA viruses. Furthermore, the propose synthesis is modular and short which will allow the easy and fast preparation of new series of isonucleosides after the initial biological evaluation in order to get the best drug candidate.

**Resumen del Curriculum Vitae:**

The candidate, Silvia Cabrera, studied Chemistry at the Universidad Autónoma de Madrid (UAM, Spain) and was graduated in 2000. During the last year of her bachelor, she joined Prof. Juan C. Carretero's group at UAM with an undergraduate fellowship from the Spanish Ministry of Science (MEC). In the same group, she obtained her M.Sc. in 2002 and afterwards the Ph.D. in Chemistry (2006) with the best qualification ( $\zeta$ Sobresaliente Cum Laude $\zeta$ ) under the supervision of Prof. Juan C. Carretero and Dr. Ramón Gómez-Arrayás. In both, M.Sc. and Ph.D, she was focused on the synthesis of a new family of chiral ligands, Fesulphos, and their application in asymmetric catalysis. In 2005 she was awarded the Lilly Research Award to be considered one of the best three Ph.D. students of Spain. Furthermore, during her Ph.D. studies, she carried out a predoctoral stay in the group of Prof. Lanny S. Liebeskind at Emory University (Atlanta, USA) working on cross-coupling reactions under copper catalysis. After her Ph.D., she decided to research in organocatalysis, an emerging area and one of the hottest topics in the field of catalysis. For this purpose, she joined the group of Prof. Karl A. Jørgensen in the Centre for Catalysis (Aarhus University, Aarhus, Denmark) for a two year postdoctoral stay (2006-2008). In this group, she was working on the development of new reactions using chiral amines and thioureas as organocatalysts. Then, she moved to the medicinal chemistry area, a challenge in her scientific career. Thus, from May 2008 until now, she is researching in Prof. M<sup>a</sup> José Camarasa's group at Instituto de Química Médica from CSIC (Spain) with a  $\zeta$ Juan de la Cierva $\zeta$  contract. She is currently focused on the synthesis of new inhibitors of the dimerization of the HIV-1 reverse transcriptase and on the synthesis of new prodrugs based on the DPPiV/CD26 enzyme. As a result of the scientific career of the candidate, she has been awarded the Suschem-INNOVA Award for young chemist researchers in 2009. She is author of 24 publications at the highest level and one more has been submitted. Most of her publications belong to the top-ten journals of different chemistry areas: 4 Angew. Chem. Int. Ed., 3 J. Am. Chem. Soc., 2 Chem. Commun., 2 Org. Lett., 1 Chem. Eur. J., 3 J. Org. Chem., 1 J. Med. Chem. Furthermore, she is the first author of 10 articles and the corresponding author of 4 articles. During all her career, she has been working in hot topics in catalysis and medicinal chemistry areas. Due to her important contributions to these areas, 6 publications have been highlighted in Synfacts, one of them has been selected for the cover picture and she has received 813 citations since her first publication in 2001. The candidate has participated actively in six projects and the best results obtained in them have been presented in 9 congresses (6 internationals and 3 nationals) in which the candidate is author of 2 oral communications and 4 posters. She has also received fellowships and contracts from the Spanish Ministry of Science (undergraduate and post-doctoral fellowships and  $\zeta$ Juan de la Cierva $\zeta$  contract) and from Universidad Autónoma de Madrid (pre-doctoral). Furthermore, she has also experience at academic level as assistant teacher.