AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Trayectoria Guillermo Minguez

Resumen de la Memoria:

The scientific career of Guillermo Minguez, which has resulted in 39 publications of which he is corresponding author in 13 of them, can be divided in three parts: i) at the University of Seville as an undergraduate; ii) at the University of Sheffield (UK) as a PhD student and then a short post-doc; iii) at the University of Valencia as a Juan de la Cierva researcher and then a senior post-doc. In these periods he has worked in different aspects of Inorganic Chemistry.

During his degree in Chemistry at the University of Seville he was initiated in research in several European laboratories, working on polyoxometalates, modern NMR techniques and crystal engineering. In his PhD he was involved the study of interactions and reactions of novel metal-organic networks and their behaviour under extreme conditions, developing expertise in ab initio structure solution and refinement from X-ray powder diffraction data and high-pressure crystallography. Afterwards, in Valencia he made a change in his research line moving towards Molecular Magnetism. There he has initiated an independent research that intends to use his previous expertise in inorganic chemistry and crystallography in combination with the acquired knowledge in molecular magnetism in order to develop novel stimuli-responsive molecular materials exhibiting multifunctional properties. In addition, he is implementing the concepts of halogen bonding into the field of molecular magnetism in order to control the magnetic properties.

Resumen del Currículum Vitae:

Guillermo Mínguez studied Chemistry at the Universidad de Sevilla (Spain) (1999–2004) where he performed two 1-month placements in France and a research project in the UK, which resulted in the publication of three papers. He graduated at the top of his year winning numerous awards, including the "Premio Extraordinario" and "Segundo Premio Nacional de Fin de Carrera". Then, he returned to the UK in October 2004 to start a PhD in the group of Prof. Lee Brammer at the University of Sheffield, which he completed in November 2007. His work involved the study of halogen bonding of metal-containing systems and reactions in molecular crystals. The scientific quality of his PhD was recognized by two international awards: the 'Ludo Frevel Crystallography Scholarship' to the high accomplishments in applying the different diffraction techniques (he was the only European of the 2007 Award) and the Gold Medal at the European Young Chemist Award organized by the European Association for Chemical and Molecular Sciences (EuCheMS). After finishing his PhD, he held a 6-month post-doctoral position at the University of Sheffield, and from September 2008 until the present he has been working in the group of Prof. Eugenio Coronado at the Instituto de Ciencia Molecular of the University of Valencia, where he has held a Juan de la Cierva fellowship. He is currently working on the synthesis and physical characterization of dynamic magnetic MOFs. Guillermo Mínguez has published 35 articles (plus 2 submitted) in journals of high impact factor, and 4 chapters in books. These include 1 Nature Commun., 1 Nature Photon., 3 Angew. Chem., 5 J. Am. Chem. Soc. (one of them highlighted by the editors of Science and another by the editors of Nature Chemistry), 1 Chem. Soc. Rev., 2 Chem. Sci., 2 Chem. Eur. J., 1 Chem. Commun. (selected as hot paper), 4 Inorg. Chem. and 8 CrystEngComm, receiving a total of 680 citations with an h-index = 15. He is the corresponding author of 13 publications (plus 2 submitted), including 1 Nature Commun., 1 J. Am. Chem. Soc., 1 Chem. Soc. Rev., and an invited contribution to the New Talents Issue of CrystEngComm. In addition, he is the single author of two chapters in books. He has attended several international congresses, presenting 19 oral communications of which he has been an invited speaker in 13 (one of them as a Keynote speaker). Guillermo has participated in 3 European research projects, and has co-directed 1 PhD student (defended in Nov. 2013), 1 MSc student and six final undergraduate research projects. As a result of his scientific career, the candidate has been selected as the winner of the prestigious 2009 Dalton Young Researchers Award awarded by the Royal Society of Chemistry, the 2010 "Real Academia Sevillana de Ciencias Award" for young researchers, the 2011 "Xavier Solans Award" for the best scientific publication in Crystallography, and the "Premio Talento Joven CV" in 2013. In 2013, he was selected to attend the prestigious 63rd Meeting of Nobel Laureates in Lindau. He has also performed reviewer tasks for several journals, including Chem. Soc. Rev., Angew. Chem. Int. Ed., Acc. Chem. Res. and Chem. Commun., and has been the guest editor of a special issue of Coord. Chem. Rev.

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Metal-catalyzed asymmetric reactions. Design of new asymmetric methodologies and chiral ligands

Resumen de la Memoria:

During his career, Abel Ros has worked in different topics in the field of asymmetric organic synthesis. The experience acquired during this time has allowed him to open a new research topic in his group in the field of fluorescent dyes as molecular switches and sensors.

The candidate carried out his doctoral Thesis under a project funded by BayerCropScience involving the synthesis of chiral herbicides. As a result, a new methodology based on the asymmetric transfer hydrogenation (ATH) via dynamic kinetic resolution (DKR) of ketones and imines was developed. This work generated an international patent and the subsequent commercialisation of the herbicide Indaziflam; in USA. Afterwards, the candidate got consecutive postdoctoral contracts with BayerCropScience and the University of Seville, which he spent in the Instituto de Investigaciones Químicas working in the development of new families of chiral NHC ligands and their metal complexes, as well as in the catalytic applications in asymmetric reactions such as non-asymmetric and asymmetric Suzuki reaction, Tsuji-Trost reaction, asymmetric hydrosilylation of ketones and asymmetric 1,3-cycloaddition reaction between azomethine ylides and α,β−unsaturated esters. It is important to highlight from this period the development of the first asymmetric Suzuki-Miyaura reaction with high levels of enantioselectivity using phosphine-free ligands. This methodology has been highlighted in ChemInform and Organic Chemistry Portal. Abel Ros joined then the group of Prof. Aggarwal (Bristol), as a Marie Curie IEF, where he worked on the synthesis of chiral Csp3-boron and sulfur ylides derivatives and their application in organic synthesis. It is noteworthy that this work led to the first 1,2-addition of alkyl boron-derivatives to aldehydes and the development of a new, cheap and readily available chiral reagent [today commercially available in TCI], and its application to the total synthesis of Quinine and Quinidine employing sulfur ylide chemistry. After his postdoctoral stay in Bristol, the applicant returned to Spain and continued working on the asymmetric Suzuki-Miyaura reaction topic, developing a dynamic kinetic asymmetric cross-coupling strategy which constitutes a breakthrough in the metal-catalyzed asymmetric reactions and set up a new research area in the field. Based on the knowledge he acquired on boron chemistry during his postdoctoral stay, the candidate triggered the development of a new research topic in the group: New methodologies for the ortho-regioselective C-H borylation of arenes. In collaboration with Dr Uwe Pischel, the applicant started a new research topic, fluorescent boron-based dyes as molecular switches and sensors, using the borylated arylisoquinolines (BAI) products synthetized by the C-H borylation methodology previously described. The applicant has demonstrated to have a wide background in the field of asymmetric organic synthesis, which has provided him with leadership, management, problem-solving and project planning skills.

Resumen del Currículum Vitae:

After obtaining his Bachelor degree in Chemistry at the University of Seville (1996-2001), Abel Ros joined the research group of Dr. José María Lassaletta at the Instituto de Investigaciones Químicas (CSIC-US), where he worked on a project funded by BayerCropScience involving the asymmetric synthesis of chiral triazine-based herbicides. This work, which eventually allowed the candidate to obtain the doctoral degree in 2006, resulted in an internacional patent [PCT/WO 2006/072374], of which he is a co-author, and the subsequent commercialisation of the herbicide Indaziflam; in USA since 2011. After a selection process in Frankfurt (Germany), the candidate got a postdoctoral contract funded by BayerCropScience during the period May 2006-May 2007. Afterwards, he joined the group of Prof. Rosario Fernández (June 2007-Feb. 2008) at the University of Seville to work on the synthesis of a new family of chiral NHC ligands and their metal complexes, as well as on the development of new metal catalyzed asymmetric reactions employing chiral NHC- and hidrazone-based ligands. On March 2008 the candidate joined the research group of Prof. Varinder Aggarwal at University of Bristol (UK) as a Marie Curie-IEF postdoctoral fellow (March 2008-March 2010). During this period he worked on the development and application of new chiral organometallic reagents, in special boron derivatives, and in the application of the chemistry of sulfur ylides to the total synthesis of natural products. There he supervised some PhD and Ms students. In March 2010, the candidate returned to the IIQ with a postdoctoral contract funded by the regional government (April 2010-March 2012) and later as a JAE-Doc fellow (March 2012-currently), working on the topic of new asymmetric C-X bond forming reactions, in particular on the asymmetric Suzuki coupling reactions and directed borylations of C-H bonds. He also was awarded with a Marie Curie RG (May 2010-April 2013), which helped him to start an independent research project, in collaboration with Dr. Uwe Pischel at University of Huelva, in the area of new borylated compounds as fluorescent dyes, molecular switches and sensors. The applicant has participated in 12 research projects, two of them funded by private companies, among which is worth highlighting the

Marie Curie RG fellowship, of which he is PI. The scientific quality of his research is supported by the number of publications in high-impact journals (24 published, 2 accepted, 1 submmited): ACIE (2), JACS (4), Chem. Eur. J. (2), Chem. Soc. Rev. (1), Adv. Synth. Cat. (1), Org. Lett. (1), J. Org. Chem. (3), Organometallics (3), Dalton Trans. (2), Tetrahedron (3), Synlett (1), Tet. Asymmetry (2), e-ROS enciclopedia (1), in 15 of them appearing as a first author, 6 as second author and 3 as corresponding author, and receiving a total of 456 citations with an h-index of 13. Abel Ros is also co-author of 2 book chapters (in press) and 3 patents (1 PCT and 2 are under review). During his scientific career he has presented 33 communications in national and international congresses, including 4 oral communications. Furthermore, the applicant has co-supervised one PhD and one master thesis, and is currently co-supervising two PhD students. Additional, the applicant collaborated in the teaching activities of the University of Huelva in 2010-2011. Research ID: E-9256-2011

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Light-driven nanotechnology: sensors and photocatalytic processes

Resumen de la Memoria:

The main research line Dr. González-Béjar has carried out serves from light-driven strategies to design nanosystems and/ or develop novel photocatalysts and bioapplications by using the interaction of nanosystems or molecules with light. During these years, she has consolidated her expertise in photochemistry and photophysics and has developed a solid background in nanotechnology and in the design of efficient methods for making and modifying nanostructures; i. e., she has learned how to design these materials. Currently, she can make and characterize metallic, semiconductor and up-conversion nanoparticles with exceptional control and perform their custom designed modification for targeted applications.

During her PhD, the candidate was able to work on the development of positive photocatalysis in the framework of preparative organic chemistry; in particular cycloaddition reactions promoted by new organic photocatalysts.
Later on, during her postdoctoral stay in Canada she developed new sensors based on quantum dots (QDs) and got involved in many subprojects and exposed to different high-class and top-quality research related mostly (but not only) with metallic nanoparticles. Thanks to this environment, she could also combine her previous knowledge on photophysics with plasmonics to invent new nanocatalysts to explore new chemical transformations or to improve known ones. Last but not least, she performed several studies merging her knowledge about photochemistry with biological purposes (cells, human serum albumin, collagen, etc.) and started to develop a project related with upconversion nanoparticles.
Now, in her returning phase, she is being involved in the development of colorimetric sensors based on metallic nanoparticles, photodynamic therapy with upconversion nanoparticles and photosensitizers, methods to make colloidal nanoparticles using light and plasmon mediated catalysis.
Therefore, she has contributed to key areas of photochemistry (mechanisms and photosynthetic processes) and nanotechnology (antenna/transmitter effect, sensors, bioapplications and (photo)catalysis).

Resumen del Currículum Vitae:

Dr. González-Béjar joined Prof. Perez-Prieto¿s research group in 2003 at the Department of Organic Chemistry/ The Institute for Molecular Science (ICMOL) at the University of Valencia, and got a FPI predoctoral fellowship from the Spanish Ministry of Science and Technology. From June 2005 to August 2005 she was working at the Technische Universität München under the supervision of Prof. Bach. She earned her PhD in Chemistry in 2007, with the highest mark (European Doctorate and Extraordinary Prize) and was awarded with a post-doctoral grant from the Spanish Ministry of Science and Technology to develop new sensors based on quantum dots at the University of Ottawa under the supervision of Prof. Scaiano where she continued working as a Research Associate for another 2 years.
Dr. González-Béjar was awarded with a Marie Curie Career Integration Grant within the 7th European Community Framework (FP7-PEOPLE-2011-CIG) to support her research and actually holds a Juan de la Cierva contract at the University of Valencia.
The relevance of her work is testified by good quality papers (31, 17 of them in the last 3 years and 4 as a corresponding author) published in top-class international peer-reviewed chemistry journals, 4 more under review, one book chapter and by the number of presentations and seminars given to nationally and internationally established conferences and workshops and universities: 64, 25 orals (4 invited). She has been an active part of 16 funded projects with several researchers from University of Valencia (11, 2 of them head researcher), University of Ottawa (2), Universidad de Santiago de Chile (1), The University of Liverpool (1) and Canada National Research Council (1).
She has also established national (Prof. García-Verdugo¿s group, Instituto Cavanilles de Biodiversidad y Biología Evolutiva, Valencia; Prof. Pilar Campíns, Faculty of Chemistry, Valencia; Dr. Julio Lloret, Universitat de Girona and Dr. Marta Liras, Instituto de Ciencia y Tecnología de Polímeros, CSIC, Madrid) and international collaborations (Prof. Scaiano, University of Ottawa; Prof. Pino, Universidad de Santiago de Chile and Dr. Lopez-Sanchez, The University of Liverpool). Moreover, she participates as a referee in several scientific journals such as, International Journal of Nanomedicine, Photochemistry and Photobiology Sciences, The Journal of Organic Chemistry and Chemical Reviews among others. She has also been member of the examination panel in a thesis and has been invited to evaluate a proposal for Concurso Regular 2014, FONDECYT Program (CONICYT) from Chile, which funds national research projects.
Since 2007, she has trained and co-supervised new group members in Spain and Canada (3 postdoctoral fellows, 12 graduate and 3 undergraduate students) and taught in the Department of Organic Chemistry (Degree) and in a master in Sustainable Chemistry.

Indeed, she has received a visiting professor from Chile and an Argentinean student during her returning phase.
During the last ten years working in physical and organic chemistry laboratories, the candidate has received training in several techniques, which include chromatographic purifications (HPLC and GC), spectroscopic techniques (UV, Circular Dichroism, IR and NMR), fluorescence, LFP, and NIR-Phosphorescence, as well as techniques for nanomaterials characterization (SEM, TEM, DLS, Zeta Potential).

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Nuevas Metodologías para la Síntesis de Péptidos Cíclicos Bioactivos

Resumen de la Memoria:

Obtuve la licenciatura en Química en junio de 1994. Tras una breve estancia en la industria farmacéutica, me trasladé a Estados Unidos para realizar mis estudios de doctorado en la Universidad de Minnesota en el grupo del prof. George Barany, anterior colaborador de Bruce Merrifield. Mi trabajo de tesis se centró en la síntesis de análogos de una pequeña proteína, BPTI, y en el posterior estudio de su plegamiento, en que estuve codirigida por la Prof. Clare Woodward. Se desarrolló también una metodología de síntesis de péptidos cíclicos en fase sólida por ligación química. De esta etapa surgieron 7 publicaciones como por ejemplo: Biochemistry 2004, 43, 1591-1598 y J. Org. Chem. 2004, 69, 4101-4107 entre otras. Durante mi etapa predoctoral tuve la oportunidad de realizar una estancia con la prof. Mercedes Álvarez donde trabajé en química de paladio en fase sólida. De este trabajo surgió la publicación Org. Lett. 2004, 6, 1405-1408. Tras finalizar mi doctorado (Febrero 2004) me incorporé al grupo del prof. Fernando Albericio en el Institut de Recerca Biomèdica en el Parc Científic de Barcelona.

El principal proyecto de investigación ha consistido en la síntesis de análogos de péptidos y depsipéptidos cíclicos antitumorales de origen marino (17 publicaciones). Del subproyecto de la tiocoralina, un péptido bicíclico antitumoral, se obtuvieron las siguientes publicaciones: Chem. Eur. J. 2006, 12, 9001-9009, J. Am. Chem. Soc. 2007, 129, 5322-5323, J. Comb. Chem. 2008, 10, 69-78, Chem. Eur. J. 2008, 14, 4475-4478, J. Med. Chem. 2009, 52, 834-839 y Angew. Chem. Int. Ed. 2013, 52, 5726-5730 entre otras. En la mayoría de estas publicaciones soy la primera autora así como la codirectora del trabajo ya que era la responsable de esta línea de investigación. La síntesis de los péptidos naturales Stellatolide y Pipecolidepsin A, estructuralmente muy complejos, se consiguió y dio lugar a la publicación: Nat. Commun. 2013, 4:2352, con reseñas en varios medios de comunicación.

El desarrollo de la resina ChemMatrix para péptidos complejos dió lugar a varias patentes y publicaciones, siendo la mas relevante J. Comb. Chem. 2006, 8, 213-220, destacada por la revista como un de los manuscritos más citados del 2006 i de los 20 más citados de los últimos 3 años (80 citaciones). Esta es la resina utilizada normalmente ahora para la síntesis de péptidos complejos y se ha utilizado en la producción de varios activos farmacéuticos (APIs): Thymosin alfa1, Pramlintide y Linaclotide.

Otra línea de investigación ha consistido en desarrollar metodología de síntesis de péptidos, como nuevos grupos protectores de cisteína y espaciadores bifuncionales para la preparación de fragmentos protegidos para su posterior utilización en síntesis convergentes. De este trabajo surgieron publicaciones como Chem. Eur. J. 2012, 18, 16166-16176, Chem. Commun. 2012, 48, 2313-2315, y Chem. Rev. 2014, 114, 901-926.

Los resultados de las investigaciones de mi etapa postdoctoral se han presentado en 30 conferencias, la mayoría internacionales.

Finalmente, he de destacar que durante my postdoctorado he disfrutado de un contrato postdoctoral Beatriu de Pinós (Generalitat de Catalunya, 2006-2007) y de un contrato Juan de la Cierva (MEC, 2008-2011), y que en dos ocasiones (2005 y 2008) disfruté de bajas maternales.

Resumen del Currículum Vitae:

De mi currículum cabe destacar la publicación de 45 artículos de investigación en revistas internacionales que hasta el momento acumulan 375 citaciones, siendo la primera autora en 14 de ellas y codirectora de investigación en 21. De ellas las más relevantes son las siguientes:

- Miriam Góngora-Benítez,* Judit Tulla-Puche,* and Fernando Albericio.* Multifaceted Roles of Disulfide Bonds. Peptides as Therapeutics. Chem. Rev. 2014, 114, 901-926.

- Marta Pelay-Gimeno, Yésica García-Ramos, María Jesús Martín, Jan Spengler, J. M. Molina-Guijarro, Simon Munt, Andrés M. Francesch, Carmen Cuevas,* Judit Tulla-Puche,* and Fernando Albericio.* The First Total Synthesis of the Cyclodepsipeptide Pipecolidepsin A. Nat. Commun. 2013, 4:2352.

- Judit Tulla-Puche,* Miriam Góngora-Benítez, Núria Bayó-Puxan, Andrés M. Francesch, Carmen Cuevas, and Fernando Albericio.* Enzyme-labile Protecting Groups for the Synthesis of Natural Products: Solid-Phase Synthesis of Thiocoraline. Angew. Chem. Int. Ed. 2013, 52, 5726-5730.

- Miriam Góngora-Benítez, Michèle Cristau, Matthieu Giraud, Judit Tulla-Puche,* and Fernando Albericio.* A Universal Strategy for Preparing Protected C-terminal Peptides on the Solid Phase through an Intramolecular Click Chemistry-based Handle. Chem. Commun. 2012, 48, 2313-2315.

- Judit Tulla-Puche,* Núria Bayó-Puxan, Juan A. Moreno, Andrés M. Francesch, Carmen Cuevas, Mercedes Álvarez, and Fernando Albericio*. Solid-Phase Synthesis of Oxathiocoraline by a Key Intermolecular Disulfide Dimer. J. Am. Chem. Soc. 2007, 129, 5322-5323.

También se han presentado 7 patentes, 6 en explotación (4 por Lonza AG y 2 por PharmaMar S.A.) y he tenido la oportunidad de coeditar un libro y de participar en la escritura de 3 capítulos de libro.

Otro aspecto que cabe destacar es la codirección de numerosos estudiantes de doctorado (4 tesis doctorales ya finalizadas, 3 en curso, y 5 estudiantes de doctorado pertenecientes a universidades extranjeras dirigidos durante la realización de una estancia pre-doctoral en el grupo).

Por otra parte, he participado en varios proyectos de investigación tanto de financiación publica como privada, internacionales (1 de ellos europeo) y nacionales. He presentado my trabajo de investigación en 30 conferencias, la mayoría internacionales (con presentaciones orales en 8 de ellas, dos como invitada, 1 de ellas como Keynote Speaker).

También he actuado como censor de la ANEP y revisor para la American Chemical Society y Springer.

Por último debo mencionar que he disfrutado de los contratos postdoctorales Beatriu de Pinós y Juan de la Cierva, obtenidos en convocatorias competitivas.

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Multiscale computational approach to reaction mechanisms, new catalysts and designed enzymes

Resumen de la Memoria:

The transformative capacity of multiscale computational methods to understand and predict experimental phenomena has been acknowledged through the Nobel Prize in Chemistry 2013 awarded to Karplus, Levitt and Warshel.

Throughout my 13-year career, I have witnessed the huge technological progress that nowadays allows chemists to face computational challenges that were merely a dream a few years ago: the navigation through constellations of reaction pathways in multistep stereoselective reactions, the accurate description of solvation, the simulation of sub-millisecond dynamics of proteins and photovoltaics, the characterization of the bioactive conformations of glycopeptides, etc. Through the years, I have shown that all these phenomena can indeed be studied from a computationally perspective.

However, computational protocols were not implemented in my original group, so I took the responsibility of filling this gap. I quickly realized that computations could be used to understand the striking results that I was obtaining in the lab, such as a counterintuitive SN2 reaction in a quaternary center. My experimental work, and also that from my colleagues, benefited largely from the interaction with QM and MD calculations. We were able, for instance, to propose a highly pyramidalized enolate as the source of the unexpected stereoselectivity, and we "saw" water molecules interacting intimately with a glycopeptide and sculpting its bioactive conformation. The direct observation of these structural features is highly elusive through experimental techniques. As a result of these joint experimental and theoretical studies, I published around 15 collaborative papers, and the group productivity increased significantly both in quantity and quality.

I also performed innovative work during my first postdoc at University of Zaragoza, where I developed a totally new and challenging research line, namely the computational elucidation of the effect of heterogeneous support in the stereodirecting properties of chiral organometallic complexes. Through state-of-the art hybrid and DFT methods, I was able to characterize, for the first time, the structures of the reactive Cu(I)-carbene species in the presence of the solid support. These models provided an explanation of the striking effect of the clay support on the stereochemical outcome of cyclopropanation reaction.

Finally, I took innovation a step further and moved to UCLA to work on the understanding of stereoselective transition metal and organocatalyzed reactions, which constitute the ideal platform for the longstanding goal of rational, computer-aided design of enzymes and metalloenzymes. The massive supercomputing capabilities available at the Houk lab and the great network of collaborations I was able to create, allowed me to learn almost every single computational technique necessary to tackle problems of very distinct nature. These included the quantum dynamics of photochemical rearrangements, and the role of remote mutations in engineered acyltransferase and iron-dependent cytochromes by microsecond MD. These investigations produced around 10 high-impact papers so far, and many more are submitted or in preparation. Ultimately I am leading a small subgroup devoted to designing new metalloenzymes for Diels-Alder reaction, with the aim of achieving a superior catalytic activity. These studies are now at the experimental validation stage, and we hope to get promising results soon.

Resumen del Currículum Vitae:

My curriculum is dense and heterogeneous, which reveals my multidisciplinary profile ranging from organic and organometallic, to green and theoretical chemistry, molecular recognition, enzymology, materials science, etc. These are arguably the most significant papers for both the groups I worked for and the community:

A. Avenoza, J. H. Busto, F. Corzana, G. Jimenez-Oses, J. M. Peregrina (in alphabetic order). "S(N)2 vs. E2 on quaternary centres: an application to the synthesis of enantiopure b(2,2)-amino acids." Chem. Commun. 2004, 980.

With this highly cited paper (26 citations) I started 10 years ago a new research line in my group that is still active. The intriguing SN2 reaction occurring at the most hindered carbon, which I also analyzed computationally, was a very productive topic that has been revisited recently by other authors in high-impact journals.

F. Corzana, J. H. Busto, G. Jimenez-Oses, J. L. Asensio, J. Jimenez-Barbero, J. M. Peregrina, A. Avenoza. "New insights into a-GalNAc-Ser motif: Influence of hydrogen bonding versus solvent interactions on the preferred conformation." J. Am. Chem. Soc. 2006, 128, 14640.

This pioneering and highly cited paper (38 citations) was an experimental and theoretical collaborative effort that finally explained a very intriguing geometric feature of antifreeze proteins determined by the presence of structured water in the glycopeptide pocket. My contribution was to demonstrate through QM calculations that the role of solvent is actually crucial to maintain the experimental structure.

G. Jiménez-Osés, A. J. Brockway, Jared T. Shaw, K. N. Houk. "Mechanism of Alkoxy Groups Substitution by Grignard Reagents on Aromatic Rings and Experimental Verification of Theoretical Predictions of Anomalous Reactions." J. Am. Chem. Soc. 2013, 135.

This recent paper constitutes a valuable example of how experiments and computations can interact synergistically to elucidate the mechanism of a given reaction, and how calculations can be used to correct misinterpreted experimental results, and even predict anomalous reactivity.

G. Jiménez-Osés, P. Liu, R. A. Matute, K. N. Houk. "Competition Between Concerted and Stepwise Dynamics in the Triplet Di-π-Methane Rearrangement." Angew. Chem. Int. Ed. in press.

This just accepted paper has been ranked as "highly important" (<10%) and will probably create an impact on the photochemical community, since non-statistical effects are found to be significant in this paradigmatic reaction, through massive propagation of QM trajectories. Classical theories (TST, RRKM) fail to reproduce the reactivity of dibenzobarrelene, which shows a non-negligible "dynamically concerted" component.

G. Jiménez-Osés, S. Osuna, X. Gao, M. R. Sawaya, L. Gilson, S. J. Collier, G. W. Huisman, T. O. Yeates, Y. Tang, K. N. Houk. "The Role of Distant Mutations and Allosteric Regulation on LovD Active Site Dynamics." Nat. Chem. Biol. in press.

This just accepted paper is my biggest accomplishment in Chemistry so far. The efforts of four groups were combined to come up with a paradigm shift in enzyme design: instead of mutating the active site to promote reactivity, mutations should be incorporated in remote regions. Microsecond MD simulations explained why the x-ray structures of active and inactive variants look identical: protein-protein interactions allosterically regulate the dynamics of the active site, and remote mutations overcome this effect in the most e

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Catálisis en Síntesis Orgánica

Resumen de la Memoria:

The candidate was early intrigued for the connections between homogeneous and heterogeneous reactions, and a rational explanation of the mechanisms operating in both has constituted the body of work during his career. Catalysis is a transversal subject in many fields of chemistry, i.e., bulk manufacturing, fine and total organic synthesis, waste process, and others, and understanding the analogies and differences in homo- and heterogeneous catalysis and how to unify the best of these worlds is a worthy challenge from a scientific and practical point of view.

The candidate completed his Ph. D. studies in 2005 under the supervision of Prof. Hermenegildo García working on catalytic palladium-containing solids for the construction of carbon-carbon bonds. A stay at Prof. Buchwald s laboratories in the Massachusetts Institute of Technology (Boston), a well-reputed group in palladium catalysis, complemented these studies. The final Thesis deserved the Extraordinary Prize of the Universidad Politécnica de Valencia 2006. The candidate s research during this period also covered organocatalysis, basic and acid catalysis, synthesis of photomaterials and the use of non-conventional solvents.

After working during 6 months for Repsol Co. in the activation of carbon dioxide, the candidate moved for a post-doctoral period in The University of Cambridge with Prof. Ley for the total synthesis of natural products. The candidate s decision for a post-doctoral stay in The University of Cambridge was based on the quest of a better knowledge of synthetic chemistry. Prof. Ley s group is world-leading in the synthesis of complex natural products, and the candidate designed and completed the synthesis of three different natural products, (-)-Epypiriculol in 17 steps, and Bongkrekic and Isobongkrekic Acid, in 28 steps. The total synthesis of the anti-apoptosis reagents used in medicinal chemistry- Iso- and Bongkrekic Acids remains a challenge since their isolation from natural sources gives a final price of 1000 euros per milligram (Sigma-Aldrich). The shorter synthesis of these products was accomplished following the planned retrosynthesis.

In 2008, the candidate joined the Prof. Corma s group and launched a new line of work based on homogeneous gold catalysts. New recyclable organogold compounds showed high catalytic activity and lead to unexpected reactions forming new C-O, C-N and C-B bonds. This line of research crystallized with the discovery that some metallic homogeneous catalysts aggregate to small metallic clusters that catalyze very efficiently a series of reactions, published in Science and Angew. Chem. Int. Ed., among other journals. In parallel, the use of a friendly metal such as iron for organic catalysis was envisaged and implemented in different reactions, and constituted the Thesis of the candidate s first student to be defended (2013). This catalytic success has been implemented by us for the search of new molecules with pharmacological activity, the latter being measured by us or externally.
A critical review about the analogies and differences of gold clusters and gold nanoparticles in catalysis has been recently accepted in Acc. Chem. Res. and opens the way to establish a pattern of catalytic behavior for gold clusters and nanoparticles in many reactions.

Resumen del Currículum Vitae:

The candidate s Ph. D. studies at the ITQ, working in Prof. García s group, were focused on the synthesis of novel palladium-supported solids for catalysis in cross-coupling reactions, a hot topic in that time that was later recognized (2010) with the Nobel Prize in Chemistry (Professors Heck, Suzuki and Negishi). The candidate completed these studies with a stay at Prof. Buchwald s laboratories in the Massachusetts Institute of Technology (Boston), a world-reputed group in palladium catalysis, and all the results together constituted the candidate s Thesis, which deserved the Extraordinary Prize of the Universidad Politécnica de Valencia 2006. The body of ten publications within the thesis dealing with palladium supported catalysts has received in total ~800 citations. The order of authors is alphabetical and not representative of each one s contribution, and the candidate appears as the last author of the published work during the thesis period. The candidate s research during this period also covered organocatalysis, basic and acid catalysis, synthesis of photomaterials and the use of non-conventional solvents.

The candidate did a post-doctoral stay in The University of Cambridge. Prof. Ley s group is world-leading in the synthesis of complex natural products, and the candidate designed and completed the synthesis of three different natural products, (-)-Epypiriculol in 17 steps, and Bongkrekic and Isobongkrekic Acid, in 28 steps, the latter constitutes the shorter route to date to these commercial products.

The candidate then joined the Prof. Corma s group and launched a new line of work based on homogeneous gold catalysts. This line of research crystallized in a series of publications in top journals and finally in the review entitled "Gold-catalyzed carbon-heteroatom formation" (2011) which has received 325 citations. A later critical review in Angew. Chem., Int. Ed. (2012) examined why and how gold is generally a better catalyst than the corresponding platinum and mercury counterparts, the so-called "relativistic triad". The knowledge acquired during these years permitted the identification, synthesis and use in catalysis of very small gold clusters of 3 to 10 atoms that are able to produce millions of catalytic cycles at room temperature. This work was accepted in Science and a related patent has been sent. Not only this reaction but also some other representative transformations in gold catalysis has been found to be catalyzed by these small gold clusters formed in-situ in solution either form gold salts, complexes or nanoparticles, reactions including carbon-carbon, carbon-oxygen and carbon-bromo formation. These works have been publishes in top journals such as Angew. Chem., including three font convers.

54 publications and 2 patents illustrate the diverse work accomplished by the candidate within the field of catalysis, organic synthesis and materials, with a total of ~1300 citations and a H index= 21. The candidate s contribution in at least the 80% (43/54) of the works is high, either as the intellectual and/or experimental author, appearing as either the intellectuall and/or experimental author, and being the corresponding author in 10 out of them. The candidate is currently directing one post-doc, three Ph.D. students (fourth, third and first year) and two last year students, in either homo- or heterogeneous catalysis.

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

From supramolecular chemistry and asymmetric catalysis to technology transfer

Resumen de la Memoria:

Since I was appointed in April 2011 as project researcher at the Catalyst Selection and Optimization Laboratory (CSOL) at the Institute of Chemical research of Catalonia (ICIQ), I have been working in the optimization of the chemical technology (catalysts and processes) developed at ICIQ to transfer it to the society. In CSOL I have coauthored 2 patents and 1 Nature Protocols article. In addition we have put 6 asymmetric catalysts into the market.

Previously, I had worked on 2 main research lines: 1) self-assembly as a tool to achieve functional materials with special emphasis in helical assemblies and, 2) asymmetric catalysis using organic molecules and its application in reactions in continuous flow conditions.

During my PhD thesis work as an FPU predoctoral fellow in the group of Prof. J. L. Serrano in the University of Zaragoza (2002-2005), I used the self-assembly properties of liquid crystalline dendrimers to achieve nanostrustured anisotropic materials. As an example, we developed an easy manner to obtain thermotropic liquid crystalline dendrimers, by converting the dendrimer surface (-NH2) to hydrophobic (alkyl chains). The resulting materials can be easily macroscopically aligned and present anisotropic ionic conductivity. In this period I coauthored 9 publications, most of them in high impact journals (1 JACS, 1 Chem. Soc. Rev., 1 Macromolecules, 4 Chem. Mater.), and took part in several projects, 2 of them international.

In March 2006 I started my postdoctoral stage in the group of Prof. E. W. Meijer in the Eindhoven University of Technology (2006-2008) first with a contract within a European project, later as a MEC/Fulbright postdoctoral fellow, and finally as a Marie Curie fellow. Prof. Meijer group is a world-wide leading group in supramolecular chemistry and in dendrimers research, which gave me the opportunity of taking part in a broad variety of projects, especially in the field of supramolecular chemistry. My main research line was the self-assembly of C3-symmetrical molecules based on a central benzene-1,3,5-tricarboxamide core. We were especially interested in how the chiral information is transferred from the alkyl chains in the periphery to the helical stacks that these molecules form in the solid state and in solution. We described for the first time the helical stacks in the liquid crystalline state. These molecules have been later used for the application of their self-assembly properties in NMR contrast agents and in single polymer chain nanoparticles with use as site isolators in catalysis. After 25 months I coauthored 10 publications: JACS, Chem Sci., Chem. Eur. J. (4), Langmuir, Macromolecules, J. Mater. Chem., Org. Biomol. Chem.

In April 2008, I joined the group of Prof. M. A. Pericàs as Juan de la Cierva researcher (2008-2011) at ICIQ. There, I started my research work on asymmetric catalysis and its application in continuous flow processes. Flow conditions usually facilitate the isolation of the product and allow an easier scale up. We have developed enantioselective immobilized organocatalysts for the following reactions on carbonyl substrates in flow: a-aminoxylation, anti-selective Mannich reaction, and domino Michael–Knoevenagel reaction. The folowing publications result from my work in this period: Green Chem. (corresponding author), Chem. Eur. J., J. Mater. Chem., Synlett, Beilstein J. Org. Chem.

Resumen del Currículum Vitae:

I obtained my degree in Chemistry at the University of Zaragoza (UZ) in 2001. During my last year as undergraduate student I started my research career, in the field of coordination chemistry, first with a "Beca de colaboración" under the supervision of Prof. M. A. Ciriano (UZ) and later as an Erasmus student in the group of Prof. B. Lippert in the University of Dortmund. In 2002 I started my PhD studies with a FPU scholarship in the group of Prof. J. L. Serrano at the Organic Chemistry Department of UZ. My PhD thesis was supervised by Dr. M. Marcos and Dr. A. Omenat and involved the design, synthesis and characterization of liquid crystal dendrimers. In 2005 I did a predoctoral stay in the group of Prof. H. Finkelmann in the University of Freiburg and in December 2005 I obtained my PhD degree from UZ with the Cum Laude qualification. For my PhD thesis I was awarded with the "Premio Extraordinario de Doctorado" (UZ) and the 2nd prize from the "Grupo Especializado de Polímeros" of the "Real Sociedad Española de Química" to the best PhD thesis in the 2-year period 2005-2006. In March 2006 I started my postdoctoral stage at the Eindhoven University of Technology (TUE) in the group of Prof. E. W. Meijer, which is a world-wide leading group in the fields of supramolecular chemistry and dendrimers. After being working there first as a contracted researcher and then under a MEC postdoctoral scholarship, I gained a Marie Curie Intra-European Fellowship in January 2007 to work in the same group. My research focused on the self-assembly behavior of C3 symmetrical molecules. In addition to this, I also took part in other projects related to supramolecular chemistry. From the TUE I moved in April 2008 to the Institute of Chemical Research of Catalonia (ICIQ) to work for 3 years in the group of Prof. M. A. Pericàs under a "Juan de la Cierva" contract. There I worked in the development of asymmetric catalysts and of continuous flow processes. In April 2011 I was appointed as project researcher in the newly created Catalyst Selection and Optimization

Laboratory (CSOL), a technology transfer unit where I am currently working in the further development of chemical technologies owned by ICIQ. From my period at CSOL, I have 2 patent applications (2012, 2014). During my scientific career I have coauthored 26 communications in conferences (13 oral communications, 4 of them invited lectures) and 25 publications in scientific journals, one as corresponding author and 22 indexed in the first quartile of the subjects Chemistry and Materials Science according to the Journal Citations Report: Nature Prot. (1), JACS (2), Chem. Sci. (1), Chem. Soc. Rev. (1), Green Chem. (1), Chem. Eur. J. (5), Chem. Mater. (4), J. Mater. Chem. (2), Langmuir (1), Macromolecules (2), Org. Biomol. Chem. (1), Macromol. Rapid Commun. (1), Synlett (1), Beilstein J. Org. Chem. (1) and Liq. Cryst. (1), which have overall received to this date 574 citations with an h-index=15 (Web of Science). These publications are well-distributed along my scientific career. I have participated in 10 scientific projects (4 of them international: one Integrated Action and 3 European projects). I have been referee for Langmuir and for the Journal of Polymer Science Part A, and hold the ANECA accreditation for becoming "Profesor Ayudante Doctor" and "Profesor de Universidad Privada" in Spanish Universities.

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Microcoils of Nuclear Magnetic Resonance Spectroscopy and concomitant applications

Resumen de la Memoria:

The Applicant's main research line is focused on the use of planar and spiral microcoils, a relative novel concept to enhance the sensitivity of NMR spectroscopy, main limitation of the technique. The radiofrequency microcoils are integrated on top of a glass-substrate defining
the called ﷺNMR-chipﷺ, which allows the analysis of mass- and volume-limited samples. She works in the optimization of the NMR probe (that holds the NMR-chip) as such, in parallel to its application in different fields. Related to the optimization of the probe, three generations of NMR-chips have been designed and fabricated, recently multinuclear 1D and 2D NMR experiments have been carried out with a single microcoil, and an international project has recently been granted for the incorporation of gradient coils. The hyphenation of different energy sources, like microwaves, UV-visible light and conventional heating to the NMR-chip is the main topic of study, and it is focused on the online/in situ monitorization by NMR of chemical processes for a swift optimization of reaction conditions, for automation of a chemical reaction, for detection of short-life intermediates and for extraction of kinetic information within the first seconds of the reaction.
This research line started with a Marie Curie Reintegration Grant (ERG) granted to the applicant at the Regional Institute for Applied Scientific Research (IRICA, University of Castilla-La Mancha), as a new research line within the Microwave and Sustainable Organic Chemistry group (www.umsoc.com). The current position of the applicant, as INCRECYT researcher, allowed her to continue with the ERG project. This project is an application of the NMR-chip concept optimized during the applicant's postdoctorate at University of Twente (The Netherlands) supported by an individual Marie Curie IntraEuropean Fellowship (EIF). For the development of this research line, the applicant supervises two PhD projects (and a third is starting shortly), one of them recently defended with the maximum qualification. A project granted by JCCM on the field helped to the implementation of this new research line. In addition, international R+D contracts and projects fund the execution of this research. The applicant is principal investigator within the UCLM of that international project, to be developed within the cited research line.
In addition, the candidate is focused on the application of NMR spectroscopy in fields like supramolecular chemistry, metabolomics and food science in collaboration with other research groups and participating in other projects. High impacts publications, book chapters, patents, direction of PhD projects, participation in European, International and national projects are the highlighted achievements related of the research line of the applicant.

Resumen del Currículum Vitae:

Chemistry degree at the Faculty of Chemistry (University of Castilla-La Mancha, UCLM) in June 2001; PhD in Chemistry (UCLM), Cum Laude in 2006. Title: Use of Microwave Irradiation and Supported and/or Acid Catalyst in Environmentally friendly Organic Chemistry; Postdoctorate as MARIE CURIE INTRAEUROPEAN (EIF) FELLOW at the University of Twente from 2006-2008. Title of the project: Micro & Nano NMR;Reintegration as MARIE CURIE REINTEGRATION GRANT at the UCLM from 2009-2012. Title of the project: On-line monitoring of microwave-assisted chemical reactions by small-volume NMR techniques; INCRECYT Senior Researcher from Albacete Science and Technology Park working at UCLM from 2011 up to date. PAST SCIENTIFIC EXPERIENCE: Predoctoral stay at the University of Oxford (England) in 2001; PhD student (F.P.U from "Ministerio de Educación, Cultura y Deporte") from 2002-2006; Predoctoral stay at the Chemistry Technology Institute (ITQ) (CSIC-UPV, Valencia) in 2003. PARTICIPATION IN R&D&I PROJECTS: 19 projects (PI in an international one within UCLM, 15 in competitive tenders & 3 no competitive). Three of the competitive projects (International, European and regional projects) were funded to support the new research like I am implementing at the Microwave and Suistainable Chemistry group (UCLM). PATENTS: A dutch patent granted and an international one (PCT) filed, a another one under preparation. PUBLICATIONS: I am author of 27 international publications (three of them are book chapters) and another 2 submitted and 6 under preparation. First author in 10 of the articles, corresponding author in 2 of the articles, and only 4 scientific articles are not within the 25% higher impact factor in its knowledge area. CONFERENCES: Contribution in 59 international/national conferences (2 as invited speaker). THESIS AND OTHER WORK AS SUPERVISOR: Director of a PhD project just defended (Cum Laude), supervision of a second PhD project, and a third to start shortly. I have supervised 1 postdoc student, 2 students in their final project to get the bachelor degree, 2 students in their final master project, 1 student in the work leading to an Advanced Studies Diploma, 7 students from the last course of Chemistry degree. TEACHING: I have participated in three projects for innovation in teaching, I was awarded the positive evaluation from the ACUM (Quality agency from Castilla-La Mancha) for the positions of "Profesor Contratado Doctor" and "Ayudante Doctor", I have given teaching in a total of 11 subjects, what corresponds to more than 300 hours of teaching to students

of Chemistry, Chemistry Engineering and Food Science; In addition, I was hired as "Profesor Asociado" for a few months at the UCLM. QUALIFICATIONS AND AWARDS: Honourable mention to my academic marks, and Erasmus project prize at the Erasmus 25th anniversary. REVIEW OF ARTICLES. I partipate in the peer review of articles submitted to ACS journals. ENGLISH COURSES. I have the oficial diploma (English) from the Oficial School of Languages, and an Advanced Course from Wall Street Institute with a duration of 11 months. SCIENTIFIC COMMITTEE: I have participated in a PhD defense committee, and in seven defenses of a research subject.

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Synthetically Engineered Transport Across Lipid Membranes

Resumen de la Memoria:

· My PhD (FPU $, Prof. S. López) was focused in the synthesis and biological evaluation of bioactive retinoids. I published 5 papers in the retinoid field (Org. Lett., J. Org. Chem., Chem. Eur. J. (2x), Chembiochem, RSC Advances submitted). I have also published one paper for each of my abroad predoctoral stages in top-level institutions of Europe and USA: one Org. Lett. in Total Synthesis with Prof. Steven Lay (Cambridge, UK) and one Org. Biomol. Chem. in Supramolecular Chemistry with Prof. Reza M. Ghadiri (Scripps USA). In 2009 I moved to the University of Geneva for my post-doc (NSF $, Prof. Stefan Matile).

· 1 Nat. Chem. 2010, 2, 533-538. During my post doc I was directly involved in the synthesis and characterization of supramolecular molecules and membrane transporters. I learnt about transport experiments (U-tube and/or nanometric liposomes), fluorescence techniques, characterization of supramolecular assemblies and quantification of weak interactions. The 135 citations this paper has received in the last three years clearly reflect the great significance of this breakthrough.

· 2 Chem. Sci. 2011, 2, 303-307. I was also involved in more applicable and functional projects such as differential bio-sensors where I worked in the synthesis and transport experiments for series of cationic dynamic amphiphiles (hydrazones). The differences of the DNA transport fingerprints in fluorogenic vesicle were used to differentiate closely related structures (i.e. enantiomers) and complex mixtures (i.e. perfumes). This paper (1st author*) triggered diverse applications in biomembrane research and several papers were published extending this methodology (Chem. Eur. J. (2x) and Org. Biomol. Chem. (2x) and Chem. Asian J.

· 3 J. Am. Chem. Soc. 2013, 135, 9295-9298. (1st author*) During my postdoc I was promoted (NCCR $) as a coordinator of small group of chemist and biologist working together to implement the dynamic cytofectins prepared in the siRNA-mediated transfection of He-La cells. Our identified hits performed much better than the commercially available kits (lipofectamine).

· 4 J. Am. Chem. Soc. DOI: 10.1021/ja410901r. I moved back to Spain to work with Prof. Juan Granja (JdC $). In this paper (nanotechnology and materials science) I am first and corresponding author reflecting my decisive contributions in design, experimental, research coordination and manuscript writing.

· 5 Systems Chemistry for the Synthesis of Dynamic Cell Penetrating Polymers (Ref: IE130688). Grant award (PI) from the International Scheme Program (Royal Society) aimed to establish long-term collaboration between the UK and overseas brilliant young researchers. We will try to implement my know-how in polymer assisted DNA transport across (bio)-membranes. The clear-cut objectives proposed and my expertise in dynamic (hydrazone) chemistry, membrane biophysics and biological screening unmistakably justified the award received.

I have also combined my background to benefit ongoing projects of my current lab and other labs of my research center (vesicle transport: E. M. Vázquez; cell transfection protocols: J. M. Martínez-Costas). Nevertheless, my main efforts are focused in research direction. The Master Thesis of Juan Priegue (9.6 mark) was intended towards DNA sensors using membrane transport protocols (Angewandte Chemie sumitted) and I am currently supervising two more final projects and one PhD student.
* Shared.

Resumen del Currículum Vitae:

I obtained my PhD degree in 2009 (Santiago de Compostela, Prof. Susana Lopez, FPU fellowship) in the field of Organic Synthesis and Protein Chemical Biology publishing seven papers in high impact factor journals (Org. Lett., J. Org. Chem., Chem. Eur. J. (2x), Chembiochem, RSC Advances submitted). I did two predoctoral stays in top-level Universities and Research Institutes of Europe and USA. In Cambridge University with Prof. Steven V. Ley publishing the first Total Synthesis of Millingtonine (Org. Lett.) and in the Scripps Research Institute (Prof. Reza Ghadiri) publishing a first design of biodegradable supramolecular polymers (Org. Biomol. Chem.). I spend 3 years as Post-Doctoral fellow in the University of Geneva (Prof. Stefan Matile) publishing 12 papers in the best chemical journals (JACS; Nat.; Chem.; Chem. Sci.; Chem. Eur. J. (2x); Org. Biomol. Chem. (2x); Langmuir; Chimia (2x); Chem. Soc. Rev.;

Chem. Asian J.). I then joined the laboratory of Prof. Juan R. Granja as a Juan de la Cierva fellow (2012) publishing two high impact articles (JACS and Acc. Chem. Res.) and two more papers already submitted (Angew. Chem. Int. Ed. and Curr. Opin. Med. Chem.).

I directly secured my first year Post-doc funding resources from the highly competitive international funding program of the Swiss National Science Foundation (http://www.snf.ch). Furthermore, in the next two following years I was promoted as a research associate of the most prestigious Swiss National Centre of Competence in Research (NCCR) for Chemical Biology (http://www.nccr-chembio.ch/).

I have directed one master thesis (Biosensors, Juan Priegue) and I have also directed one final project of an interexchange student from Argentina (Protein recognition, Alexis Wolfel). I am corresponding author of my last paper published in 2014 (JACS) as well as my two last submitted manuscripts (RSC Advances, ACIE). The Royal Society of Chemistry has recognized the maturity and international projection of my independent research with an International Exchange Scheme award entitled "Systems Chemistry for the Synthesis of Dynamic Cell Penetrating Polymers" (Ref: IE130688, http://royalsociety.org/grants/schemes/international-exchanges/).

I have been invited to present my research in one invited lecture in the University of Geneva (one more in Birmingham University, June 2014). I have been invited to international symposiums performing a total of six oral communications and I have accomplished 340 hours of teaching duties in Spain and 120 hours in Switzerland. I was awarded with the cover picture of prestigious journals such as Acc. Chem. Res., Chem. Asian J. and Nat. Chem.

In summary my research efforts are "genuinely" interdisciplinary and based in a strong background in organic synthesis and supramolecular chemistry applied to chemical biology and nanotechnology. I have strong level of high quality productivity (21 papers published, 3 papers submitted). I have been awarded with different fellowships during all the stages of my carrier (FPU, SNF, NCCR, JdC). I have performed a total of 3.7 years abroad research stages in top-level Institutions of Europe and USA. I have supervised PhD and master students and I have obtained funding for my independent research from prestigious international funding agencies.

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Pump-probe spectroscopy of organic molecules with applications as molecular wires, in photovoltaics and photoinitiators in 3D photolithography

Resumen de la Memoria:

Dr. de Miguel did his PhD in the Department of Physical Chemistry of the University of Córdoba under the supervision of Prof. Luis Camacho. He defended his PhD Thesis in 2007 with outstanding distinctions. His PhD thesis was entitled "Calixarenes as host molecules of porphyrins: characterization and organization of thin films". The main research line carried out during this period was the fabrication of Langmuir-Blodgett films of amphiphilic calixarene molecules with the acidic group in the lower ring and the tert-butyl groups in the upper ring together with different types of porphyrins (amphiphilic, hydrophobic and charged hydrophilic). Dr. de Miguel employed a vast arsenal of characterization techniques to investigate the organization and interactions of the molecules within the films. In addition, the gas sensing and photovoltaic properties of porphyrin/calixarene and porphyrin/calixarene/fullerene thin films have also been studied to develop the potential applications.

In June 2008, he started his first postdoctoral period at the Department of Chemistry and Pharmacy of the Friedrich-Alexander University of Erlangen-Nuremberg under the supervision of Prof. Dirk. M. Guldi. Dr. de Miguel was a daily user of a vast arsenal of transient absorption and emission techniques, from the femto- to the microsecond resolution, e.g., femtosecond transient absorption spectroscopy, nanosecond flash photolysis, fluorescence up-conversion spectroscopy, and picosecond time-correlated single photon counting. Dr. de Miguel implemented this spectroscopic approach to a wide variety of organic molecules: porphyrins, phthalocyanines, fullerenes, cyclophanes, -extended tetrathiafulvalene, oligofluorenes, rotaxanes, triazole linkers, etc, describing the different excited state reactions taking place after photoexcitation: forward and backward electron transfer, energy transfer, intersystem crossing, twisted intramolecular charge transfer (TICT), cis-trans photoisomerization, intramolecular vibrational energy redistribution (IVR), etc

In September 2010, he joined the Department of Physical Chemistry of the University of Castilla-La Mancha for his second postdoctoral position, working at the research group of Prof. A. Douhal. The main objective of his researcht was to characterize the photodynamics of the different electron transfer reactions that take place in squaraine and porphyrin-based dye sensitized solar cells. These studies are critical to shed light on the limitations of SQs as sensitizers in DSSCs and help to design new SQ molecules with optimized properties for high efficiency DSSCs.

In April 2013, he moved to the Nanophysics Department of the Italian Institute of Technology with a research position. This more stable position is already allowing him to be more independency and develop his own research projects. Thus, Dr. de Miguel is applying his wide expertise in the field of femto- to milli- second transient absorption spectroscopy (pump-probe) to disentangle the kinetics of the photoinitiators used in the polymerization of curable resins (photolithography). In this sense, the funding program which has been awarded (Marie Curie CIG grant) is strongly supporting the on-going research through the personal budget. Thus, the CIG project is providing him the tools to gain leading capabilities which can increase his

Resumen del Currículum Vitae:

Dr. Gustavo de Miguel Rojas was born in Zaragoza on 20th January 1979. He graduated in Chemistry with honours at the University of Córdoba in September 2002. Right after that, he started his PhD in the Department of Physical Chemistry of the same University under the supervision of Prof. Luis Camacho. He got his PhD Thesis in 2007 with a grade of summa cum laude. During his PhD he did three research stays in international labs (3 months each) with Prof. Tim Richardson (University of Sheffield, UK), Prof. Helge Lemmetyinen (University of Technology, Finland) and Prof. Hiroshi Imahori (Kyoto University, Japan).
His teaching experience can be summarized as follows: during the PhD, he was collaborating in two experimental subjects in the Degree of Chemistry with 200 hours in total; during his time in Erlangen, he enjoyed a position as temporary assistant professor, teaching two experimental subjects in the Master Degree of Chemistry and Molecular Science for three consecutive semesters (320 hours in total); in the 2011/2012 and 2012/2013 academic years, he was involved in the official teaching program of the Department of Physical Chemistry of the University of Castilla-La Mancha with the subjects "Laboratorio Integrado I" and "Termodinámica" with a total of 150 hours; since the 2013/2014 year, he teaches in the Biochemistry Degree of the University of Córdoba with a part-

time lecturer position (Profesor sustituto interino).
Dr. de Miguel has published 29 articles in peer-reviewed journals including an invited review: 4 Journal of the American Chemical Society, 1 ACS nano, 4 Chemistry – A European Journal, 1 Chemistry of Materials, 5 Journal of Physical Chemistry C, 3 Journal of Materials Chemistry, 2 Journal of Physical Chemistry B, 1 Electrochemistry Communications, 1 Langmuir, 1 ChemPhysChem, 2 PhysChemChemPhys, 1 Electrochimica Acta, 2 Journal of Colloid and Interface Science and 1 Journal of Porphyrins and Phthalocyanines. The 90% of the articles are published in journals within the first quartile (Q1). The 69% of the articles are published in journals with an impact factor greater than 4.1. His h-index is 10, and his papers have been cited more than 350 times. He has 18 contributions to national or international conferences, including 8 oral presentations and 1 invited lecture to an international conference. He is the principal investigator (PI) of an European Project entitled "Nanometer Resolution in Two-Beam Direct Laser Writing Lithography". The funding agency is the European Commission through the Career Integration Grant (CIG) programme of the Marie Curie Actions. The duration of the project is four years and is funded with 100.000 €. He has also participated in two international, five national and four regional research projects. Dr. de Miguel has been awarded during his research career with different prestigious and competitive grants and prizes: The predoctoral fellowship from the "Ministerio de Ciencia e Innovación", "Formación de Profesorado Universitario" (FPU); the postdoctoral fellowship from the Alexander von Humboldt Foundation and the "Juan de la Cierva" grant from the "Ministerio de Ciencia e Innovación". He holds a part-time lecturer position in the University of Córdoba, "Profesor Sustituto Interino". Finally, his research and teaching activities have been accredited by the ANECA (Prof. Ayudante Doctor and Contratado Doctor).

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Physical chemistry of biological systems

Resumen de la Memoria:

My main research line deals on experimental physical chemistry of biological membranes. My long term goal is to fabricate membrane-based bioinspired artificial systems able to interact with cultured cells, to improve the treatments currently available for different diseases. To achieve this ambitious objective on biotechnology, the approach must be necessarily interdisciplinary bringing together strong expertise in biophysics with a profound understanding of the biological role of membranes in important cellular functions as membrane trafficking. I bring together both scientific profiles. My biophysical approach is bottom-up, from the single molecular components to the biomimetic (multicomponent) systems. Tight control of the physico-chemical parameters is only achieved from adequate formulation, thus a reductionist understanding of the important elements and of the first behavioural principles requires such a bottom-up approximation. The main model is based on giant unilamellar vesicles (GUVs), which can be easily formed by electroformation and microfluidic methods. This membrane model is extremely useful as it can be formulated in a controlled way and its mechanical properties measured by microscopy-based techniques. These artificial vesicles size from 1 to 100 microns, just the optimal range to perform relevant cytomimetic studies. As the lipid distribution as the protein localization can be easily monitored under the fluorescence microscopy mode. These optical techniques quantitatively assess about changes in shape, membrane deformations, spatial distribution of fluorescent species, and in the fast acquisition mode, about the dynamics of the different membrane processes. The artificial function depends on building blocks forming the bio-inspired object and can be modified chemically. As proven by my background in membrane mechanics, membrane interactions can be monitored using micropipette techniques, shape analysis (flickering spectrosocpy), whereas dynamics is easily accessible from stochastic analysis of the membrane motions. My major achievements relevant to this research line include: new protocols and preparative methods for biomimetic assays, developing experimental methodologies for measuring membrane mechanics and dynamics, understanding how molecular composition affects the mechanics and dynamics of lipid membranes, as well as quantitative descriptions of the mechanical impact of protein supramolecular assemblies in model membranes. On the physicochemical basis of self-organisation of multicomponent systems, I will set up a novel approach to fabricate smart liposomes for health improvement.

Resumen del Currículum Vitae:

After completion of my B.Sc. in Physics (Condensed Matter Physics) at Universidad Autónoma de Madrid (UAM) in 2001, I applied to an interdisciplinary doctoral school in biophysics at Paris. My DEA was pursued in Molecular Biophysics (Université Pierre et Marie Curie) under a competitive schema and I was awarded by a predoctoral fellowship from the French Ministry of Education. My PhD (2002-2005) was supervised by Prof Philippe F. Devaux at Institut de Biologie Physico-Chimique (CNRS-Université Paris 7), co-supervised by Marisela Vélez (UAM). My PhD thesis focused on lipid asymmetry and transport on lipid membranes. I defended my PhD thesis in February 2006 with the highest honors. My predoctoral training was particularly fruitful as I acquired strong theoretical and experimental skills in membrane biophysics, which are allowing further developing of my postdoc career in Spain. Just after, I joined the group of Prof. Francisco Monroy at the Universidad Complutense de Madrid (UCM). I was reintegrated through a postdoctoral contract from a Research Network Program financed by Comunidad de Madrid (NANOBIO-M, leaded by José López Carrascosa (CNB-CSIC)). Within this network, I was hired for two years in a bilateral schema (2006-2008; 1st year at UCM → 2nd at UAM). My research efforts focused the specific problem of the mechanics of cell division. In 2007 I was awarded in the Juan de la Cierva program. During this time (2008-2013), I have contributed to start up the emerging group leaded by F. Monroy "Mechanics of biological Systems" as one of the most active teams in the physical chemistry of biological membranes. Additionally, I have mentored up to 10 undergraduate students and co-supervised with FM two PhD thesis. Lately, granted by the Jose Castillejo program, I have spent seven months (February-August 2010) at the group of Patricia Bassereau, an international reference in membrane mechanics and in-membrane synthetic biology. In 2013, I have been awarded with an ERC Strating Grant from the European Research Council (Physical and Analytical Chemical Sciences Evaluation Panel) to go deep into the fabrication of membrane-based bioinspired artificial systems able to interact with cultured cells, with the final goal to improve the treatments currently available for mitochondrial diseases. During my period at UCM, where I am ascribed in the present as a Visiting Professor, I have actively participated in the docent program of the department of Physical Chemistry I. The gain experience in teaching has enabled me to be certified by ANECA as "Profesor Contratado Doctor". Derived from my research, I have published 28 scientific publications international peer-reviewed journals with high impact factor (within the 25% best) in the fields of Physical Chemistry, Biophysics, Soft Matter, Materials and Biological Chemistry. I have also received more than 380 cites (h index = 13). For their impact

index and journal's quality I emphasize 1 PNAS, 1 PRL, 1 JPC Letters, 3 Langmuir, 2 Soft Matter, 2 J Biol Chem, 3 Biophys J., 3 BBA Biomembranes among others. I have participated or still participate in several research projects funded by MINECO. In addition, I have presented 39 communications in international and national meetings (5 of them as invited speaker).

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Título:

Nanomaterials for energy

Resumen de la Memoria:

Research relating to photovoltaic devices based on molecular components continues to be an area attracting considerable interest from chemists, physicists and engineers.

This area can be considered to have begun with the development of the Dye Sensitized Solar Cell (DSC) by Gratzel and O'Regan in 1991. In their work their innovation was to sensitize a high surface area mesoporous metal-oxide film with a Ru(II) dye allowing for a dramatic increase in film light absorption and device photocurrent. The efficiency recorded in their work of 7-9% was a genuine breakthrough in the area of photovoltaics based on cheap materials and simple processing methods. An advantage that DSCs have over more established photovoltaics based on silicon and thin films is that they continue to show high efficiency even at low light levels.

Since the seminal work by Gratzel and O'Regan, many efforts have been undertaken to improve the efficiency and stability of this emerging technology. This have included the development of new sensitizers, red-ox couples, metal-oxide films and counter electrode materials. Currently the best DSC efficiency using a liquid electrolyte is over 12%. However, to be more commercially attractive this technology will need to eventually substitute the liquid electrolyte for a solid hole transporting material. Many efforts have been devoted to this involving polymer materials (e.g. P3HT) and small molecules (e.g. oMeTAD). However, the best efficiencies of DSCs containing solid hole transporting materials continue to be considerably lower than those of their liquid electrolyte counterparts (about 7%).

Efforts have also been undertaken to substite the molecular sensitizer with semiconducting materials with quantum confinement properties (&#65533;quantum dots&#65533;) can be used instead as light-harvesters. These have the advantage that they can be prepared using simple precurser reagents and their color can be tuned depending on the material in question and also on the diameter of the nanoparticles formed. Though this is a promising strategy, the best efficiencies are still low (about 7%).

More recently, a new type of device has been developed independently by Gratzel and Snaith based on a perovskite material, typically CH3NH3PbCl3. These devices show remarkable efficiencies of up to 15%. In these devices the inorganic perovskite performs the light-harvesting function but is also an ambipolar conductor of holes and electrons. Though the exact physics of these devices is still to be known these devices represent a breakthrough in the field.

Finally, other promising device architectures include bulk heterojunction organic photovoltaics based on either polymers or small molecules. In these devices these materials generally act as electron donors and are coupled with fullerenes which act as electron acceptors. The best efficiencies are currently about 10% for these devices.

Resumen del Currículum Vitae:

My research work has focussed on the development of novel light-harvesting systems. My contributions to this research have been broad, ranging from material synthesis and characterization, to device design and assembly, through to device testing using advanced photochemical and electrochemical techniques.

PhD research involved the investigation of electron transfer processes in TiO2 Dye Sensitized Solar Cells with the aim of controlling such processes for optimized device performance. These processes were treated in terms of Marcus non-adiabatic electron transfer theory in order to elucidate the underlying parameters controlling them (i.e. free energy ΔG0 versus distance r). Other activities included the development of novel methods to deposit insulating blocking layers such as Al2O3 on TiO2 films to control interfacial charge trasfer processes and the development of new sensitizers such as phthalocyanines and porphyrins.

Postdoctoral research at ISOF (CNR) was concerned with the photophysical characterization of novel C60 fullerene donor-acceptor complexes. The competition of electron transfer and energy transfer processes in these systems, as well as the influence of solvent environment in modulaing such processes, was invesigated. Fullerene C60 dyads containing star-shaped conjugated oligomers with strong multiple-photon absorption (MPA) cross sections were also investigated for generating singlet oxygen for use in photodynamic therapy (PDT).

Postdoctoral research at KU Leuven was concerned with single-molecule spectroscopy (SMS) and the study of luminescence "photoblinking" of moleular probes. This blinking was monitored using Confocal Microscopy to investigate the underlying causes of this phenomenon in order that it could be better understood to design more stable probes. Other activities included spectroscopic and electrochemical characterization of fluorescent BODIPY (difluoroborondipyrromethene) dyes with phenyl, ethenylphenyl, and ethynylphenyl substituents.

My research activities at ICIQ are focussed on the design and characterization of novel materials for molecular photovoltaic devices. Such materials include quantum confined semiconductor nanocrystals (e.g. CdS, CdSe "dots"), perovskites (e.g. CH3NH3PbCl3) hole-conducting polymers (e.g. P3HT) as well as molecular dye sensitizers such as D-pi-A dyes, porphyrins, phthalocyanines, indolines, squarines and Ru(II)polypyridals. Other activities include the study of novel dimer Ru(II) complexes for the oxidation of water in the production of H2 as a fuel, the use of "click chemisry" to fabricate C60-QD dyad systems and the assembly of fullerene C60-porphyrin supramolecular complexes in solution and on surfaces.

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Título:

Study of Reaction Intermediates in Homogeneous Catalytic Processes

Resumen de la Memoria:

The research career of the candidate is divided into four stages.
In the first stage, (May 2004 – March 2009, Instituto de Ciencia de Materiales de Aragón (University of Zaragoza - CSIC)) the candidate carried out his PhD studies. He was working on asymmetric catalysis mediated by transition metal complexes developing enantioselective 1,3-dipolar cycloaddition reactions of alkenes with nitrones as well as Diels–Alder reactions between enal and dienes mediated by one-point-binding half-sandwich catalysts.

The second stage (April 2009 – August 2012, Laboratoire Hétérochimie Fondamentale et Appliquée (University Paul Sabatier - CNRS)) corresponds to a postdoctoral period. His research work was focused on the study of stabilised-silylenes and their transition-metal-like behaviour and of low valent silicon derivatives as precursors for preparing unique molecules. He was supervisor of two PhD thesis.

The third period (September 2012 – December 2012) was a placement in RIKEN Advanced Science Institute, Wako (Japan) studying the ligand effect on the reaction of phosphine stabilised-silicon(II) compounds as well as the bonding modes of several low coordinated Si compounds by X-ray electron density distribution analyses.

Finally, in the fourth period (January 2013 – present, Instituto de Síntesis Química y Catálisis Homogénea (ISQCH) (University of Zaragoza - CSIC)) the applicant develops his own research topics and supervises PhD thesis as a JAE-postdoc fellow.

Resumen del Currículum Vitae:

Ricardo Rodríguez completed his graduate studies in chemistry at the University of Zaragoza (UZ) in 2003. He then started his Ph.D. studies at the Instituto de Ciencia de Materiales de Aragón (UZ-CSIC), under the supervision of Prof. Daniel Carmona and Prof. Pilar M. Lamata, with an FPI pre-doctoral scholarship. His Thesis work was focused on organometallic chemistry and asymmetric catalysis, with special interest towards the organometallic intermediates involved in the catalytic reactions. He obtained his Ph.D. in Chemistry from the University of Zaragoza in March 2009, receiving the Cum Laude qualification.

From May 2009 to August 2012, the applicant performed his postdoctoral research with Prof. Antoine Baceiredo at the Laboratoire Hétérochimie Fondamentale et Appliquée (Université Paul Sabatier - CNRS) This laboratory, undoubtedly, has a national and international reputation in main group chemistry, especially in the stabilisation of highly reactive species. His research was focused on the study of stabilised-silylenes and their transition-metal-like behaviour and using low valent silicon derivatives as precursors for preparing unique molecules.

From September 2012 to December 2012, he worked at RIKEN Advanced Science Institute funded by the Japanese Society for the Promotion of Science. There, he studied the bonding modes of several low coordinated silicon compounds by X-ray electron density distribution analyses.

Since January 2013, he has been performing research at the Instituto de Síntesis Química y Catálisis Homogénea (ISQCH). This placement is supported by a Jae-Doc fellow, funded by the Spanish Council for Scientific Research. His research work is focused on the study of asymmetric catalysis processes mediated by transition metal complexes.

The applicant is co-author of 20 publications and 4 patents, one of them international; in multidisciplinary chemistry journals (8) Angew. Chem. Int. Ed., (3) J. Am. Chem. Soc., (2) Chem. Eur. J. and in specialised journals (1) Adv. Synth. Catal., (3) Organometallics, (2) Dalton Trans. and (1) Tetrahedron: Asymmetry. The average impact factor of his publications is 9.0. He has attended several international and national congresses and has performed 3 oral presentations.
Finally, the applicant has supervised the research work of two Ph.D. students at the University Paul Sabatier. He is also currently a co-director of a Ph.D. student at the University of Zaragoza.

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