



AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2015

Turno de acceso general

Nombre: CALLE VALLEJO, FEDERICO
Referencia: RYC-2015-18996
Área Científica: Química
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Título:

Toward structure-sensitive and composition-sensitive computational designs of (electro)catalysts

Resumen de la Memoria:

1. Brief description of research activities
1.1. Chemical engineering studies (2002-2007)
I studied chemical engineering in Colombia at UPB. My thesis was entitled **Simulating stirred-tank reactors under dynamic conditions**.
1.2. PhD at DTU (2007-11). Thesis title: **DFT perspectives on the activity and stability of electrocatalysts**.
Supervisors and collaborators: Jens Norskov, Jan Rossmeisl and Ib Chorkendorff
I made a PhD on the design of catalyst materials at the DTU, Denmark. I learned to carry out DFT calculations to study the activity and stability of heterogeneous catalysts. I also learned about the d-band model, scaling relations, Brønsted-Evans-Polanyi relations and volcano plots, methodologies on which I have published 2 articles. I studied 3 classes of catalysts:
1) Perovskite oxides. 9 articles, front cover of ChemCatChem 2011.
2) Alloys of platinum. 5 articles, inside cover in Angewandte Chemie 2012.
3) Graphitic materials functionalized with nitrogen and transition metals. 2 articles.
1.3. Postdoctoral studies
1.3.1. Leiden University (2011-2013)
Supervisor and collaborators: Marc Koper and Aliaksandr Bandarenka
I focused on:
1) Electrochemical reduction of CO on copper single-crystal electrodes. 4 articles, inside back cover of Angewandte Chemie 2013 and front cover of J. Phys. Chem. Lett. 2015.
2) The exceptionally high activity of (100) facets of certain transition-metal electrocatalysts. 2 articles.
3) Platinum and its near-surface alloys. 3 articles.
4) Enhanced catalytic activity of various alloys for the electrochemical reduction of nitrate. 2 articles, front cover of ChemCatChem 2013.
5) Gold oxidation and the mechanism of the oxygen evolution reaction. 1 article featured in the front cover of Chemical Science 2013.
1.3.2. ENS Lyon (2013-2015)
Main collaborators: Philippe Sautet and David Loffreda.
In the framework of an FP7 European contract, I collaborated with researchers from LRCS in Amiens and CEA/LITEN in Grenoble and co-authored an article with them. Besides, I worked on:
1) Development of **generalized coordination numbers**. 2 articles, front cover of Angewandte Chemie 2014.
2) Incorporation of structural sensitivity into scaling relations between adsorption energies. 1 article in Nature Chemistry 2015.
3) Development of realistic models of NSAs of Pt and Cu. 2 articles.
1.4. Principal Investigator at Leiden University (April 2015-present).
Main collaborators: Marc Koper (Leiden University) and Aliaksandr Bandarenka (now at TUM, Munich, Germany).
In 2014 I obtained a 3-year Veni grant from NWO. Only 10% of the applications are successful for this prestigious grant. It provided me with 250.000 €. I have worked on:
1) Coordination-activity plots for the oxygen reduction reaction. 1 article in Science 2015.
2) Oxygen evolution activity of nickel double hydroxides. 1 article.
3) Structure-sensitive electrochemical reduction of acetaldehyde on copper. 1 article.
1.5. Additional collaborations
I have also participated in other projects that are not part of my habitual lines of research. Those led to 6 publications on borohydrides (performed at DTU during my PhD, front cover of J. Chem. Phys. 131, 2009), Cu-Te thin films (in collaboration with Aliaksandr Bandarenka), Al-H clusters and SiO₂, RuO₂ and SiO₂@RuO₂ nanotubes and nanowires (in collaboration with José Ignacio Martínez, CSIC, Spain).

Resumen del Currículum Vitae:

I use Density Functional Theory (DFT) and atomistic thermodynamics to make structure- and composition-sensitive models of electrocatalytic processes. I focus on trends in catalytic activity rationalized in terms of electron-counting rules and coordination numbers. Models based on these intuitive and insightful descriptors are robust, more predictive and computationally affordable than other state-of-the-art models.
I am able to perform DFT calculations at the generalized gradient approximation (PBE, RPBE) and hybrid levels (B3LYP). I have also expertise on transition-state search (nudged elastic band method). I have worked with the codes VASP, GPAW and Dacapo in supercomputers in Denmark, Holland and France. I can perform vibrational-frequency and Bader analyses, and estimate work functions



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and band moments.

I currently hold a 3-year VENI grant (worth 250.000 euro) for young researchers from the Netherlands Organization for Scientific Research. At the same time, I also obtained a Marie Curie COFUND grant and a Mobilex grant at DTU, Denmark. During my career, I have collaborated with widely known theoreticians in Denmark (PhD supervised by Jens Norskov and Jan Rossmeisl, 2007-11), The Netherlands (postdoctoral researcher at Leiden University, supervised by Marc Koper, 2011-13) and France (associate researcher at ENS Lyon, supervised by Philippe Sautet, 2013-15). I have also devoted part of my career to collaborating with experimentalists to design new materials and help explain experimental observations in electrocatalysis and heterogeneous catalysis. In fact, 17 of my 44 articles have been made in collaboration with experimentalists.

My scientific achievements are twofold: on the one hand, I have pushed forward the state of the art by providing predictive and innovative models to understand the adsorption processes that ultimately determine the catalytic activity of materials. On the other hand, I have provided theoretical input to my experimental collaborators to rationalize experimental observations and design improved catalysts. My approach can take the computational design of catalysts to the next level, as demonstrated by my publications in Science (1 article), Nature Chemistry (1), Chem. Soc. Rev. (1), J. Am. Chem. Soc. (4), Angewandte Chemie (5), ACS Catalysis (3), Chem. Sci. (2), Phys. Rev. Lett. (1), and J. Phys. Chem. Lett. (2), among others. Besides, I have got 8 journal covers (6 front covers, 1 inside cover, 1 inside back cover), have 1380 citations and my H index is 18. I have given 12 oral presentations at international scientific events, 4 of which were invited.

I am interested on extended surfaces and nanoparticles of transition metals, their monoxides, dioxides and perovskite oxides. I have also worked on bulk alloys, near-surface and surface alloys and on porphyrins and graphitic materials functionalized with nitrogen and transition metals.

Regarding analyses of catalytic activity and reactivity, I have expertise in assessing free energies, computational hydrogen electrode, d-band model, Bronsted-Evans-Polanyi relations, scaling relations and volcano-type activity plots.

I am interested on catalytic reactions related to fuel cells, electrolyzers and pollution control such as the oxygen reduction and evolution reactions, hydrogen evolution, CO oxidation and reduction, and nitrate reduction.



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Nombre: RIMOLA GIBERT, ALBERT

Referencia: RYC-2015-18885

Área Científica: Química

Correo Electrónico: albert@klignon.uab.es

Título:

Computational Chemistry Of Bio/Inorganic Systems: From Metal-Ion Interactions To Surface-Induced Primordial Chemical Evolution Processes

Resumen de la Memoria:

The research activity of Dr. Albert Rimola has focused on the use of molecular and periodic quantum mechanical calculations on chemical problems involving bio/inorganic-related systems to obtain atomistic insights on their fundamental physico-chemical properties. His PhD was devoted to the interaction of metal cations with biomolecules, in which quantum chemical calculations were essential to interpret the complex outcome of mass spectrometry experiments and to understand the electronic structure of metal complexes relevant to metal-promoted neurodegenerative diseases. During this period he acquired a complete knowledge of different quantum mechanical methods for the treatment of open-shell systems and gained experience in the simulation of chemical reactivity. During his post-doc, Dr. A. Rimola studied the electronic structure of different solid-state extended systems and of their physico-chemical properties, including adsorption and chemical reactivity features, getting deep experience in the modeling of surfaces of different nature; e.g., ionic/covalent, crystalline/amorphous, defective, etc. The expertise of Dr. A. Rimola is thus on the simulation of chemical reactivity and modeling of complex surfaces and his current research activity merges and exploits these two skills, which are of great interest in several fields like heterogeneous catalysis and surface science. His current research lines focus on the modeling of processes related to primordial chemical evolution (i.e. astrochemistry and prebiotic chemistry), in which solid state matter plays an important role. Related to this subject, Dr. A. Rimola presented proposals in the ERC Starting Grant 2013 and 2014 calls, which in both cases received the maximum qualification of A but they were not retained for funding, and he is currently leading two financed research projects (CTQ2014-60119-P and CTQ2015-62635-ERC). He holds several international collaborations with quantum chemists (Prof. P. Ugliengo, Univ. Turin; Prof. A. Michealides, Univ. College London), experimentalists (Prof. T. Chiavassa, Univ Marseille; Prof. N. Balucani, Univ. Perugia; Prof. F. Dulieu, Univ. Cergy-Pontoise) and astronomers (Prof. C. Ceccarelli, Grenoble Observatory; Prof. J. Cernicharo, CSIC; Dr. J.M. Trigo-Rodríguez (ICE-CSIC). Since 2004, Dr. A. Rimola has coauthored 52 international peer-reviewed papers and 2 book chapters, and has given 12 invited international conferences. According to SCOPUS indicators, he has an h-index of 20 and has been cited 1144 times (22.00 average citation/item). He is also involved in activities of dissemination science, such as giving conferences in secondary schools and is coauthor of 4 popular science articles.

Resumen del Currículum Vitae:

Dr. Albert Rimola graduated in Chemistry at the Universitat Autònoma de Barcelona (UAB, 2002) and got a PhD in Theoretical and Computational Chemistry (UAB, 2007) under the supervision of Prof. M. Sodupe and Dr. L. Rodríguez-Santiago. During the PhD period he did short visits at foreign laboratories: 3 months at Univ. Évry ♦ Val d'Essone (2004); 3 months at Univ. Turin (2005); and, 2 months at Univ. Kent (2006). Then he carried out a post-doctoral work (2007 ♦ 2009) in the group of Prof. Piero Ugliengo (Univ. Turin), and in 2010 he returned to UAB. During all these years Dr. A. Rimola has obtained several grants and contracts achieved through competitive international calls, among them the Juan de la Cierva contract. He is currently a Distinguished postdoctoral researcher by UAB.

The focus of the research of Dr. A. Rimola has always been on modeling chemical processes by accurate quantum chemical calculations using both molecular and periodic ab initio approaches. His PhD was devoted to the metal-ion gas-phase chemistry, in which quantum chemical calculations were essential to interpret the complex outcome of mass spectrometry experiments. During this period he acquired a complete knowledge of different quantum mechanical methods for the treatment of open-shell systems and gained experience in the simulation of chemical reactivity. During his post-doc, Dr. A. Rimola studied the electronic structure of different solid-state extended systems and of their physico-chemical properties, getting deep experience in the modeling of surfaces of different nature. His current research lines focus on the modeling of processes related to primordial chemical evolution (i.e. astrochemistry and prebiotic chemistry), in which solid state matter plays an important role. Related to this subject, Dr. A. Rimola presented proposals in the ERC Starting Grant 2013 and 2014 calls (DUSTAR, proposal nº 337052; QUANTUMDUST, proposal nº 638189), which in both cases received the maximum qualification of A but they were not retained for funding. He has led one financed research project (CTQ2013-40347-ERC) and he is currently leading two financed research projects (CTQ2014-60119-P and CTQ2015-62635-ERC). He holds several international collaborations with quantum chemists (Prof. P. Ugliengo, Univ. Turin; Prof. A. Michealides, Univ. College London), experimentalists (Prof. T. Chiavassa, Univ Marseille; Prof. N. Balucani, Univ. Perugia; Prof. F. Dulieu, Univ. Cergy-Pontoise) and astronomers (Prof. C. Ceccarelli, Grenoble Observatory; Prof. J. Cernicharo, CSIC; Dr. J.M. Trigo-Rodríguez (ICE-CSIC).

Since 2004, Dr. A. Rimola has coauthored 52 international peer-reviewed papers and 2 book



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chapters, and has given 12 invited international conferences. According to SCOPUS indicators, he has an h-index of 20 and has been cited 1144 times (22.00 average citation/item). He is also involved in activities of dissemination science, such as giving conferences in secondary schools and is coauthor of 4 popular science articles.

Dr. A. Rimola holds the outstanding PhD thesis award (2006/07 course) and the European Doctorate Mention.



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Turno de acceso general

Nombre: ALBERTAZZI , LORENZO
Referencia: RYC-2015-18989
Área Científica: Química
Correo Electrónico: lalbertazzi@ibebarcelona.eu

Título:

Design of supramolecular assemblies for biomedical applications guided by super resolution imaging

Resumen de la Memoria:

My research activity has always been characterized by a multidisciplinary approach, at the interfaces between chemistry and biophysics. In particular I am interested in the application of biophysical techniques, such as advanced fluorescence microscopy, to the study of chemical synthetic systems. One of the great goals of my research is the understanding at the molecular level of the behavior of complex materials in vitro and in the biological environment using super resolution microscopy. This knowledge will allow to unveil the design principles for the next generation of synthetic materials for biomedical applications such as drug delivery.

During my PhD at Scuola Normale Superiore (Pisa, Italy, 2007-2011) and my stay at University of California Santa Barbara (USA), I studied a variety of synthetic materials based on polymers and dendrimers, understanding their behavior in vitro and in the biological environment. The understanding of the structure-activity relations guided the synthesis of novel synthetic devices for drug delivery (Angew. Chem. 2011) and molecular sensing (JACS 2010).

In the group of Prof. Bert Meijer at Eindhoven University of Technology (Netherlands) I focused on self-assembled materials with particular emphasis on supramolecular polymers. These materials are endowed with unique properties (modularity, dynamics, adaptivity) but their complexity pose a serious challenge towards the understanding of such molecular architectures. To tackle this challenge I developed novel biophysical methods to investigate the properties of supramolecular polymers. With our unique tools I solved open questions related to the self-assembly phenomena in aqueous environment (e.g. PNAS 2013 and Nat. Comm. 2015). In particular, the biggest achievement in this field has been the super resolution imaging of supramolecular polymers (Science 2014). I applied for the first time this innovative technique to supramolecular systems allowing the visualization and the understanding of the self-assembly mechanism at the molecular scale.

On this basis I recently started my research group at the Institute for Bioengineering of Catalonia (IBEC). The main goal of my research group at IBEC is the Nanoscopy for Nanomedicine Group is to generate knowledge about structure-activity relations in self-assembled nanomaterials (supramolecular polymers, nanoparticles) using advanced optical microscopy techniques such as super resolution imaging. This information is used for the formulations of novel nanomaterials based on self-assembly for the treatment of cancer and infectious diseases, i.e. translating fundamental knowledge about supramolecular chemistry into medically relevant applications.

Resumen del Currículum Vitae:

I obtained my BSc in Chemistry at the University of Pavia (Italy) and MSc in Chemistry at the University of Pisa (Italy) in 2007. After my MSc I won a fellowship of the Italian Institute of Technology and joined a graduation program in Molecular Biophysics at Scuola Normale Superiore (Pisa, Italy) where I obtained my PhD cum laude in 2011. My scientific education has been characterized by the combination of training in chemistry and biophysics and I carried out my PhD project at the National Enterprise for Nanoscience of Nanotechnology (NEST), a multidisciplinary institute of Scuola Normale where chemists, biologists and physics join forces to tackle scientific challenges. The output of my PhD research was published in several high impact journals including JACS, Angewandte Chemie and Nature Methods. During my PhD I worked as visiting fellow at the University of California Santa Barbara (USA) under the supervision of Prof. Craig Hawker, a world-renowned polymer chemist. In Hawker's group I focused on the design and synthesis of novel polymer- and dendrimer-based structures with potential for drug delivery applications and published relevant papers on Angewandte Chemie and Biomacromolecules. Subsequently, I moved as postdoctoral fellow to the group of Prof. Bert Meijer at Eindhoven University of Technology (Netherlands) one of the world leading groups of the field of supramolecular chemistry. In the Netherlands I obtained two grants as PI to support my research (ICMS fellowship 200k and Veni Grant 250k) focused on the applications of advanced fluorescence techniques such as super resolution microscopy to the study of synthetic self-assembled structures in water. This innovative approach led to several discoveries reported in high impact publication on JACS, PNAS and Nature Communication with a breakthrough represented by the first super resolution imaging of a synthetic material published on Science in 2014. With these premises I recently moved to Spain as a junior group leader at the Institute for Bioengineering of Catalonia (IBEC). The combination of supramolecular chemistry and biophysics is at the basis of my research group at IBEC (Nanoscopy for Nanomedicine group, <http://www.ibebarcelona.eu/nanoscopy>) where I currently supervise a senior post doc, one PhD student and 2 Master Students. Up to date I published 31 peer-reviewed articles (plus 5 papers submitted), of which 12 as first author and 11 as corresponding author. More than 90% of them were published in first quartile journals. They attracted 730 citations corresponding to an H-Index of 16.



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Nombre: BOUTUREIRA MARTÍN, OMAR

Referencia: RYC-2015-17705

Área Científica: Química

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Título:

Chemical Biology - Chemical protein modification and the use of halogens & chalcogens as well as metal-mediated strategies in glycoconjugate synthesis and carbohydrate chemistry

Resumen de la Memoria:

Summary of current research interests: My main research interests are in the exciting interface between Chemistry and Biology. I have established a research programme using Organic Chemistry as a key research tool to strength the Chemical Biology and Biomedicine fields, including chemical protein modification [Chem. Rev. 2015, 115, 2174] (with a particular emphasis on the development of targeted therapeutics for cancer treatment) [Nat. Chem. 2016, DOI: 10.1038/nchem.2393] and the use of halogens & chalcogens as well as metal-mediated strategies in glycoconjugate synthesis and carbohydrate chemistry. I am currently developing novel aqueous bioorthogonal reactions and carbohydrate chemistry probes that can be used for the understanding of important biological processes and also enable the development of specific tools for imaging, diagnosis, and treatment of important diseases (HIV, Tuberculosis, Cholera, Cancer, and vascular conditions such as stroke, etc.). 1) Development of cutting-edge techniques for targeted cancer therapeutics \diamond delivery of cytotoxic drugs and proinflammatory cytokines into malignant tissue with the intention of creating safer, more potent, and efficient cancer treatments. 2) Development of F-sugar probes [Org. Lett. 2015, 17, 2836] for evaluating carbohydrate-protein interactions by cutting-edge NMR methods and molecular dynamic calculations. 3) Synthesis of complex fluorinated and 2-C-branched carbohydrate epitopes [Org. Lett. 2012, 14, 1728] for the development of homogeneous non-self glycoconjugate vaccines using challenging metal-mediated trifluoromethylation approaches. 4) Development of glycoconjugates as inhibitors of carbohydrate binding & processing proteins. 5) Se-sugars as redox modulators for vascular and neurodegenerative disease treatment

Summary of early achievements: During my Ph.D. and postdoctoral training I gained a strong synthetic chemistry background at URV in Tarragona, Spain as well as in Chemical Biology at Oxford, UK. 1) Development of synthetic methodology for the preparation of Fglycosides and trehalose analogues for the direct imaging of M. tuberculosis in vitro and in vivo without disturbing bacterial growth and viability [Nat. Chem. Biol. 2011, 7, 228]. 2) \diamond QuaNCAT: a method for quantitating proteome dynamics in primary cells \diamond [Nat. Methods 2013, 10, 343] represents a novel, robust methodology for quantitating (by MS techniques) proteome dynamics in primary cells. 3) Development of protein modification methods and selective transformations for the synthesis of homogeneous proteins. These methodologies have been successfully applied to the chemoenzymatic glycoprotein synthesis [Chem. Sci. 2010, 1, 709], incorporation of F- and Se-sugars [Angew. Chem. Int. Ed. 2012, 51, 1432], metal-catalyzed reactions [J. Am. Chem. Soc. 2013, 135, 12156], 18F-radiolabelling of proteins [Chem. Commun. 2011, 47, 10010 & 2010, 46, 8142] and the preparation of homogeneous glycoconjugate vaccine candidates [Angew. Chem. Int. Ed. 2011, 50, 4127]. Importantly, I was the intellectual and experimental responsible in developing, for the first time, the introduction of such an elaborated F- and Se-glycosides into proteins within the Davis group

Resumen del Currículum Vitae:

I received my B.Sc. in Chemistry (2002) and completed my Ph.D. (2007, Summa Cum Laude with European Mention) at the Universitat Rovira i Virgili (URV) with Prof. Sergio Castellón working on the stereoselective synthesis of 2-deoxyoligosaccharides. I conducted postdoctoral research (2008-11) as a Marie Curie IEF fellow at the University of Oxford, UK with Prof. Benjamin G. Davis, where I was involved in several multidisciplinary projects within the Chemical Biology field; these included the development of new trehalose probes for the direct detection of M. tuberculosis and the development of chemical, metal-catalyzed, and enzymatic protein engineering methods for the introduction of F & 18F- and Se-sugars into proteins. In August 2011, I returned to the URV and started my independent line of investigation as a Marie Curie CIG and Juan de la Cierva fellow. From August 2014, I am a Senior Scientist holding a Marie Curie IEF within the Bernardes Group at the University of Cambridge, UK. I am co-author of 34 papers in international peer-reviewed journals, 3 book chapters, and 3 conference proceedings: Nat. Chem. (1), Nat. Chem. Biol. (1), Nat. Methods (1), Angew. Chem. Int. Ed. (2), J. Am. Chem. Soc. (1), Chem. Rev. (1), Chem. Soc. Rev. (1), Chem. Sci. (3), Chem. Commun. (5), Org. Lett. (3), J. Org. Chem. (3), Org. Biomol. Chem. (2), ChemBioChem (1), Eur. J. Org. Chem. (5), RSC Adv. (1), and Carbohydr. Res. (3), receiving a total of 574 citations (average impact factor 8.90) and h-index = 16 (source: Scopus, 14/01/2016) despite the fact that 73% of the publications are very recent (>2010). I am the first author of 13 articles and the co-corresponding or senior author of 6 articles. My work has been highlighted in scientific blogs (6) & spotlights (9), featured on the cover (2), selected as hot papers (3) and among the most accessed papers of the journal (3) and also form the subject matter of highlight articles (2) and patents (1). I am currently co-principal investigator in 2 academic research projects and participate as a researcher & project manager in 2 more. I have participated actively in several research projects (12 in total, ca. 9.9 M \diamond), of particular relevance are 3 Marie Curie European projects (2xIEF at Oxford & Cambridge, which currently support my independent line of investigation and 1xCIG at Tarragona), 1 International project (Bill and Melinda Gates Foundation, USA), and 8 National Projects (including FCT-Portugal and EPSRC-UK). I have presented my work in 41 conferences & meetings (21 international and 20 national) including 5 invited



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lectures, 20 oral communications, and 28 posters. I also perform peer-review services for Bioorg. Med. Chem., Appl. Organomet. Chem., Curr. Org. Chem., Org. Biomol. Chem., Organometallics, and Helv. Chim. Acta and my research and teaching activities have been accredited (Lecturer and Research accreditations) by the Catalan University Quality Assurance Agency (AQU). I am currently co-supervising 3 Ph.D. students, 1 Postdoc & 1 Master student. I have supervised in total 7 Master students and 10 last year undergraduates, summer, and Ph.D. visiting students (in 3 different institutions & 2 countries)



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Nombre: DEL BARRIO LASHERAS, JESUS

Referencia: RYC-2015-18471

Área Científica: Química

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Título:

Control Over Material Properties Through Light-Driven Molecular Switching

Resumen de la Memoria:

I am a polymer scientist with ample experience in organic and polymer synthesis, macromolecular self assembly, optical and dynamic stimuli-responsive materials and rheology. I aim to apply my scientific understanding to produce innovative ideas that can potentially be developed into practical technologies and solve societal problems. Following a Chemistry degree at the University of Zaragoza (Spain), I worked towards a PhD degree under the supervision of Dr. Luis Oriol (Department of Organic Chemistry) and Dr. Carlos Sánchez (Department of Condensed Matter Physics) from January 2006 to February 2010. Having two supervisors from different academic departments provided me with plenty of opportunities, invaluable skills and a truly interdisciplinary context to my PhD research. At Zaragoza I designed polymeric materials for optical technologies including azobenzene-containing side-chain and hydrogen-bonded homopolymers, dendrimers and block copolymers (BCs). I also investigated the transfer of chiral information from light to soft matter as well as the photoinduction of birefringence in polymeric thin films through a unique combination of techniques including linear and circular dichroism spectroscopy and a range of different light sources. One of my major achievements was the introduction into the area of photochromic polymers of the concept of linear-dendritic BCs and its self assembly. The unique linear-dendritic structure combines the perfectly branched architecture and high functionality degree of dendrimers with the phase separation behavior of traditional linear-linear BCs thus enabling access to functional BCs in a controlled and reproducible manner. At Zaragoza I also pioneered the area of polymer micellization in aqueous environment and investigated the self assembly of amphiphilic BCs into a wide range of micellar structures. The hydrophobic domains of these micelles are composed of isomerizable azobenzenes therefore cargo encapsulation and light-triggered release can readily be achieved. After finishing my PhD in 2010, I moved to the UK to work on aqueous self assembly, host-guest chemistry and supramolecular polymers with Dr. Oren Scherman at The University of Cambridge. As a postdoc, I significantly contributed to the expansion of cucurbituril (CB) host-guest complexation into polymer and materials chemistry by exploiting the fundamentals of aqueous self-assembly with complementary motifs. I devised a wide variety of noncovalent polymer constructs including supramolecular single-chain polymer nanoparticles, polymer-peptide and doubly-hydrophilic BCs which were applied to the stabilization of biologically active basic fibroblast growth factor, and the controlled encapsulation and release of insulin and the chemotherapeutic drug doxorubicin; and therefore significantly advanced the state of the art in the area of stimuli-responsive compartmentalized structures in aqueous media. At Cambridge, I also had the opportunity to marry the concepts of azobenzene isomerization with CB host-guest chemistry and apply them to develop light-controlled macromolecular self assembly and dynamic polymerization. In 2014 I joined the Schlumberger Gould Research Centre (Cambridge, UK) where I am leading projects aimed at developing innovative hydrogels and other polymer fluids with enhanced performance for the upstream oil and gas industry.

Resumen del Currículum Vitae:

I have ca. 10 years of active research experience in the fields of organic chemistry, polymer chemistry, supramolecular self assembly and photochemistry. In addition, training and carrying out academic and industrial research, both in Spain and the UK, allowed me to gain an international perspective, hone my scientific and communication skills, and develop international professional relationships which will be extremely helpful while returning to academic laboratories in my native country. My PhD research at the University of Zaragoza was in the area of light-responsive polymers and macromolecular self assembly with applications in optical and encapsulation technologies. At Zaragoza, I developed a variety of well-defined photochromic polymers and investigated the transfer of chirality from light to matter and the photoinduction of birefringence in polymeric thin films. I also pioneered research in the area of light-responsive block copolymer micelles for controlled release of encapsulated cargo. In recognition of my outstanding achievements and innovation, I was awarded the prize for the best PhD thesis in polymer science in 2010 (Grupo Especializado de Polímeros de las Reales Sociedades Españolas de Química y de Física). After finishing my PhD in 2010, I moved to the UK to work on supramolecular materials at the Department of Chemistry of The University of Cambridge. In 2011, I was awarded a Marie Curie Postdoctoral Fellowship to explore dynamic polymeric materials and had the opportunity to apply my PhD knowledge of photochromic polymers with supramolecular self assembly, to build a unique set of light-controlled hierarchically organized polymers in water. In addition, I was instrumental in the preparation of several major grant proposals, including a recently funded Marie Curie Initial Training Network, and the coordination of international projects. In 2014, I was selected from a large international pool of highly qualified applicants to be a Research Scientist at the Schlumberger Gould Research (SGR) Centre (Cambridge, UK), a world renowned R&D center devoted to original research into oil and gas exploration and production. At SGR, I am leading projects aimed at developing innovative fracturing systems and polymer fluids through fundamental understanding of aqueous macromolecular self assembly and dynamic hydrogels. The large number of articles that I have co-authored in leading journals and several oral contributions at international conferences are a testament of my scientific aptitude: I have co-authored one book chapter on supramolecular hydrogels and 33 publications [Chem. Rev. (1), Chem. Soc. Rev (1), J. Am. Chem. Soc. (3), Angew. Chem. Int. Ed. (2), Chem.



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Sci. (1), Chem. Mater. (1), Chem. Commun (2), Macromolecules (3) to name a few], two of them as corresponding author and 28 indexed in the top quartile of the subjects Chemistry and Polymer Science (Journal Citation Reports). My h-index is 15 and my publications have been cited 815 times (Web of Science). I have participated in 7 national and international projects, including one exchange program with the Tsinghua University (Beijing, China). Additionally, I have significantly contributed to the educational advancement of undergraduate and PhD students both at Zaragoza and Cambridge, where I served as supervisor for several courses and master projects.



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Nombre: GÓMEZ RAMOS, MARÍA JOSÉ
Referencia: RYC-2015-17959
Área Científica: Química
Correo Electrónico: m.gomezramos@uq.edu.au

Título:

Advanced mass spectrometry

Resumen de la Memoria:

My lines of research are analytical and environmental chemistry. During my PhD thesis and postdoctoral studies at IMDEA-Agua my work was mainly focused on developing and establishing innovative analytical methodology for the rapid and simultaneous analysis of hundreds of environmental contaminants and to identify nontarget hazardous contaminants, mainly in environmental matrices. This was an improvement of the analytical methods developed at that time, where only a relatively small number of known target environmental contaminants were included. Using such methods I was able to evaluate the fate and impact to the environment of a vast range of chemicals, including pharmaceuticals and personal care products, endocrine disruptor compounds, pesticides, dioxins, polycyclic aromatic hydrocarbons, bisphenols, and other industrial contaminants. I worked with a broad range of sample preparation techniques, instruments and software for analysis and in close collaboration with experts in advanced oxidation processes, ecology, toxicity, risk assessment and from industry. I made significant contributions in my field by pioneering the development of screening methods for the detection of nontarget contaminants in various environmental matrices, helping to identify potentially hazardous organic contaminants in surface water. I developed the first accurate-mass database for the automatic screening of emerging contaminants and their transformation products. I have also evaluated the risk of hazardous chemicals in recycled water. Many important contaminants and transformation products that were identified in my studies have not been previously reported. I contributed to the establishment of the first Spanish hazard ranking of contaminants in wastewaters. I contributed also to develop analytical methods to quantify contaminants in complex food matrices, substantially improving previous methods. Since joining the interdisciplinary group of Prof Mueller at Entox (UQ, Australia), I have had the opportunity to establish collaboration with senior scientists at Entox and researchers from other international groups and I have expanded the capabilities for analytical non-target analysis in the Centre, establishing and leading a new line of research. I have developed innovative research in biomonitoring analyses, developing improved analytical methods for the analysis of a broad range of polar and non-polar chemicals in biological matrices, and one of the first international methods for nontarget screening in biota and humans. I have developed an innovative strategy in the environmental field, adopted from the omics field, to identify hazardous unknown chemicals in biological samples. Applying this methodology we have discovered 4 novel per- and polyfluorinated alkyl substances in human blood, not previously reported in any chemical database. We have also identified new important biomarkers of exposure and effect in marine turtles from the Great Barrier Reef. In addition, I have developed new methods for the analysis of emerging contaminants in urine samples, using these methods, I have provided previously unavailable but much needed information on contaminant status in Australian populations. This information is being used by collaborating researchers from the medical field to link these exposures to adverse health outcomes.

Resumen del Currículum Vitae:

Following my degree in Chemistry in the University of Almeria, I joined the Prof Fernandez-Alba group in the Analytical Chemistry Department at the same university. In 2004 I was granted a FPI fellowship from the MCYT to conduct a PhD under the supervision of Prof Fernandez-Alba and Prof Ana Agüera. During my PhD I was involved in several Spanish projects and I carried out two pre-doctoral stays, a 5 months stay at the Instituto de Investigaciones Químicas y Ambientales de Barcelona (IIQAB), and a 6 months stay at the École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris. In 2008, I obtained my PhD at the University of Almeria, with *cum laude* distinction, for my study on determination of organic pollutants in wastewater and their environmental impact assessment. The quality of the research performed during my PhD was recognized by 9 publications, all of them are highly cited. Having finished my thesis I continued in the Prof Fernandez-Alba group carrying out postdoctoral research and coordinating the chemical analysis component of a CONSOLIDER project, awarded with the IWA prize 2010 for innovation in the practical realisation of sustainable urban water management. At the end of 2008 I was awarded a highly competitively Juan de la Cierva contract to work at the newly established Madrid Institute for Advanced Studies (IMDEA-Water). I was in charge of the newly installed instruments and staff. I was also supervising a PhD student and a Master student in addition to leading a project from the National Plan of the MICYT of Spain, from which I was Principal Investigator. Since August 2012, I have been employed as postdoctoral fellow at the National Research Centre for Environmental Toxicology, Entox (University of Queensland, UQ), where I have established my own and independent line of investigation based on developing innovative techniques for the non-targeted analysis of environmental pollutants in biological samples and in the environment. To conclude, along all these years of the scientific path, my work has been published in 47 peer-reviewed journal publications in high tier journals (37 of which I was between the first 3 authors or as senior author) and I have another 3 publications as senior author currently under preparation. I have also contributed on two invited chapters to prestigious scholarly book series. Jointly, these publications have been cited more than 2516 times, with an average of about 54 citations per article, leading to an H-index of 24. I have contributed to 58 presentations (28 oral and 30 poster presentations) in International and National Conferences and Workshops. I was invited to deliver oral presentations (fully funded) in 2 international and 1 national meetings. Three of my poster presentations received awards. I have actively contributed to the design and



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execution of 15 research projects and 9 research contracts, usually involving interdisciplinary research collaboration. I was principal investigator of a national project and one of the chief investigators of 3 Australian projects and 2 Australian contracts. I have co-directed 1 PhD thesis, 1 MSc thesis and I am currently supervising another 2 PhD theses at the UQ. I am a regular reviewer for the top journals, including Water Research, Analytical Chemistry, Journal of Chromatography A, Science of the Total Environment, Chemosphere.



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Nombre: VAYÁ PÉREZ, IGNACIO
Referencia: RYC-2015-17737
Área Científica: Química
Correo Electrónico: igvapre@qim.upv.es

Título:

Functionalisation of photoactive hybrid metal nanoparticles with drugs and specifically biological targets for their use in biomedical applications

Resumen de la Memoria:

Dr. Ignacio Vayá started his research career the last year of his higher studies as an Erasmus student to carry out the final project degree at the University of Leiden. He started his PhD at the Department of Chemistry/Institute of Chemical Technology (DQ-ITQ) at the UPV. His research was focused on the investigation of the specific interactions between drugs and proteins by means of spectroscopic techniques such as fluorescence (steady state and time-resolved) and laser flash photolysis. To this aim, a number of model systems composed of a drug covalently linked to an amino acid were first designed following different organic synthetic routes. Special emphasis was provided on chiral recognition in the excited states, photo-induced hydrogen and electron transfer as well as in the study of photosensitised processes. The real drug/protein interactions were also investigated by means of the laser flash photolysis technique, where a novel methodology was first developed to get key information about strength of binding, selective occupation of the binding sites by the drug, etc. This approach became as a general tool to study this type of complexes. In 2006, Dr. Vayá joined Prof. Olivucci's research group (Italy) with the aid of grant from MEC as a pre-doctoral visitor to work in the field of computational chemistry. In September 2008, he moved to the Laboratoire Francis Perrin (France) as a postdoctoral researcher. During this period, he improved his expertise in spectroscopy by using ultrafast techniques. His research was focused on the photoreactivity of natural DNA and DNA model helices as well as G-quadruplexes under different environments and conditions. His investigations aided to give a more detailed view of the complex deactivation pathways arising from excited DNA systems; herein, the role play by high energy emitting long-lived mixed states was proposed, their involvement being supported by theoretical calculations. In April 2012, Dr. Vayá was awarded with a JdC contract and joined the DQ-ITQ at the UPV. He was given the freedom to initiate his own research line on the biological consequences of the photoinduced processes occurring in drug/biomolecule systems (photoallergy, phototoxicity, etc.). In this context, he supervised the research project (TFM and TFG) of two students. One of the collaborations he strengthen with Prof. Markovitsi gave him the opportunity to design a project (funded by the EU) that aimed to investigate the primary processes, such as electron or energy transfer, occurring between photo-excited drugs and proteins by femtosecond fluorescence upconversion spectroscopy, resulting in the publication of several papers in high impact journals. With the aim of expanding his multidisciplinary formation and with the purpose of seeking a technological application of the expertise acquired along his research career, Dr. Vayá designed a new project about the synthesis of photoactive multi-functionalised metal nanoparticles for their use in biomedical applications. He got funding from the EU and moved to the University of East Anglia (UK) as a MSC-IF researcher. The main objective is the design and investigation of the photoreactivity of the new metal nanomaterials under biological conditions and perform intracellular studies to explore their use for photodynamic or photothermal therapies, as biosensors, etc.

Resumen del Currículum Vitae:

Dr. Ignacio Vayá started his research career the last year of his higher studies, carrying out the final project degree at the University of Leiden (Erasmus student). He was awarded with several fellowships, among them the FPU to develop his PhD at the Universitat Politècnica de València (UPV). His research aimed to investigate the photoreactivity of drug/biomolecule models and the real complexes by means of spectroscopic techniques. One of the main achievements was the development of a novel methodology to study the photoreactivity of drug/protein complexes by the laser flash photolysis technique. In 2006, Dr. Vayá joined Prof. Olivucci's research group (Italy) with the aid of grant from MEC as a pre-doctoral visitor to work in the field of computational chemistry. He earned his PhD in Chemistry (European Doctorate) in November 2007 with the highest mark. In September 2008, Dr. Vayá moved to the Laboratoire Francis Perrin (France) as a postdoctoral researcher funded by an international project supported by the French National Research Agency and continued as a laureate of the most prestigious postdoctoral grant from the Generalitat Valenciana (GV, VALi+D program). He focused his interests in the photoreactivity of natural DNA and DNA model helices as well as G-quadruplexes in different media and conditions. One of the main goals of his investigations was the proposal that the deactivation pathways of the emitting states of DNA model helices can arise from excited states higher in energy and longer-lived than those of the monomeric units. This effect was also observed in natural DNA, which may have implications in its photoreactivity and therefore in its damage. Another important outcome of his research was the prove that pairing of bases in models composed of adenine and thymine enhances the fluorescence of base pairs upon irradiation with UVA light, which also favours the formation of cyclobutane pyrimidine dimers, the main photochemical products responsible for the DNA damage. In April 2012, Dr. Vayá was awarded with a Juan de la Cierva contract and joined the DQ-ITQ at the UPV. He was given the freedom to independently design various research projects aiming to study the photoreactivity of drugs in the presence of biomolecules. Indeed, he obtained financial support to develop his own research line as Principal Investigator (PI) from the European Union (Marie Curie CIG) and from national institutions (GV, Proyectos Emergentes; and UPV, Primeros Proyectos). Besides, he also obtained funding from a European SLIC



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project to continue his collaboration with Prof. Markovitsi. In May 2015, Dr. Vayá was awarded by the EU as a Marie Skłodowska-Curie IF researcher and moved to the University of East Anglia (UEA) to expand his research experience in the field of functionalised metal nanoparticles for their use in biomedical applications. He has published among 31 peer-reviewed articles in high impact journals and he has been invited to international conferences and seminars. Dr. Vayá has supervised the research projects of students, being the co-director of a TFM project and of a TFG of an Erasmus student, in addition of leading the laboratory work trainees. He has also been recognised by ANECA as a researcher professor, assistant professor and private University professor.



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Nombre: ROCA SANJUÁN, DANIEL

Referencia: RYC-2015-19234

Área Científica: Química

Correo Electrónico: daniel.roca@uv.es

Título:

Computational Photochemistry and Chemiluminescence of Molecules of Interest in Biology and Technology

Resumen de la Memoria:

The main research line carried out by Dr. Daniel Roca-Sanjuán corresponds to the Computational Photochemistry and Chemiluminescence of Molecules of Interest in Biology and Technology. During the last five years, the candidate has extended his PhD studies on the UV-induced chemistry of the DNA/RNA nucleobases to the reactivity with reactive oxygen species and free radicals and the modeling of more complex nucleic acid systems, including whole DNA/RNA double strands. He has also coordinated a new and promising line of research aimed to study the interaction between photosensitizers and DNA/RNA and to accurately determine the chemical mechanisms of photodynamic therapy by means of the tools of Computational Photochemistry. Moreover, the candidate has continued with the postdoc research on chemi- and bioluminescence and has extended it to works aimed to exploit the synergy between the photochemical and chemiluminescent phenomena. The training acquired in his doctoral and postdoc research provides Dr. Roca-Sanjuán with optimal knowledge to carry out high-impact studies which shall help to increase the efficiency of the conventional techniques of photodynamic therapy and to discover new ones based on chemiluminescence principles.

Resumen del Currículum Vitae:

Dr. Roca-Sanjuán has a great potential to carry out high-quality and high-impact research as demonstrated in his CV. Thus, he has produced 46 articles in international peer-reviewed SCI journals, 5 more to be published soon (15 with IF>5 and 22 % as first author). In addition, he contributed with 5 book chapters. His skills as coordinator of research and the ability to produce independent research are also remarkable for a researcher at his career stage. Thus, he is corresponding author of 39% of the articles and 47% of works have been carried out independently without his PhD supervisors. Dr. Roca-Sanjuán participated in congresses/symposiums/workshops as author or co-author with 63 conferences, oral communications and posters. He was invited speaker in 2 congresses and to give 5 invited conferences/seminars at European universities plus one-week course at an international university. This potential of the candidate has been supported by the Spanish MINECO through the FPU predoctoral fellowship and the Juan de la Cierva postdoc fellowship, by the European Commission through the Marie Curie postdoc fellowship, by the Generalitat Valenciana through the project GV2015-057 in which he was PI, and recently also by the Spanish MINECO through the project CTQ2014-58624-P in which he is PI. He has been involved in a total amount of 15 funded research projects.

Finally, Dr. Roca-Sanjuán has acquired a great experience teaching and supervising master and PhD students. He participates as local tutor at the Universitat de València in the EM-TCCM master program and the IJD-TCCM doctorate program funded by the European Commission. The candidate has supervised 3 doctoral theses, 1 more to be defended shortly, another ongoing, and 5 EM-TCCM master theses. He has been examiner of 6 Doctoral Theses, 6 EM-TCCM Master Theses, and 2 national proposals of research projects. Dr. Roca-Sanjuán has participated as reviewer in 14 distinct journals.



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Nombre: FERNÁNDEZ TEJADA, ALBERTO
Referencia: RYC-2015-17888
Área Científica: Química
Correo Electrónico: alberto.fernandezt@gmail.com

Título:

Synthesis and Conformational Analysis of Glycopeptides Incorporating Unnatural Amino Acids & Development of Synthetic Saponin Vaccine Adjuvants and Carbohydrate/glycopeptide-based Vaccines

Resumen de la Memoria:

My research experience and interests are at the interface of chemistry and biology, applying chemical tools and advancing organic synthesis to address important biological problems, always under the broad headings of carbohydrate and peptide chemistry. Initially, I enjoyed two undergraduate research fellowships in Biochemistry/Molecular Biology & Organic Chemistry, respectively. My PhD research at the University of La Rioja, mentored by Profs. Jesús M Peregrina & F Corzana, focused on the synthesis and conformational analysis of diverse O-glycopeptides to study the influence of glycosylation and the incorporation of unnatural amino acids on the conformational properties of the corresponding peptide. Beyond gaining insights into the complex interplay between peptide and glyco domains underlying important biological processes, my PhD work also offered potential applications towards glycopeptide-based drug design by enabling access to glycopeptide systems with tailored conformational preferences.

The research line that I led during my first postdoctoral experience in the group of the late Prof. David Gin at Memorial Sloan Kettering Cancer Center has brought the power of high-level organic synthesis to the saponin adjuvant field for the first time. I took the lead in this project and in collaboration with immunologists and clinicians, I established detailed structure-activity relationships of QS-21 and identified of novel, synthetically accessible saponin variants with improved activity/toxicity profiles for potential clinical exploitation. In addition, I have developed the first saponin chemical probes for early mechanistic studies of these synthetic adjuvants, which will constitute my main research goal in the medium-term together with the development of novel, more effective subunit antigen vaccines based on such saponin adjuvants.

Continuing with my focus on medicinal/biological chemistry and the vaccine field, in my second postdoctoral stage in the laboratory of Prof. Danishefsky, I exploited the power of chemistry for the total synthesis of biologic-level structures such as homogeneous glycoproteins and fully synthetic, glycopeptide-based vaccines against cancer and HIV. Besides further honing my chemical synthesis skills contributing new advances to organic chemistry, key interdisciplinary collaborations at MSKCC for the biological evaluation of these molecules have provided me sound knowledge and experience in the immunological/biological arena that will be applied in my future multidisciplinary research. This work resulted in a fruitful collaboration with a biotechnology company towards the development of human monoclonal antibodies using my synthetic molecules. In the return phase of my Marie Curie Fellowship in the group of Prof. Jiménez-Barbero (CIB-CSIC & CIC-bioGUNE), I carried out the conformational analysis of the saponin variants synthesized at MSKCC, providing a molecular rationale and key correlations between three-dimensional structure and adjuvant activity.

To expand further my scientific repertoire, I am now working in the group of Prof. Ben Davis (University of Oxford) on a chemical-biology project that uses enzymatic approaches and bioorthogonal chemistry to explore and unravel the molecular basis underlying the beta-O-GlcNAc glycosylation of proteins, a key medicinally-relevant posttranslational modification.

Resumen del Currículum Vitae:

I graduated in 2004 from the University of La Rioja (B Sc in Chemistry with Distinction & Honors), where I carried out my graduate research with a MEC-FPU fellowship on the synthesis and conformational analysis of natural and unnatural peptides and O-glycopeptides, mentored by Profs. JM Peregrina & F Corzana. In 2008, I spent 4 months at Memorial Sloan Kettering Cancer Center (MSKCC, USA) working on the synthesis of complex saponin immunostimulants under the guidance of Prof. David Gin. After obtaining my PhD (Cum Laude) in 2009 at the University of La Rioja, I carried out a brief postdoctoral stay on the synthesis of biomimetic molecular machines with Profs. PJ Campos & D Sampedro.

In 2010, I returned to MSKCC for postdoctoral studies in the laboratory of the late Prof. Gin with a MEC-Fulbright fellowship, working independently and leading my research on the development of improved saponin vaccine adjuvants. This research line has become my main scientific interest and will be a significant part of my research portfolio with the goal of developing novel, saponin-based subunit antigen vaccines and unraveling the mechanism of action of saponin adjuvants. In 2012, I moved to the Danishefsky laboratory (MSKCC) as a Marie Curie International Outgoing fellow (MC-IOF) to work on the total synthesis of complex homogeneous glycoproteins and carbohydrate/glycopeptide-based vaccines. In all these multidisciplinary projects at MSKCC, I participated actively in the immunological evaluation of these therapeutically important molecules, gaining key knowledge in the biological arena that will be highly beneficial in my future interdisciplinary research. In 2014, I returned to Spain for the reintegration phase of my MC-IOF to work with Prof. Jiménez-Barbero (CIB-CSIC & CIC-bioGUNE) on the conformational analysis of the saponin adjuvants synthesized at MSKCC, further improving my skills in NMR and molecular modeling. Since 2015, I am working in the group of Prof. Ben Davis (University of Oxford) with another Marie Curie Fellowship (MC-IEF) on the development of novel chemoenzymatic approaches to probing protein O-GlcNAc glycosylation. Thus, my research interests and experience are at the interface of chemistry, immunology and biology, and the main research line that I will be



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pursuing in my career is in the field of chemical immunology and chemical glycobiology, developing chemical tools to address long-standing immunological/biological questions, such as the enigmatic mechanism of saponin immunopotentialiation.

As a result of my +10-year research career, I have a proven track-record of oral communications in international symposiums (8 in the last four years) and 20 publications in top journals (11 in the last two years, including 2 book chapters and 3 review articles) plus 1 submitted and 3 in preparation. Of these, 13 are as first-author (notably, 9 without my PhD advisor, and 7 as corresponding author), standing out 1 Nature Chem, 1 J Am Chem Soc, 1 Chem Commun and 1 Chem Eur J (see section 6 of the CVN for details). My research has resulted in 4 patents/patent applications and has been greatly disseminated by the press (newspapers, radio and television). I have been awarded the SusChem Divulga & Postdoc Awards (3rd place) and obtained the CAP Certificate from the University of La Rioja as well as the Profesor Ayudante Doctor qualification by ANECA.



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Turno de acceso general

Nombre: FRATILA , RALUCA MARIA

Referencia: RYC-2015-17640

Área Científica: Química

Correo Electrónico: rmfratila@gmail.com

Título:

Bioorganic chemistry and multifunctional nanomaterials for biomedical applications

Resumen de la Memoria:

During my research career I built a unique, multidisciplinary expertise in (bio)organic and bioconjugate chemistry, NMR spectroscopy/imaging and nanotechnology, my competence spanning different fields allowing me to set up my current research line on multifunctional nanomaterials for biomedical applications.

PhD (2001-05): My PhD thesis involved experimental, computational and NMR studies of the asymmetric reduction of carbonyl compounds with NADH peptidomimetics, establishing for the first time the structural characteristics of the ternary complexes NADH/Mg²⁺/substrate and the transition states thereof. My PhD thesis obtained the highest distinction awarded by the University Politehnica Bucuresti.

2006-08: My main research line during this first postdoctoral period (Prof. J. M. Aizpurua, Universidad del Pais Vasco) consisted in the development of a new click synthetic strategy to obtain unsymmetrically disubstituted bistriazoles. Additionally, I actively participated in different projects involving the functionalization of carbon nanotubes and polymers for biomedical applications, as well as the use of click chemistry to obtain surfaces with antibiotic properties.

2009-13: In my first postdoctoral stay at University of Twente (The Netherlands) I worked in the group of Prof. David Reinhoudt and Dr. Aldrik Velders on a challenging \blacklozenge NMR-on-a-chip \blacklozenge project focused on the development of small-volume NMR probes for integration with microfluidic devices. During my second post-doc in Twente I expanded my research interests towards biomedical applications of nanomaterials, therefore starting to build up my current research. At the NeuroIMaging group (Prof. Bennie ten Haken) I worked on the use of magnetic nanoparticles (MNPs) as contrast agents for magnetic resonance/multimodal imaging applications.

2013-current: In November 2013 I was awarded a Marie Curie COFUND-ARAID research position at the Institute of Nanoscience of Aragon (group of Dr. Jesus Martinez de la Fuente) to carry on my project on the development of novel high aspect ratio magnetic nanomaterials as multifunctional nanoplatforams for imaging and therapy. This project opened a new research line at the host group, based on my previous experience in (bio)organic/bioconjugate chemistry and magnetic resonance imaging (MRI) using MNPs. This expertise allowed me to successfully participate in other research projects at the host group, such as the synthesis and functionalization of MNPs for combined magnetic hyperthermia-drug delivery applications. In parallel, I developed new skills in the area of synthesis and characterization of nanomaterials and their interaction with living systems (in particular transmission electron microscopy -TEM- and cell culture); this allowed me to initiate several collaborations in the field of TEM characterization of nanomaterials. In 2014 I established another new research line at the host group, based on my previous expertise in click chemistry: the use of bioorthogonal click chemistry for the covalent immobilization of MNPs on cell membranes for mild magnetic hyperthermia applications. Noteworthy, for this research I was first awarded a research grant for young researchers from University of Zaragoza and then a prestigious Marie Skłodowska Curie IE fellowship.

Resumen del Currículum Vitae:

I received my Chemical Engineer (2000) and MSc in Advanced Chemistry (2001) degrees from the University \blacklozenge Politehnica \blacklozenge Bucharest (UPB), Romania. I obtained my PhD in Chemistry (2005) with the highest distinction awarded by the UPB for my thesis on the biomimetic reduction of carbonyl compounds with NADH peptidomimetics. I carried out part of my doctoral research at the University of the Basque Country (UPV-EHU), San Sebastián, Spain, with a MARIE CURIE RTN5 individual fellowship (2002-03, Prof. C. Palomo and Prof. J. M. Aizpurua). Then I conducted several postdoctoral stays at the UPV-EHU (2006-08, Organic Chemistry Department, Prof. J. M. Aizpurua) and the University of Twente, The Netherlands (2009-11, MESA+ Institute for Nanotechnology, Prof. A. Velders and 2011-13 at the MIRA Institute for Biomedical Technology and Technical Medicine, Prof. B. ten Haken). In 2013, I was awarded a MARIE CURIE FP7 COFUND - ARAID research grant for my project on novel multifunctional magnetic nanoplatforams for biomedical applications to be developed at the Nanotherapy and Apoptosis group (Dr. J. M. de la Fuente), Institute of Nanoscience of Aragón (INA), University of Zaragoza. In 2014 I established another novel research line at the host group, focused on the use of bioorthogonal click chemistry in nanotechnology, for which I obtained a MARIE SKŁODOWSKA-CURIE fellowship (2015-17). I am also involved in the research carried out in the frame of the ERC Starting Grant project NANOPUZZLE (PI J. M. de la Fuente), developing novel magnetic nanomaterials for controlled drug release using magnetic hyperthermia.

I consider myself an ambitious, creative and curiosity-driven researcher with a multidisciplinary research expertise in bioorganic, surface and bioconjugate chemistry, NMR spectroscopy, magnetic resonance imaging and nanotechnology. During my postdoctoral stays in different research environments, I developed strong interpersonal, organizational and research management skills. To the date, I have published 32 peer-reviewed scientific papers and one book chapter (h index of 10, 5 as corresponding author, one highlighted on the cover of Langmuir, 2014) in multidisciplinary and specialized journals with impact factors above the average impact factor of the respective field. These include top-10 journals in the areas of Organic Chemistry (Org. Lett., J. Org. Chem.), Medicinal Chemistry (ChemBioChem), and General Chemistry (Nat. Commun., Angew. Chem. Int. Edit., J. Am. Chem. Soc., Nanoscale). I have more than 50 contributions at national



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and international conferences and I am co-inventor of a Dutch and an international (PCT) patent derived from my postdoctoral research on the topic of small-volume NMR spectroscopy. I am currently involved in the process of setting up the spin-off company XtraSpin BV, aiming at developing universal, magnetic field-independent NMR microprobes. I am a member of the Spanish Royal Chemical Society (RSEQ, including its Young Researchers Division), Dutch Royal Chemical Society (KNCV), the Royal Society of Chemistry (RSC) and American Chemical Society (ACS) and I have been referee for various journals. I supervised a total of 14 students (3 PhD, 6 MSc and 5 BSc) and I carried out teaching both at BSc and MSc level (practical chemistry courses at UPB and Biomedical Engineering Master courses at UNIZAR).



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Nombre: JURADO SÁNCHEZ, BEATRIZ

Referencia: RYC-2015-17558

Área Científica: Química

Correo Electrónico: beatriz.jurado@uah.es

Título:

Artificial nano/micromotors for analytical, environmental and biomedical applications

Resumen de la Memoria:

The research trajectory of Dr. Jurado can be divided in three different parts: i) PhD student and postdoc at the University of Córdoba, ii) post-doc (Marie Curie fellow) at the University of California-San Diego and iii) senior post-doc (Marie Curie fellow) at the University of Alcalá. The candidate have a highly interdisciplinary profile in very hot nanotechnology topics.

Since 2013, the candidate research line focused on the design of artificial nano/micromotors for lab-on-a-chip, sensing, environmental and biomedical applications. During 24 months, Dr. Jurado worked as a postdoctoral researcher at the University of California-San Diego with a Marie Curie IOF fellowship. She reported on a fundamental study about the enhanced transport and fluid mixing imparted by the movement of tubular micromotors, catalytic nanowires and Janus particles. This study will have important implications for the manipulation of fluids and mixing of reagents in situations where mechanical stirring is not possible (LOC formats). She also developed different Janus micromotors by sputter deposition of a catalytic layer (Pt or Ag) onto high-active surface particles (activated carbon, zeolite and magnesium). Such motors offer considerable promise for environmental remediation applications. Dr. Jurado also contributed to the development of a new sensing silver protocol based on the motion of metallic nanowires, including both numerical and experimental simulations. Tubular microengines composed entirely by one of the cutting edge nanomaterials, graphene, were also synthesized for the first time. Dr. Jurado worked actively on the development of the first biomimetic motors, prepared by the incorporation of red-blood cell particles on the surface of ultrasound-propelled Au nanowires. Such motor sponges connect artificial nanomotors with biological entities and hold great promise for bacteria isolation and detoxification applications. The applicant also reported, for the first time, the incorporation of quantum-dots in the surface of template-prepared microengines. The potential of such tiny "microsensor" has been proved for on-chip multiplexed detection of mercury and bacteria in biological samples. The dynamic movement of the microsensors through the microchip reservoirs avoid the use of pumps to move fluids, allowing further miniaturization and reducing the volume of sample required for the analysis.

In august 2015, the candidate joined Prof. Escarpa group at the University of Alcalá as a part of the return phase of her Marie Curie IOF. Dr. Jurado started a new research line, focused on the development of new nanomachine-based analytical strategies for the isolation and detection of biological threats in foodstuffs. She is also interested in the development of new lab-on-a-chip devices integrating self-propelled micromachines for rare cell isolation and analysis in complex biological samples.

Resumen del Currículum Vitae:

Beatriz Jurado Sánchez obtained her B.S. in Chemistry at the University of Jaén (2004) and her PhD in Analytical Chemistry at the University of Córdoba (2009) under the supervision of Prof. Mercedes Gallego. During her PhD period her research line focused on the development novel strategies for the control of amines and N-nitrosamines in water, food and biological samples. In 2013 she was awarded with a Marie Curie IOF fellowship (success rate <13%) to carry out research at the University of California-San Diego with Prof. Joseph Wang (pioneer in the field of artificial micromachines). She acquired a strong background in artificial micromachines, showing its applicability to design new lab-on-a-chips and for environmental remediation applications. The candidate also become an expertise in cutting edge microfabrication and characterization techniques including scanning electron microscopy, sputtering, e-beam and atomic layer deposition and PDMS microchip fabrication using soft lithography. In 2015 Dr. Jurado moved to Dr. Escarpa group at the University of Alcalá to pioneer a new nanomotors research line with promising applications in the biomedical and analytical fields.

The relevance of Dr. Jurado work is testified in the publication of over 30 scientific papers in top peer-review multidisciplinary chemical journals (h index, 14), 2 book chapters and 20 international communications in national and international conferences. The publications include 1 ACS Nano, 2 Advanced Functional Materials, 2 Small, 1 Nanoscale, 1 Chemical Communications and 1 Langmuir. Some of these publications have been highlighted in many media such Separations Now (Wiley), JSTO in the News, BBC News, Nanowerk and Science Daily. She is also co-inventor of a nanomotor-related patent application and is currently co-advising 1 PhD student, one master student and supervising one end-of-degree chemistry student. She has also participated in 12 funded projects with several researchers from the University of Córdoba, University of California-San Diego, University of Alcalá, University of Tetouan and University of Jaén. She has been recently awarded (as PI) by the Spanish Ministry of Economy and Competitiveness with a highly competitive grant for the preparation of an ERC Starting Grant (Acciones de Dinamización Europa Investigación). She has established many international collaborations with renowned international scientist (Prof. Joseph Wang, University of California, San Diego, Dr. Wei Gao, Department of Electrical Engineering & Computer Sciences, University of California, Berkeley, Prof. Zhiguang Wu, Harbin Institute of Technology, China, Prof. Deniz Aktas, Department of Biochemistry, Adnan Menderes University, Turkey). Since 2010 she acts as referee in several scientific journals such as Talanta, Analytical and Bioanalytical Chemistry, Journal of Agricultural and Food Chemistry, Microchimica Acta, Sensors and Actuators: B,



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Turno de acceso general

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Área Científica: Química

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Trayectoria Garcia Rodriguez

Resumen de la Memoria:

I define myself as a curious synthetic inorganic chemist with a broad interdisciplinary background. I have already worked in four different research groups in three different countries. As a result, my research experience has covered some of the key themes of inorganic chemistry, including multidisciplinary areas: organo-transition metal chemistry, main group chemistry, bio-inorganic chemistry and inorganic nanomaterials. I have also had the opportunity to experience very different research cultures, in the USA and in Europe.

My PhD work in the group of Prof Daniel Miguel was focused on the synthesis, characterization, and reactivity of complexes with N and O donor ligands of metals of groups 6 and 7, mainly. In the six-month interim between the defence of my PhD, which was awarded **Premio Extraordinario de Tesis Doctoral**, and the commencement of my postdoctoral position at the University of Pittsburgh (USA), I participated in an academic-industrial collaboration between Scientific Park (University of Valladolid) and Renault España S.A., conducting studies of corrosion on metal parts.

I worked as a postdoctoral researcher in the group of Prof Haitao Liu (2010-2013) at the University of Pittsburgh (USA) investigating the reaction mechanisms of the synthesis of group II-VI semiconductor nanocrystals. Although my work has been focused mainly on the investigation of the mechanism and kinetics of syntheses of cadmium chalcogenide NCs, especially CdSe, I also have studied other systems such as zinc and lead chalcogenide that share similar precursors and synthetic approaches. Some specific topics which I have explored include: identification of reaction intermediates (see, Garcia-Rodriguez, R. and Liu, H. J. Am. Chem. Soc. 2012, 134, 1400), study of solution structure of metal precursors used in NCs synthesis (see Garcia-Rodriguez, R and Liu, H. Chem. Commun. 2013, 49, 7857), stoichiometry, thermodynamics and kinetics of precursor binding (Garcia-Rodriguez, R. and Liu, H. J. Phys. Chem. A 2014 118, 7314.) and mechanistic studies of the role of additives in the nanocrystal synthesis (see, Garcia-Rodriguez, R. and Liu, H. J. Am. Chem. Soc. 2012, 134, 1400)

In October 2013 I began to work as a postdoctoral researcher in the group of Prof Dominic Wright, a world-leader in the area of metal- and nonmetal based ligand systems, at the University of Cambridge. This position was initially supported by a Marie Curie Intra-European Fellowship.

At the University of Cambridge, my main project has been focused on the synthesis and characterization of main group metal and semimetal-based tris-pyridyl ligands of the type $[E(py)_3]_n^-$ (E=main group atom or group, py=pyridyl), the study of their coordination and catalytic properties and the mechanisms of these reactions. I have also been involved in several other projects including: phosphorus bridged tris-pyridyl ligands, phosphazene chemistry and investigation of main group catalysed dehydrocoupling reactions.

This has given me the opportunity to establish collaborations with Lutz Gade (University of Heidelberg), Evamarie Hey-Hawkins (University of Leipzig), Marta E. G. Mosquera (Universidad de Alcalá), Jonathan Owen (Columbia University), Haitao Liu (University of Pittsburgh) and Brandi M. Cossairt (University of Washington), in addition to my PhD advisors in Spain.

Resumen del Currículum Vitae:

I completed my Bachelor's Degree in Chemistry (2004, average mark 2.7/4) and my PhD (2010 **Premio Extraordinario de Tesis Doctoral**) at the University of Valladolid in Prof Daniel Miguel's group. My doctoral studies were funded by a FPU fellowship and supplemented with a short stay in the group of David Leigh at the University of Edinburgh, a world-leader in organic chemistry. I also participated in an academic-industrial collaboration between Scientific Park (University of Valladolid) and Renault España S.A.

I was a postdoctoral researcher in the University of Pittsburgh (USA, 2010-2013) in the group of Prof Haitao Liu. There I studied the reaction mechanisms of the synthesis of group II-VI semiconductor nanocrystals. In this newly established group, we had to set up the lab from scratch. Despite not having previous experience in the materials field, I identified a research area suited to my organometallic background and expertise and developed several projects (see for instance, Garcia-Rodriguez, R and Liu, H. J. Am. Chem. Soc. 2012, 134, 1400 and Garcia-Rodriguez, R and Liu, H. J. Am. Chem. Soc. 2014, 136, 1968).

Since Oct 2013, I am a research associate at the University of Cambridge in the group of Prof Dominic Wright, a world-leader in the area of metal and nonmetal based ligand systems. I am also teaching and lecturing about 70 hours per year since 2014, and in addition acting as senior demonstrator. Notably, I developed the doctorate subject "New Directions in Metal and Non-Metal Catalysis": I created all original teaching content of the course and the course notes and delivered the course lectures. So far I have supervised a large number of students in Spain, the US, and the UK at different levels: PhD (6), Masters/final year (5) and undergraduate (6). I am also currently co-directing 2 PhD students, and I have obtained positive evaluation by ANECA for Profesor de Universidad Privada, Ayudante Doctor and Contratado Doctor.

My two postdoctoral research positions have been supported by very competitive fellowships: Ramón Areces and Marie Curie Intra-European. My research work has been presented at more than 24 international/national conferences including 3 oral presentations at ACS meetings, and I have acted as chair in an international conference. I have published 30 research articles, 4 as corresponding author, in high-



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impact peer-reviewed journals: J. Am. Chem. Soc. (2), Chem. Commun. (4, one featured as inside front cover), Chem. Mater. (1), Chem. Eur. J. (2), Inorg. Chem. (2), J. Phys. Chem. A (1) Dalton Trans. (14, one featured as inside front cover), Eur. J. Inorg. Chem (1) J. Organomet. Chem. (2) and Organometallics (1).