



Turno de acceso general

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Título:

Innovative Chemistry for Electrochemical Energy Storage (InnoChEES)

Resumen de la Memoria:

My research career has been linked to the development of Innovative Chemistries and Nanomaterials for Energy applications, and the implementation of Advanced Characterization tools such as in situ ssNMR.

As undergraduate, in 2002 at Univ. Complutense (UCM)+Univ. Kent (UK) as Erasmus I did a Final year project on synthesis of silica nanotubes functionalized with gold nanoparticles. In 2003 at ICMM-CSIC: synthesis and characterization of silica and polymer Nanospheres for photonic crystals (PRB, JAP). I did my PhD thesis at UCM (2003-2008). I synthesised new oxides via high-pressure and characterized them by XRD, Transmission electron microscopy, Magnetism and Resistivity measurements (JACS, InorgCh, JSSChx4, SolidStateSc). I visited CSEC, Univ. Edinburgh (UK, 2005) for Neutron diffraction studies (JSSCh) and the Lab. Crystallography, Bayreuth (Germany, 2006) for 4D superspace group analysis on single crystals of the first Sr-Cr-O misfit layer (JSSCh).

I have held 3 postdoctoral positions:

First during 2008-2010 at NanoTech Institute-Univ. Texas at Dallas (USA), where I developed: (i) novel cyclic diacetylenes for the rational chemical synthesis of carbon nanotubes by solid-state polymerization (ii) Industry: polydiacetylene co-crystallization for time-temperature indicators. (WO2010/114752) (iii) Biscrolled CNT yarns for energy applications (First μ -size CNT biscrolled Li-ion battery, WO2011/005375 A2+A3, Science) (iv) Graphene and graphene nanoribbons for energy conversion and storage. (AdvMat, JPhCh-Cx2, JMatCh-A).

Second during 2011-2015 CIC EnergiGUNE (Spain). I spent one year (2011) in the Dpt. of Chemistry at Univ. Cambridge, where I studied the mechanisms of intercalation and displacement reactions in Li-ion battery electrodes by in-situ XRD and ssNMR. After that, at CIC I was acting as co-PI of the Na-ion battery efforts, I focused on searching for new anode chemistries (EnergyEnvironSci (EES), AdvEnergyMat, JMatCh-A, ACS-Mat&Interf, MRB), especially based on Carbon-Nitrogen functionalities: Schiff-Bases (AngewChem, EES., ChemSusChem), Prussian blue (EP163826183, JPSx2, EchemActax2, 1book), Carbodiimides (JMCh-A, JPS, MRS) being thesis director of 3 PhD students (2016-2017). In 2015 I visited Warsaw Univ. chemical compatibility of anodes with novel electrolytes. Also found new active organic electrolytes for redox flow batteries (WO2016/156451, EES).

Third, 2016-2018 at the Dpt. of Chemistry Cambridge Univ., working in several projects: (i) understanding the chemistry of wet Li-air batteries (Sciencex2), (ii) novel MOFs (JACS) (iii) supervising a PhD on Si anodes (JACSx2) (iv) managing projects (AMorpheuS, CAM-IES). In 2017 I got a highly competitive Marie Curie Fellowship that allowed me to supervise students and be the PI on the Search of New chemistries (MOFs, COFs, and new inorganics phases) for Energy Storage and Understanding their mechanisms of reaction via XRD and ssNMR.

Assistant professor at UCM since sept 2018 (PI of a challenges proposal on Potassium ion batteries under evaluation), my previous experience has given me capacity to carry out independent research, attract funding and international networking (92 months abroad) needed to lead my research line: Innovative Chemistries for Electrochemical Energy Storage that embraces novel chemistry from inorganic to organic chemistry and nanotechnology.

Resumen del Currículum Vitae:

My track record includes 52 high quality publications (Sciencex3, EnergyEnvironScix3 (IF. 29.5), Adv.Mat, AdvEnergyMat, JACSx5, AngewChem, JPSx5, JSSChx4) being corresponding author in 11 of them, with >2150 citations (h-index 21) and a book with 5 chapters. I¿m co-inventor of 4 world patents, 2 being exploited and 1st inventor in one result of collaborative work with industry. I¿ve participated in national and international conferences, given 4 invited talks, and contributed with 42 oral presentations, 39 posters & 5 proceedings.

I had a high level of international mobility (92 months). Undergraduate: Erasmus fellow in Kent Univ. (UK, 2002, 9 months). During my PhD at Univ. Complutense I was awarded a FPI + 2 mobility grants: (i) Prof. Attfield¿s group at CSEC (UK, 2005, 3 months)) for refinement of neutron diffraction data (ii) Prof. van Smaalen¿s lab. of Crystallography, Univ. of Bayreuth (Germany, 2006, 2 months) to perform 4D superspace group analysis. As post-doc I got research contracts and-postdoctoral grants in Dallas, (USA, 2008-2010) and Cambridge (UK, 2011 + Dec. 2015-2018) as well as a mobility grant for Poland (2015, 2 months) and a Marie Curie Fellowship for Cambridge (UK, March 2017-Aug 2018) in total > 5 years abroad.

I have participated in research projects funded by USA bodies (Temp-Time, NSF, US-Korea, NECCES, BATT), the EU (H2020-MSCA-IF-2016-747449), and UK government (EP/P007767/1, EP/N001583/1, EP/K002252/1). I significantly contributed to the creation of 2 International energy research centres: CIC Energigune (Spain), CAM-IES (UK).





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I co-directed 3 PhD students (2016, 2017), and supervised 2 masters and 6 undergraduate students. I frequently participate in communication and outreach activities and in the organization of international meetings: 1st Symposium in Na-ion batteries (Spain, 2013). I have taught undergraduate and masteras students at Univ. Complutense, Univ. of Cambridge and CIC Energigune; Since 2016 I am Co-Founder of the Erasmus Int. Summer Course (Univ. A Coruña-Univ. Cambridge) and Iam qualified by ANECA to teach at Spanish public and private Universities. Since 2014 I m editor of Scientific Reports (Nature group) and reviewer for RSC, ACS, Wiley, Springer-Nature, Elsevier. Iave evaluated research projects from Argentina, Peru and Israel and have been jury for 3 PhD viva.

Along my research career I demonstrated creativity and excellent capacity to carry out original research, supervising a research team. I¿ve developed my career in worldwide laboratories with world-class scientists and succeeded in getting funds (>800k) through FPI-PhD and highly competitive postdoctoral fellowships (MEC and Marie Curie) contracts and projects. I¿ve participated in >20 research projects in different areas, leading the research on time temperature indicators and wearable batteries at NanoTech Institute in Dallas, the Na-ion projects at CIC Energigune and the research on MOFs and COFs for energy storage at Cambridge. I¿ve been PI of 2 PhD fellowship proposals worth ~ 100k (4 yr) and ~ 75 k (3 yr) Spain, 6 successful proposals for experiment time in neutron (ILL-France, ISIS-UK), synchrotron (Sp-8-Japan) and high pressure (BGI-Germany) facilities and my Marie Curie Fellowship. I¿ve acted as co-PI in the design and supervision of 2 projects in Na-ion Batteries (Etortek 2014, LINABATT 2013, CIC energigune, Spain).





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Nombre:BELOQUI , ANAReferencia:RYC2018-025923-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:a.beloqui@nanogune.eu

Título:

Design of robust biocatalysts for industrial and technological applications

Resumen de la Memoria:

My research work spans the field of the chemistry applied to biocatalysts: from the discovery, improvement, and characterization of biocatalysts to the application of polymer chemistry to those in order to impart new functionalities and fabricate bioresponsive materials for industry applications. I am thus an interdisciplinary researcher with experience on molecular biology methods for enzyme cloning and production, screening methods to detect enzymatic activities, chemical modification of enzymes for their immobilization, applied polymer chemistry to proteins, and fabrication of catalytically responsive materials. Hence, since the starting of my PhD, I have been exploring new avenues of improving biocatalysts, either by looking for enzymes already adapted to extreme environments or by making them working better.

Therefore, in my Postdoc stage I moved from a biochemical (including proteomics, metagenomics, and molecular biology) to a chemical approach for the fabrication of robust and responsive biocatalytic materials, with the scope of designing and improving biocatalysts for technological and industrial uses. Hence, in my current projects I apply methodologies and concepts that are atypical for the field concerned, as it is expected for frontier research. The technological applications of my research are evidenced by 3 patent applications and several scientific high-quality publications.

My current research line (and planned future research lines) includes all the knowledge harvested during the last 13 years in different research Institutes and shared with (inter-)national researchers in the field of enzymology, chemical (orthogonal) modification of biomolecules, surface-protein interaction, and applied polymer science. In this interdisciplinary field, there are 2 common and correlated aims: the immobilization of the biomolecules on supports of (in-)organic nature and the achievement of more efficient and robust catalysts. All in all, the idea is to interfere in the denaturation and thus, inactivation of the biocatalysts under extreme conditions, which usually are needed in some industrial and technological processes, such as biomass or biogas processing (low pH, around 4, and temperatures around 50°C) or the chemoenzymatic synthesis of enantiomerically pure compounds like glycans (at organic solvent concentration above 50%). At this respect, the combination of inorganic or polymeric-based materials with biomolecules to design functional nanostructures, with the formation of the so-called hybrid materials, is a fast-developing research line. With this in mind, specific topics of my current and future research lines are described below.

Resumen del Currículum Vitae:

In 2004, I concluded my studies in Chemistry at the Navarra University with distinction (awarded with Premio Extraordinario de Carrera) and concluded my PhD in 2009 at the Universidad Autónoma de Madrid with distinction as well. I have been awarded with 6 grants to conduct my research along my career and I accumulate a total of 33 months of international mobility.

I have actively participated in a total of 37 original publications (4 of them are book chapters and 1 a scientific report), I am first (co-) author of 13 and corresponding author of 2 of them. Around 30% of the works (10 out of 33, excluding book chapters) have been published in high impact factor (IF > 8) biochemistry (including Curr. Opin. Biotechnol., Curr. Opin. Microbiol., Proc. Natl. Acad. Sci USA, Trends Microbiol., Microbiol. Rev.), chemistry (Angew. Chem. Int. Ed., Chem. Sci., Small, Adv. Funct. Mat.), and general (Nature, Nat. Commun.) journals. In the last 5 years (from 2013), I have 13 scientific contributions (average IF of 7.7), and 4 are submitted or about to be submitted (1 of them is a book chapter I am corresponding author of the 4 works), from the work conducted in 3 different research institutes. There, I have applied the tools and equipments of top-research groups to develop and build my research line. I have 22 contributions to (inter)national congresses and workshops, being 2 of them as invited speaker.

I regularly conduct peer review in high impact journals and I have been part of the scientific committee of the biannual conference BioMicroWorld. Besides, I have been contacted by the Agencia de Investigación Espanola (AIE) to be part of the ANEP-Spanish experts database-. I have reviewed national projects in the CTQ area.

I have retrieved funds for >180K in the last years in national competitive calls (from Diputación de Guipúzcoa and MICINN-Retos 2017). With this, and from 2016, I was able to build the Catalytic hybrid biomaterials research line, leading my own and independent research. I am directing and supervising the work of my PhD student Andoni Rodriguez López de Abetxuko in the frame of this project, who just got

the predoctoral grant of the Basque Government (in which I sign as Thesis Director). Further, I have supervised 1 PhD student (cosupervision of Leire Barandiaran together with Prof. Raúl Perez), 4 undergraduate students and 1 Master student.

I have established consolidated collaborations with external researchers from abroad (G. Delaittre, E. Blasco, U. Nienhaus, J. Hubbuch from KIT, Germany) and new collaborations with national and local groups, and inside nanoGUNE.





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Moreover, I regularly conduct outreach activities such as the organization of "The International Day of Girls and Women in Science" (2017, 2018, 2019), participated in the Nanokomik event organized by Nanogune, and from 2018 I am the President of the Equality Committee funded at Nanogune.





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Nombre:GARCIA SEGURA, SERGIOReferencia:RYC2018-026063-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:sergigs_87@hotmail.com

Título:

Electrochemical Advanced Oxidation Processes as water treatment technologies: From fundamentals towards scaling-up

Resumen de la Memoria:

My research interests center on improving water quality by understanding mechanisms and materials that enable depollution of wastewaters through novel electrochemical devices and processes. My peer-reviewed publications (H > 30) study different electrochemical advanced oxidation and photoelectrocatalytic processes, including the first attempts reported in literature concerning scaling-up to prepilot scale.

My main line of research involves high impact fundamental science related to electrochemistry and material science, while also pursuing applied research applications of these sciences to address challenges at the nexus within food-energy-water systems (FEWS). Securing water resources and ensuring water quality is one of the global United Nations Sustainable Development Goals. Examples of the research I pursue are described in more detail in my application, but briefly include: (i) studying of novel functional catalytic and electrocatalytic materials to mitigate water contamination and their undesired effects, (ii) developing decentralized devices of water purification, and (iii) improving of the competitiveness of existing water treatment technologies by implementation of functional materials.

Resumen del Currículum Vitae:

I am currently an Assistant Research Professor at Arizona State University in the School of Sustainable Engineering and the Built Environment, and a research member of the Nanosystems Engineering Research Center for Nanotechnology-Enabled Water Treatment. I hold a Ph.D. in Chemistry from the University of Barcelona (UB), an M.S. in Electrochemistry from the University of Alicante, and dual B.S. degrees in both Chemistry and Materials Science from UB and the Polytechnic University of Catalonia, respectively. I have an international and multidisciplinary research background, having worked across four continents in international academic institutions of different countries (Spain, Australia, Brazil, Taiwan, Germany and USA).

My research line on the food-energy-water nexus focuses on the development of novel electrochemical technologies for water treatment. My research efforts resulted in over 65 peer-reviewed articles with high impact (h=30 over 2400 citations).

I have got over \$ 600.000 of funding as PI and co-PI during the last two years to conduct cutting edge research, including translational projects with industry. I mentored undergraduate students, master students, and Ph.D. students. The direct outcome of this mentoring is the publication of over thirteen articles in high impact factor and the successful defense of final projects and thesis dissertations.

My research is internationally recognized by several awards including the Environmental Electrochemistry Prize 2014 of the International Society of Electrochemistry, or the Green Talents award 2015, among others. The scientific recognition of my contributions is also demonstrated by my role as editorial board of renowned journals in my field such as Chemosphere (IF 4.42, Elsevier) and Sensors (IF 2.47, MDPI). In this frame, I have been invited speaker and key-note speaker in 7 international and national meetings since 2015.





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Nombre:ESTRADER BOFARULL, MARTAReferencia:RYC2018-024396-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:martaestrader@gmail.com

Título:

Magnetic-based hybrid nano-objects as platforms for recording media and biosensing applications

Resumen de la Memoria:

M. Estrader s (M.E) scientific career has elapsed over 14 years, throughout which she have gained a multidisciplinary background in the field of chemistry and materials science, ranging from the molecular level (coordination complexes, photoactive organic molecules) to the nanoscale (magnetic nanoparticles, mesoporous systems, thin films). M.E PhD work (Prof. J. Ribas, UB) significantly contributed to demonstrate the utility of a method, previously developed, to assess the nature of the magnetic coupling between a transition metal ion and a lanthanide ion. Targeting at a better understanding of the magnetic interaction, an experimental approach to evaluate its magnitude and the anisotropy between 3d and 4f metal ions was developed through an international collaboration. Aiming at widening her horizons in the field of magnetic materials, M.E carried out a first postdoctoral stay (2008-2011) on the synthesis and advanced characterization of magnetic nanostructures, which was a completely unknown field for her, at Institut Català de Nanotecnologia with Prof. J. Nogués. The results obtained allowed, for the first time, to demonstrate the possibility to obtain antiferromagnetic interface coupling in core/shell nanoparticles (NP). The current magnetic recording media devices made of thin film structures are based on this property. Hence, this finding represents a step forward in the race for the miniaturization of magnetic devices because it fuels the prospect of having bimagnetic NP as the ultimate small components. M.E broadened her knowledge and skills by working with other nanoscale materials, such as mesoporous transition metal oxides and electrodeposited nanocrystalline thin films alloys, for which she was responsible of the magnetic studies. M.E subsequently moved to Stockholm University (2011-2012, Beatriu de Pinós fellowship) with Prof. L. Bergström to devise and implement a new research line in the group dealing with magnetoplasmonic hybrid NPs. These hybrid materials are envisaged as excellent candidates as a biosensors, for instance, in theranostic applications. In 2012 M.E joined the group of Dr. G. Aromí at UB (2012-2015, Juan de la Cierva fellowship) where she was focused on the design and preparation of photoactive ligands aimed at the synthesis of photomagnetic coordination complexes for their use in quantum computing. In particular, a magneto-optical molecular device externally controlled through light was achieved. In 2015-2016 M.E took a career break due to pregnancy/maternity leave. Since 2016 (Marie Skłodowska-Curie fellowship) M.E is pursuing her own research project on the synthesis of metal hybrid Co-based nanorods for their application in the emerging fields of biosensing (based on magneto-optical properties) and magnetic induced catalysis at LPCNO (Toulouse) hosted by Prof. B. Chaudret and Dr. K. Soulantika. During this period, M.E has carried out two short-stages: CICbiomaGUNE (2 months, Donostia) with W. J. Parak focused on water transfer and biofunctionalization processes and at AIT (1 month, Vienna) for in vitro biodiagnostics. Overall, M.E research line is focused on the design and fabrication of magnetic based nano/molecular materials to be implemented in dissimilar applications such as magnetic recording and biosensing. Currently, from 2019 M.E is taking a second career break owing to maternity leave.

Resumen del Currículum Vitae:

I graduated in Chemistry in 2004 at the Universitat de Barcelona (UB) and immediately joined the group of Prof. J. Ribas (UB) to perform the PhD studies on molecular magnetism with a FPI fellowship. I earned the PhD degree in Chemistry with Cum Laude qualification in 2008. Subsequently, during my postdoctoral research career I ve been able to self-finance three of the four postdoctoral stages I ve performed through 3 different competitive fellowships: Beatriu de Pinós (Catalan Government, 2011-2012), Juan de la Cierva (Spanish Government, 2012-2015) and Marie Sklodowska-Curie (EU, 2016-2018), giving rise to a total of 350 k granted. The scientific production has yielded to, so far; 40 publications in international peer-reviewed journals and one book chapter: 78 % first quartile and 45 % in journals with impactfactor > 7: 1Phys. Rep. (Review), 1Nat. Commun, 1ACS Nano, 1Adv. Funct. Mater., 2JACS, 1PRL, 4Nanoscale, 1J. Mat. Chem., 2Small, 2Angew. Chem. Int. Ed. In half of the publications I'm between the firsts three authors and I'm corresponding author in 9 of them. These articles have received more than 1100 citations and I currently have an h-index of 20. I ve been invited to deliver invited talks in congresses more than 10 times although, due to either maternity leave or project funding restrictions, I could not attend to all of them. However, I presented my research work in selected prestigious conferences (MRS, E-MRS, EUROMAT, ICMM). I have been awarded 8 projects as PI to perform experiments in international synchrotron and neutron facilities (e.g., ESRF, ILL, APS). I supervised the day-to-day work of a PhD student, 5 BSc students (end-of-degree research work, TFG) and co-supervised 2 MSc students. I m regular reviewer in international peer-reviewed journals: ACS Nano, Nanoscale, Chem. Mat., etc. I have participated in 21 research projects (3 EU) and evaluated a national project (call: PICT 2016) through the Agencia Nacional de Promoción Científica y Tecnológica of Argentina. I m accredited as Tenure Lecturer and Associate Professor by the Agència per a la Qualitat del Sistema Universitari Català (AQU). I ve taken two career breaks owing to pregnancy and maternity leave (2015-2016 and currently, from 01/2019).





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Título:

Thermo-Rheology of Biopolymer-Based Matrices to Develop Innovative Functional Gelling Formulations (Termorreología de matrices basadas en biopolímeros para desarrollar formulaciones gelificantes funcionales innovadoras)

Resumen de la Memoria:

La principal línea de investigación que ha desarrollado la candidata se centra en la termorreología de sistemas biopoliméricos para desarrollar innovadoras matrices funcionales gelificantes de interés para la comunidad científica, desde un enfoque multidisciplinario. Su interés radica en la revalorización de fuentes infrautilizadas (agrícolas, marinas o forestales) para contribuir a la sostenibilidad ambiental y al bienestar de la sociedad, alineado con los retos del H2020. Su trayectoria investigadora sostenida puede resumirse en las siguientes etapas. (1) Investigación Temprana en reología, durante el Proyecto Fin de Carrera de su primera titulación en la Universidad de Santiago de Compostela, centrada en el estudio de la viscosidad de disoluciones biopoliméricas. (2) Etapa Predoctoral en la misma universidad (con estancias en el IATA-CSIC, Valencia; INRA, Montpellier y FEUP, Porto), focalizada en termorreología de masas sin gluten preparadas con matrices biopoliméricas de fuentes agroforestales infrautilizadas, dirigidas a mejorar la calidad de vida de la población celíaca. Así como, la cinética y estática de secado, el diseño de equipos o la modelización. (3) Etapa Postdoctoral en las Universidades de Lisboa, Cambridge, Minho y Santiago de Compostela, donde profundizó su conocimiento en termorreología de biopolímeros, desglosándose su actividad en las siguientes sub-etapas. (3.1) Durante su estancia en Lisboa, participó en la formulación y caracterización química, termorreológica, textural o microscópica de geles funcionales preparados con subproductos agroforestales y alimentarios. (3.2) Durante su estancia en Cambridge, se centró en la termorreología (cizalla, oscilatoria y extensional) de disoluciones acuosas de biopolímeros y sus correspondientes sistemas aireados utilizando algas como materia prima de interés, así como las simulaciones computacionales de estos fluidos complejos. (3.3) Durante su estancia en la Universidad de Minho, su investigación se amplía hacia la termorreología de geles y films de biopolímeros extraídos de algas rojas usando los conocimientos adquiridos sobre reología de cizalla y extensional de líquidos burbujeantes en Cambridge. (3.4) En su reincorporación a la Universidad de Santiago, participó en la optimización de las condiciones de procesado para obtener biopolímeros novedosos a partir de fuentes agroforestales y marinas con características termorreológicas modificadas. (4) En la actualidad, desarrolla su investigación en el Grupo EQ2- Biomasa y Desarrollo Sostenible (Departamento de Ingeniería Química, Universidad de Vigo) con un contrato "Juan de la Cierva-Incorporación". En esta etapa, continúa trabajando con los temas anteriores y ha tenido la oportunidad de ampliar su campo de investigación de manera internacional / multidisciplinar / interdisciplinar hacia el desarrollo de procesos multiproducto utilizando tecnologías respetuosas con el medio ambiente, basado en los conceptos de biorefinería y economía circular. Su interés radica en valorizar las fracciones biopoliméricas y bioactivas extraídas de fuentes naturales para ampliar sus potenciales aplicaciones del campo alimentario al no alimentario. Su trayectoria en colaboración con profesionales de reconocido prestigio, le han proporcionado capacidades esenciales, experiencia e independencia para el desarrollo de una carrera en el campo.

Resumen del Currículum Vitae:

María Dolores Torres Pérez, diplomada en Ingeniería Técnica Industrial (2004) y titulada en Ingeniería Química (2006) por la Universidad de Santiago de Compostela, se doctoró en Ingeniería Química y Ambiental (Julio 2011, sobresaliente cum laude, premio extraordinario, acreditación doctora europea) en la misma universidad. Paralelamente, realizó 2 Masters: Prevención de Riesgos Laborales y Salud Medioambiental (2009) y Formación del Profesorado en Docencia e Investigación para la Educación Superior (2010), así como numerosos cursos formativos en su campo académico e investigador. Actualmente, tiene una posición postdoctoral (Juan de la Cierva incorporación, calificación 98/100 - 50/50 para la candidata- en el área de Tecnología Química) en la Universidad de Vigo. Ha realizado 8 estancias en prestigiosos centros nacionales (CSIC-IATA, Valencia (1 mes)) e internacionales (P4G-Universidad de Cambridge, Cambridge (22 meses); INRA, Montpellier (3 meses); ISA, Lisboa (9.5 meses); IPC, Guimarães, (9 meses); FEUP, Porto (1 mes)), permitiéndole adquirir fluidez para comunicarse en Inglés, Francés y Portugués. Ha participado en 27 Proyectos (5 como investigador principal) de convocatorias competitivas europeas (2), portuguesas (2), nacionales (13), regionales (5) y de empresas o asociaciones (5). Su actividad investigadora multidisciplinar ha sido enriquecida con la asistencia a numerosas Conferencias Científicas, donde ha participado con 67 trabajos de investigación (6 orales, siendo en 2 ponente invitada y 61 carteles). Ha contribuido al mundo científico con 81 artículos (72 ya publicados, el 86% con ≤ 4 autores, el 76% Q1 y el 36% entre los 10 primeros, con 786 citas e índices h/g/r: 20/25/24) en revistas científicas internacionales con alto índice de impacto en su campo, así como 32 capítulos de libro. Además de 1 patente de empresa en proceso de solicitud. Su actividad docente se ha desarrollado en el marco nacional (Universidades de Santiago y Vigo) e internacional (Universidades de Cambridge y Minho), iniciándose de manera temprana en 2004, como becaria de prácticas en su primera Titulación. En su segunda Titulación impartió docencia, primero como colaboradora de prácticas y en su doctorado como miembro del POD, extendiéndose a su etapa postdoctoral. Ha dirigido 15 trabajos científicos (2 Tesis doctorales en proceso; 9 Trabajos Fin de Master (4 en inglés en universidades extranjeras); y 4 Proyectos Fin de carrera (2 nacionales (1 en proceso) y 2 en inglés en universidades extranjeras). Me gustaría destacar, especialmente, la codirección de los trabajos de investigación llevados a cabo en la Universidad de Cambridge, con la colaboración de otras Universidades punteras, para el





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diseño y desarrollo de un novedoso reómetro extensional portátil, sometido con éxito a procesos de verificación en laboratorio y posteriormente usado en Borneo. Así como, Miembro de la Sociedad Europea de Reología, y del Comité Internacional de Reología. Ha sido revisora de más de 25 revistas científicas, editora invitada de 4 libros y 3 volúmenes especiales (en proceso), así como evaluadora de 4 proyectos nacionales y 2 europeos. Su actividad investigadora ha sido financiada con 8 becas competitivas, y tanto su actividad investigadora como docente ha sido reconocida por premios (8) nacionales (4) e internacionales (4), así como 4 acreditaciones de la ANECA.





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Nombre:JULIA HERNANDEZ, FRANCISCOReferencia:RYC2018-024643-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:franciscojh84@gmail.com

Título:

Organometallic Chemistry: From Synthesis to (Photo)Catalytic Organic Chemistry

Resumen de la Memoria:

The research interests of Francisco Juliá Hernández (FJH) span from organometallic synthesis to the development of sustainable catalytic strategies for organic synthesis. Over his extensive and productive research career, FJH has gathered a strong background on organometallic synthesis, homogeneous catalysis and organic chemistry. After receiving his MSc, FJH secured a PhD fellowship to carry out his doctoral studies in the group of Prof Vicente at the University of Murcia on the synthesis of high-valent organometallic complexes. In 2012, he obtained his European PhD degree with Summa Cum Laude. During this period, he also visited the group of Dr Bassetti at the University of Rome to study reaction mechanisms (3 months). Afterwards, FJH carried out two postdoctoral stays in world-recognized research groups in catalytic organic synthesis. In 2012, he joined the group of Prof. Igor Larrosa (Queen Mary University of London, UK) to develop novel catalytic reactions for the arylation of unactivated C H bonds. In 2014, FJH was granted a COFUND postdoctoral grant (Marie Curie Actions) to study a variety of catalytic organic transformations with Prof. Ruben Martin (ICIQ, Spain). At ICIQ, FJH was able to develop his independent ideas and create novel research programmes on photocatalytic organic transformations. This is demonstrated with a corresponding authorship paper. Very recently, in 2018, FJH was appointed Assistant Professor at Stockholm University, contributing to further consolidate his independence. In Stockholm, FJH has created his independent research group and secured funding to develop his research on sustainable photocatalysis for organic synthesis.

At all levels of his research career, FJH has demonstrated an outstanding commitment to producing high quality research outcomes. He has published several high impact papers (8 in PhD and 11 in postdocs) including first authorships in Nature, JACS, Angew Chem and ACS Catalysis (corresponding authorship), a book chapter and 2 filled patents. The excellence of his research has been recognized with several awards including Best PhD Thesis in Chemistry, finalist and first prize in the very prestigious SusChem/RSEQ awards in PreDoc and PostDoc categories. His research has also reached public engagement with several appearances in the media including La Vanguardia de la Ciencia. FJH has disseminated his research in several scientific conferences (5 orals including a plenary speaker) and invited seminars in international research institutions. He has also delivered teaching activities in three different countries (Spain, UK, Sweden) and supervised graduate and undergraduate students (UK and Sweden).

FJH has demonstrated an extraordinary degree of scientific maturity to evolve independent research and thinking, ability to secure funding at every level of his career, produce research outcomes at the highest level and possess leadership and management skills. FJH aims to hold a Ramon y Cajal fellowship at any University or research institution in Spain where he could develop his independent ideas in catalytic organic synthesis.

Resumen del Currículum Vitae:

Francisco Juliá Hernández (FJH) is currently an Assistant Professor in the Department of Organic Chemistry at Stockholm University (Sweden). After obtaining his Chemistry degree at the University of Murcia, in 2007, FJH joined the group of Prof José Vicente at the University of Murcia, where he started MSc studies. In 2008, he received his MSc degree and obtained funding to start his PhD within the same research group on high-valent Pd complexes. In 2009, he spent 3 months in the group of Dr Bassetti at the University of Rome (Italy) where he improved his knowledge in reaction kinetics and mechanisms. This work led to the publication of a paper in Organometallics. In 2012, FJH received his European PhD degree with maximum honors, being also awarded with the best PhD thesis in Chemistry at the University of Murcia. Furthermore, in the same year, he was awarded as finalist in the IV Premio SusChem/RSEQ-PreDoc . In 2012, FJH left Spain to join the group of Prof Igor Larrosa as a postdoctoral researcher at Queen Mary University of London (UK) (ERC Starting Grant funding). In London, he attained ambitious projects related to the development of catalytic direct arylation methodologies. In 2014, FJH was awarded a COFUND postdoctoral grant (ERC Marie Curie Action) to join the group of Prof Ruben Martin at ICIQ (Tarragona), working on the development of new methods for C C and C H functionalization and carboxylation reactions. His work on the carboxylation of organic matter with CO2 has been recognized with several awards including X Premio SusChem/RSEQ-PostDoc and finalist in La Vanguardia de la Ciencia recognizing his research as one of the fundamental scientific discoveries in 2018 in Spain. Importantly, FJH was able to start exploring his independent ideas during his postdoc with Prof Martin. He successfully conceived and developed a project that was published in ACS Catalysis (corresponding authorship). Very recently, in November 2018, FJH was appointed Assistant Professor at Stockholm University as a result of a very competitive tenure-track position. In Stockholm, he has established his independent research group and secured funding (FJH as PI) to start designing new sustainable (photo)catalytic processes for organic synthesis.





Turno de acceso general

FJH has demonstrated a strong commitment in delivering high quality research outcomes in the area of organometallic synthesis, catalysis and organic chemistry, which is demonstrated with the publication of 19 papers in journals of the first quartile (1 Nature, 4 JACS, 4 Angew Chem, 1 ACS Catal, 1 ACS Cent Sci, 1 Chem Comm, 1 Chem Eur J, 1 Inorg Chem, 4 Organometallics, 1 Tet Lett), a book chapter (Top Curr Chem) and the application of 2 patents. The excellence of his research is reflected in the number of citations (627 overall with 3 papers with more than 50) with h-index of 16 (ISI, January 19). FJH has attended 13 scientific conferences (5 orals with an invited plenary speaker) and has been invited speaker in international research institutions. He often conducts peer review for international journals (ACS, Georg Thieme, Nature Publishing Group) and has also been involved in teaching activities in three different countries (Spain, UK, Sweden) and supervised graduate and undergraduate students.

All this shows his capacity to become an independent research leader in Spain by holding a Ramon y Cajal fellowship





Turno de acceso general

Nombre: VENTOSA ARBAIZAR, EDGAR

Referencia: RYC2018-026086-I

Área Temática: Ciencias y tecnologías químicas

Correo Electrónico: edgar.ventosa@gmail.com

Título:

Sistemas electroquímicos avanzandos de almacenamiento de energía

Resumen de la Memoria:

The scientific career of Dr. Edgar Ventosa is summarized in 6 stages, including over 5.5 years abroad.

1) Dr. Edgar Ventosa obtained his PhD in Chemistry under the supervision of Prof. Palacios (University of Burgos, 2009) working mainly in the development of advanced electrochemical multi-response techniques. During this time, he carried out two stays at a prestigious group (Prof. Unwin) in the UK.

2) Postdoctoral position in the group of Por. Shuhmann at the Ruhr-University-Bochum (Germany), where he was responsible for establishing a new research line: batteries.

3) Project manager at the Technologies Center of Miranda de Ebro, where he improved his skills in project development and management.4) Senior scientist at the Catalonia Institute for Energy Research, where he led the development of a disruptive battery concept

5) Junior group leader at the Ruhr-University-Bochum (Germany), which is the most productive stage. He led several research lines related to batteries and electrolysers

6) Senior assistant researcher at IMDEA Energy, where he is currently leading a small group of 5 people in the field of advanced batteries.

During this career, Dr. Ventosa has developed several research lines, highlighting 4 lines in which his leadership is reflected by 31 papers as corresponding author.

i) In-situ analytical techniques in the field of batteries

ii) Mechanistic understanding of key processes in batteries

iii) Engineering of advanced materials for batteries

iv) New concepts and chemistries in batteries

Dr. Ventosa has participated as partner or PI in > 15 projects at National as well as European level resulting in the publication of 66 papers in peer-reviewed journals such as Adv. Energy Material, Angew. Chem. and Adv. Sci., being the corresponding author of 31 of them. He has co-authored 1 book chapter and filed 2 international patents. Since his return to Spain in 2017, Dr. Ventosa has secured over 500.000 Eur

Resumen del Currículum Vitae:

Dr. Edgar Ventosa joined IMDEA Energy (Spain) in March 2017 as a senior assistant researcher. Before, he has held several positions in different organizations (CTME, IREC and Ruhr University-Bochum) accumulating over 5.5 years abroad since he obtained his PhD in Chemistry at University of Burgos (Spain) in 2009.

During his scientific career, Dr. Ventosa has participated as partner or PI in > 15 projects at National as well as European level. Since his return to Spain in 2017, Dr. Ventosa has secured over 500.000 Eur. He has co-authored 66 publications in peer-reviewed journals (61 without the presence of his PhD supervisor) such as 3 Adv. Energy Material, 2 Angew. Chem. and 1 Adv. Sci. He is the corresponding authors in 31 of them that includes 1 Angew.Chem. (IF=12.1), 1 Adv.EnergyMater (IF=21.8), 2 NanoEnergy (IF=13.9), 1 Adv.Sci. (IF=12.4), 6 Chem.Comm (IF=6.2), 1 J.MaterChemA (IF=9.9), 3 ChemSusChem (IF=7.4), 3 ACS Appl.Mater&Inter. (IF=8.1), 1 ACS Appl.EnergyMater. (no IF yet), 1 NanoResearch (IF=8.0), 3 J.PowerSources (IF=6.9), 3 Chem.Eur.J. (IF=5.1), 1 Electrochem.Comm. (IF=4.6), 2 ChemElectroChem (IF=4.4), 1 PCCP (IF=3.9) and 1 ChemPlusChem. Last year, these publications received > 300 citations leading to a H-index of 19 (Scopus). He has co-authored 1 book chapter and filed 2 international patents.

Dr. Ventosa participates actively as speaker in international conferences (14 talks) and acts regularly as referee for funding agencies, book proposals and peer-reviewed journals, e.g. Chem.Rev.Soc., Nat. Comun., Adv.Mater., Adv. Energy Mater, JACS, Angew.Chem and Chem.Sci.

Dr. Ventosa has taught master curses and practials at Ruhr University-Bochum (2015-2017). He has supervised 5 Master theses and 1 PhD thesis. Currently, he is supervising 3 PhD theses and 1 Master thesis.





Turno de acceso general

Nombre:SANCHEZ SANCHEZ, CARLOSReferencia:RYC2018-024364-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:cssanchez123@gmail.com

Título:

On-surface Bottom-up Synthesis and Characterization of Low Dimensional Materials

Resumen de la Memoria:

My research career is embedded in the field of On-surface Synthesis, focused on the exploration and exploitation of new on-surface chemical reactions for the synthesis of covalent, low-dimensional nanostructures exhibiting novel properties. I am an expert in scanning probe microscopies and synchrotron radiation techniques, thus allowing me to apply a multi-technique approach to my research.

My research career started at ICMM-CSIC (2005-2011) as a postgraduate student (CSIC grant, 4 months) and as a Ph.D. student with a FPU fellowship (4 years), both being competitive grants. During this period, I studied the interaction and reaction of different organic and inorganic materials when supported on technologically relevant dielectric substrates (TiO2). Then, I moved to the ICMSE-CSIC (2011-2012, 15 months) as the responsible of the STM laboratory, where I studied the Sonogashira cross-coupling of alkynes and aryl halides on metallic surfaces under the supervision of Prof. R. Lambert (Cambridge University). Then, I accepted a position as responsible of the VT-STM Lab at Empa, belonging to the ETH-domain (Switzerland, 2012-2015, 39 months), where I worked on the on-surface bottom-up synthesis of atomically precise graphene nanoribbons and other graphene-based nanostructures. Since January 2016, I am co-responsible of the On-surface Synthesis research line in the ESISNA group (ICMM-CSIC), focused on the study of new covalent reactions for the fabrication of novel, technologically relevant nanoarchitectures on surfaces (Juan de la Cierva Incorporación and postdoctoral contract).

I have established collaborations with renowned researchers in the field such as Richard Lambert (Cambridge University, UK), Roman Fasel (Empa, Switzerland), Klaus Müllen (Max Planck Institute, Germany), Mar García Hernández (ICMM-CSIC), Vincent Meunier (Rensselaer Polytechnic Institute, USA), Jonas Björk (Linköping University, Sweden), Johann Coraux (Institut Neel, France), Araceli Campaña (Univ. Granada), Philipp Aebi (University of Neuchatel, Switzerland), Pavel Jelinek (Institute of Physics, Czech Republic), and Luca Floreano (Elettra Synchrotron, Italy), latter three being host institutions of my three pre-doctoral stays (18 weeks); and with top companies like BASF.

27 publications which accumulate 937 citations (48% with IF>12: 2 Nature, 4 ACS Nano, 4 JACS, 1 Advanced Energy Material, and 1 Nano Letters). H-index: 14. Q1 papers: 88%, D1: 48%. First and second author in 52% and 24% of my papers, respectively. Mean IF: 10.69 (14.1 during postdoc). Participation in 11 research projects (1 as IP, 64k , and 1 Plan Nacional-Retos-Jóvenes Investigadores pending resolution), including ERC-Synergy (EU), Office of Naval Research (USA), Swiss National Science Foundation (Switzerland), 2 Consolider (Spain), Plan Nacional, and an industrial project (BASF). 2 patents (1 with BASF) and 14 oral contributions to national and international conferences (4 invited). Supervisor of two MSc projects (September 2016 and September 2018).

Resumen del Currículum Vitae:

I obtained my bachelor in Physics in 2005 from the Universidad Autónoma de Madrid (UAM) and my PhD in Condensed Matter Physics in 2011 (supervisors: Prof. J. A. Martín-Gago and Dr. M. F. López Fagúndez, ICMM-CSIC) also from UAM. I have carried out 3 postdoctoral stages under the supervision of prestigious researchers in the field of On-surface Synthesis: Prof. Richard Lambert (University of Cambridge/ICMSE-CSIC, 2011-2012, 17 months), Prof. Roman Fasel (EMPA, Switzerland, 2012-2015, 39 months) and Prof. J. A. Martín Gago (ICMM-CSIC, since January 2016), the latter as a Juan de la Cierva Incorporación researcher. My whole research career is embedded in the emerging field of On-surface Synthesis and it is focused on the exploration of new on-surface reactions for the fabrication of novel atomically-precise low-dimensional covalent nanostructures.

I have 27 publications in peer-reviewed international journals, including 2 Nature, 1 Nano Letters, 4 ACS Nano, 4 J. Am. Chem. Soc., 1 Adv. Energy Mater., 1Chem. Comm., 1 Nanoscale, 1 Chem. Eur. J., 5 J. Phys. Chem. C, among others (Total mean IF: 10.69; Postdoc mean IF: 14.1), as well as 2 patents, one with BASF SE. I accumulate 937 citations and an H index of 14 (39.04 citations/paper). I am IP of a research project (Juan de la Cierva Incorporacion, 64k) and I have participated in 11 national and international research projects and 1 industrial project with BASF SE. I have 41 contributions to national and international conferences including 4 invited talks. Highly involved in the supervision of a PhD thesis at EMPA and supervisor of twoMSc project at ICMM. I have been the responsible of different scanning tunneling microscopy laboratories during my postdoctoral stages. I am frequent reviewer for top journals in the field of On-surface Chemistry as Angewandte Chem. Int. Ed., ACS Nano, J. Am. Chem. Soc., Chem. Commun., PCCP, J. Phys. Chem. C, among others. I am member of the Spanish Vacuum Society (ASEVA), of the organizing committee of the European Workshop of Epitaxial Graphene and 2D Materials (EWEG2D 2018), of the organizing committee of the III Young Scientist Meetings at ICMM, and of a thesis committee. I am an expert in scanning probe microscopies and a frequent experienced user of Synchrotron Radiation facilities. I am highly active in outreach





Turno de acceso general

activities like the European Researchers Night, Semana de la Ciencia, lab tours, etc. Currently, I am the co-responsible of the On-surface Synthesis research line in the ESISNA group. I have several collaborations with prestigious researchers in the field of On-surface Synthesis and Surface Science such as Prof. Richard Lambert (University of Cambridge, England), Prof. Roman Fasel (EMPA, Switzerland), Prof. Klaus Müllen (Max Planck Institute for Polymer Research, Germany), Prof. Vincent Meunier (Rensselaer Polytechnic Institute, USA), Prof. Xinliang Feng (Center for Advancing Electronics Dresden, Germany), Prof. Diego Peña (Universidad de Santiago de Compostela, Spain), Dr. Jonas Björk (Linköping University, Sweden), and Dra. Araceli Campaña (Univ. Granada, Spain), among others. All these achievements evidence scientific maturity, independency, and leadership, as required by an independent researcher.





Turno de acceso general

Nombre: FERNANDEZ SALAS, JOSE ANTONIO Referencia: RYC2018-026178-I

Área Temática: Ciencias y tecnologías químicas

Correo Electrónico: fernandez-salas@hotmail.com

Título:

From sulfoxide-promoted transformations to metal- and organo-catalysis

Resumen de la Memoria:

In July 2008, Dr. Fernández started his PhD under the supervision of Prof. Jose Luis Garcia Ruano at Universidad Autónoma de Madrid. The PhD research consisted of studies of asymmetric synthesis using enantiomerically pure sulfoxides as chiral auxiliaries, allocated in either a remote position (1,4 induction) or directly bonded to imines (sulfinyl imines). These studies involved both ionic and radical transformations. The work carried out during this period gave rise to 8 publications. In addition, during his PhD, the candidate completed a 3 months stay at the University of Groningen, where he worked under the supervision of Ben L. Feringa. Dr. Fernández was involved in the enantioselective synthesis of Almorexant via an iridium-catalyzed intramolecular allylic amidation. This work led to 1 publication. After receiving his PhD (2012, Cum Laude), Dr Fernández joined the group of Prof. Steven Nolan at the University of St Andrews as a postdoctoral researcher. The candidate was involved in the development of new catalytic applications, as well as in the ligand design with the final aim of developing new multitasking catalysts based on ruthenium and nickel. In this regard, the candidate developed a new series of organoruthenium and organonickel compounds that enabled numerous important organic transformations. This postdoctoral period proved to be very productive, featuring 12 papers in international top journals, while also appearing as first author in 7 of them.

In 2015, Dr Fernández moved to the University of Manchester to work in the group of Prof. David Procter. His research was focused on the development of new methodologies using sulfoxides as platforms to trigger the formation of sulfur-stabilized reactive intermediates, which has allowed him to develop processes for the formation of challenging C C bonds (to aromatics and heteroaromatics and C heteroatom bonds). Taking that into consideration, he studied and reported a metal-free CH CH-type strategy that allows the selective coupling of aromatic centers to propargylic centers in alkynes at the expense of two C H bonds CAr(sp2) H and C(sp3) H bonds. Taking advantage of this strategy, Dr. Fernández described an interrupted Pummerer/nickel-catalyzed cross-coupling. This postdoctoral period was very productive, featuring 5 papers published in international top journals.

In February 2017, Dr Fernández started at the UAM as Profesor Titular Interino. Since March 2018, he has become a Juan de la Cierva-Incorporación fellow. During this time, Dr. Fernández has been involved in the development of new organocatalytic transformations by using bifunctional catalysis. Dr. Fernández s research interest within this field has been devoted to the discovery of new modes of activation that would help to overcome previous limitations and unlock new reactivities in organocatalysis.

Since February 2017, and as a result of the supervision of his own working team, which currently includes 2 PhD students and a postdoctoral research fellow, Dr. Fernández has published 5 articles, 3 of them as corresponding author. In addition, the candidate has already supervised and directed 2 master students and has participated and contributed as senior researcher in a research project.

Resumen del Currículum Vitae:

Dr. Fernández received his B.Sc. in Chemistry from the Universidad Autónoma of Madrid (Spain, 2002-2006). Then, he joined the group of Prof. Jose Luis García Ruano at the same university, and obtained the M.Sc. in 2008. In 2010, he spent three months in the laboratory of Prof. Ben L. Feringa (Nobel Prize in Chemistry, 2016) at University of Groningen (Netherlands) working on Total Synthesis, and published one article. In 2012, he finished his PhD thesis with the highest qualification (Cum Laude). The PhD research was focused on asymmetric synthesis by using enantiomerically pure sulfoxides as chiral auxiliaries, studying their influence on different asymmetric transformations including polar and radical processes. These studies led to the publication of 8 articles.

In 2013, Dr. Fernández gained a competitive two-year postdoctoral position within a European project (ERC-Advanced Researcher Grant-FUNCAT) to work in the group of Prof. Steven P. Nolan at the University of St. Andrews (Scotland, 2013-2015), where he had the opportunity to co-supervise two PhD students. The research the candidate was involved in during that period was focused on the design and synthesis of new organometallic complexes with a special regard in their catalytic applications. This period (2013-2015) led to the publication of 12 scientific articles.

In 2015, the researcher gained an open call three-year postdoctoral position within a British Engineering and Physical Sciences Research Council (EPSRC) project in the group of Prof. David J. Procter at the University of Manchester (United Kingdom, 2015-2017), where he was involved in the study and development of new metal-free cross-coupling procedures. This stay successfully conducted to the publication of 5 articles in journals with high impact factor (2x Angew. Chem., Int. Ed. 2018; Nat. Commun., 2017; J. Am. Chem. Soc., 2016).

In February 2017, the candidate was appointed to a Profesor Titular Interino position at the UAM. Since March 2018, he is a Juan de la Cierva-Incorporación researcher at the same university. During this period, he has been supervising two PhD students and has already directed two master students. Since February 2017 and as a result of the supervision of his own working team, which currently includes 2 PhD students and a postdoctoral research fellow, Dr. Fernández has published 5 articles.





Turno de acceso general

His time as a researcher has been distributed in five research groups (in four different countries) and worked in projects that belong to many different areas, including asymmetric synthesis, total synthesis, metal catalysis, ligand design, labelling and organocatalysis.





Turno de acceso general

Nombre:EIBES GONZALEZ, GEMMAReferencia:RYC2018-024846-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:gemma.eibes@usc.es

Título:

Bioreactors in pursuit of a cleaner environment and a better quality of life

Resumen de la Memoria:

My research career has been focused on the design, modelling and optimization of bioreactors in pursuit of a cleaner environment and a better quality of life. My personal development as a researcher has been accomplished in four stages, where I progressively achieved the necessary capabilities to become a strong decision-maker, innovative and successful scientific leader.

I acquired a deep knowledge of environmental biocatalysis, organizational and time management skills and high level experimental abilities and at the Group of Environmental Biotechnology at the University of Santiago de Compostela, where I obtained my PhD degree dealing with the conception, modelling and operation of enzymatic reactors for removal of hydrophobic pollutants. Along this period, I had the opportunity to join internationally-renowned research groups in the Academy of Sciences of Czech Republic (Prague, Czech Republic) and Queen s University (Kingston, Canada). The subsequent 2-year postdoctoral research stay at Institute for Biotechnology and Bioengineering (Instituto Superior Técnico, Lisbon), was oriented to the design and operation of bioreactors for stem cell culture, for biomedical applications. This stage served to broaden my knowledge in a new field, biomedical engineering, and helped me to become an interdisciplinary thinker.

I rejoined the group of Environmental Biotechnology in a position of professional maturity, promoting new ideas which were the basis for opening new research lines. I was first awarded with a postdoc fellowship from Xunta de Galicia and later, as principal investigator of two research projects in prestigious and selective calls: project Jóvenes Investigadores sin vinculación (JIN) funded by MINECO and a European ERA-IB2 project. My current research focuses on novel enzymatic reactors directed to four applications: i) Removal of endocrine disrupting compounds based on enzymatic magnetic nanoparticles; ii) Pretreatment of lignocellulosic material using oxidoreductases and valorization in a biorefinery framework; iii) Extraction of bioactive compounds from agro-industrial residues and enzymatic improvement of their biological properties; and iv) Enzymatic modification of lignin for the formulation of bioadhesives.

I am currently a recognized researcher in the area of biorefinery and biocatalysis with a solid scientific production (52 JCR articles with more than 1000 citations), with demonstrated capacity of technology transfer (6 patents), an experienced supervisor (3 PhD, 3 MSc and 12 visiting students), with an important teaching experience (more than 400 hours in Chemical Engineering Degree), a wide and well developed network of contacts (collaborating with 23 prestigious international research groups from 13 countries and active participation in two national excellence networks) and an engaged member of the international scientific community, participating in PhD committees, organizing national and international conferences, reviewing papers for more than 30 international journals (Q1) and evaluating project proposals for the Spanish State Research Agency (AEI) and five public research bodies from other countries.

Resumen del Currículum Vitae:

My track can be summarized as:

1) PhD candidate with an FPI fellowship (2002-2007) at Universidade de Santiago de Compostela. Removal of polycyclic aromatic hydrocarbons by oxidative enzymes.

2) Postdoctoral fellow from Spanish Ministry of Education and Science (2007-2009) at Institute for Bioengineering and Biosciences. Production of human stem cells in bioreactors

3) Postdoctoral fellow from Xunta de Galicia, type A (2010-2013) and type B (2014). Design of bioreactors for the transformation of emerging pollutants.

4) Principal investigator of two projects: program Proyectos I+D+i jóvenes investigadores , Mineco (2015-2018) and the European program ERA-IB2 (2015-2019). Biocatalysis in biorefinery processes.

The main results of my research activities can be summarized as:

i. The supervision of three PhD theses (2013, 2015 and one still on-going), three MSc theses (2011, 2017 and 2018) and 12 visiting researchers.

ii. Principal investigator of two projects: JIN program from Mineco and ERA-IB2 program. Participation as team member in one international project (ERACoBioTech), 7 from R+D Spanish Government, 4 from the Galician Government and 2 from the Portuguese Government.

iii. Publication of 52 peer-reviewed articles (40 Q1, 5 Q2, 5 Q3 and 2 Q1), 32 of them as first or second author, 8 as last author; 23 of the total as corresponding author. Publication of 4 chapters of international books (Springer and Wiley; 2 as second author, and one as last author), one technical report (Springer Protocols) and one chapter of an Encyclopedia (Springer)

iv. 56 participations in international congresses, plus 17 oral communications in national congresses





Turno de acceso general

v. 6 granted patents of invention (4 with application to international extension)

vi. Co-authority in peer-review articles with 72 researchers from Spain (four different institutions), Portugal (three institutions), Netherlands, Czech Republic, Switzerland, Canada (two institutions), Chile (two different institutions), Mexico, Colombia, India and Japan. Current collaboration in projects with institutions from Germany (four different institutions), France (two different institutions), Slovenia and UK.

General quality indicators of scientific production (Scopus): Sum of the Times Cited: 1047 Citing Articles: 737 Average Citations per Item: 18.36 H-index: 17 Top 5% most cited publications: 5 Top 25% most cited publications: 24

Concerning teaching activities, I have been qualified as "Profesor contratado doctor" by the Spanish agency ANECA. I have taught different subjects in Chemical Engineering Degree (USC) for a total of 454 h. Regarding management activities, I have been Coordinator of Teachers in 3rd year of Chemical Engineering Degree.





Turno de acceso general

Nombre:MAYORAL GARCIA, ALVAROReferencia:RYC2018-024561-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:amayoral@shanghaitech.edu.cn

Título:

Nanochemistry at atomic level

Resumen de la Memoria:

Inicié mi carrera investigadora gracias un proyecto de un año de duración bajo la supervisión del Dr. Yasuhiro Sakamoto en la Universidad de Estocolmo, sintetizando nuevos materiales mesoporosos ordenados, analizando las transformaciones de fase y entendiendo el crecimiento cristalino de los mismos prestando especial atención a la microscopía electrónica. Este proyecto dio lugar a la publicación de dos artículos científicos (Stud. Surf. Sci. Catal. 2007 and Micropor. Mesopor. Mater. 2008, citado 85 veces). En Noviembre de 2005 fui seleccionado por el programa europeo FP5 Nanocage Materials Research and Training Network para comenzar mis estudios de doctorado en la Universidad de Birmingham dentro del grupo de Dr. Paul A. Anderson. En dicha tesis estudiaba la introducción de metales en distintos materiales porosos y su posterior caracterización mediante difracción de rayos X, análisis termogravimétricos y microscopía electrónica (Nanotechnology, 2007; Crys. Eng. Comm. 2010).

En Noviembre del 2008 fui contratado por la Universidad de Texas en San Antonio (UTSA) para trabajar dentro del grupo del Prof. Miguel Jose-Yacaman. Durante los casi dos años que estuve en su grupo estudié la síntesis, estructura y reactividad de nanopartículas metálicas con tamaños que variaban entre los pocos átomos hasta los cien nanómetros, publicando 16 artículos científicos (destacando a modo de ejemplo una revisión en Nanoscale, 2010, 59 citas o el análisis de la intercara entre nanopartículas bimetálicas de Au y Co publicado en Nanoscale, 2010, 27 citas).

En 2010, me incorporé a la Universidad de Zaragoza dentro del Instituto de Nanociencia de Aragón, como especialista en microscopía de aberración corregida aplicada a los campos de la química y ciencia de materiales. En dicho laboratorio me establecí como científico independiente orientando mi investigación en dos líneas fundamentales como son: (i) el análisis de clústeres y nanopartículas metálicas con aplicaciones en energía, biomedicina y catálisis (Nature Chem. 2013 que acumula 169 citas; Dalton Trans. 2013, portada de la revista). Y (ii) el desarrollo métodos para el análisis estructural de materiales altamente sensibles al haz electrónico como son las zeolitas (y derivados), los materiales mesoporosos y los metal organic frameworks (MOFs); todos con grandes aplicaciones en campos de la energía, catálisis y medio ambiente. Desde el punto de vista de la caracterización, la mayor complicación radica en su fragilidad bajo el haz electrónico lo que hacía imposible beneficiarse de las ventajas de los microscopios de aberración corregida. Sin embargo, entre 2010 y 2011 desarrollé una nueva técnica que permitió obtener por primera vez resolución atómica en una zeolita así como la observación de clústeres octaédricos (6 átomos) de plata formada en los poros, (Angew Chem. Int. Ed. 2011. 38 citas). Desde entonces son numerosos los artículos en los que he participado en esta temática lo que me ha llevado a establecer numerosas colaboraciones en el ámbito internacional (Prof. Xiaodong Zou, Suecia; Prof Jiri Cejka, Rep. Checa; Prof. Russell Morris, Reino Unido, o el Prof. Suk Bong hong, Korea, etc).

Desde el 1 Enero de 2018 soy Research Associate Professor en la ShanghaiTech University, donde pretendo explotar nuevas propiedades de los materiales porosos dopados con metales a un nivel atómico.

Resumen del Currículum Vitae:

El candidato es licenciado en Química, Universidad de Alcalá (2003), donde también realizó un postgrado en Ingeniería Química (2004). Simultáneamente, 2003, recibió una beca para trabajar en el departamento de investigación de CEPSA, para el desarrollo y caracterización de catalizadores para la mejora de la gasolina. En 2004 inició su carrera científica realizando un proyecto de investigación en la Universidad de Estocolmo, bajo la supervisión del Dr. Yasuhiro Sakamoto y en 2005, fue galardonado por el programa FP5 Nanocage Materials Research and Training Network para realizar sus estudios doctorales en la Universidad de Birmingham (Reino Unido) con el Dr. Paul A. Anderson como director. En Noviembre de 2008, después de depositar la tesis, obtuvo una plaza como Investigador postdoctoral en la University of Texas at San Antonio (USA) en el grupo del Prof. Yacaman. Durante ese periodo el Dr. Mayoral lideró la construcción del actual Kleberg Advanced Microscopy Center donde era responsable de los microscopios TEM y SEM además de participar en actividades de formación, mediante la supervisión de 3 estudiantes de proyecto dentro del departamento de física.

En 2010 fue contratado por el Instituto de Nanociencia de Aragón como científico especialista para el uso de los dos primeros microscopios de aberración corregida instalados en España. Aquí ha llevado a cabo su investigación de manera independiente desarrollando métodos de análisis de materiales porosos convirtiendo a dicho laboratorio en referencia mundial para el estudio de este tipo de solidos. El impacto científico queda reflejado en la publicación de 119 artículos SCI (destacando 2 Nature Chem., 3 Angew. Chem. Int. Ed., 1 ACS Nano, 8 Nanoscale, etc.). Así mismo, ha sido invitado por la revista Chem. Cat. Chem. en dos ocasiones a participar en el número especial Advanced Microscopy and Spectroscopy for Catalysis . También ha contribuido a 3 revisiones invitadas Micron, Nanoscale y Z. Anorg. Allg. Chem. En 30 de los artículos figura como primer autor acumulando 1762 citas con un h-index de 22. El Dr. Mayoral ha participado en 22 proyectos tanto nacionales como internacionales siendo IP en 3 de ellos, 2 públicos y otro con empresa, obteniendo como IP 226000 .





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También ha sido invitado a diferentes conferencias internacionales teniendo actualmente 61 contribuciones a congresos, 36 orales donde 19 han sido impartidas por el Dr. Mayoral y dentro de las cuales 9 han sido invitadas/keynote. Ha sido organizador en dos ocasiones del simposio sobre microscopía electrónica y materiales dentro del IMRC 2013 y 2016 y de la conferencia de la sociedad de microscopía española en 2017. En 2015 fue editor del libro: Advanced Transmission Electron Microscopy: Applications to nanomaterials , Springer al cuál además contribuyó con la escritura de un capítulo.

Ha sido tutor en diferentes cursos y profesor certificado por el ANECA. Tiene experiencia como gestor de instalaciones ya que fue responsable científico de los microscopios electrónicos en UTSA. Actualmente es Research Associate Professor en la ShanghaiTech University y desde 2019 también consultor externo de la empresa Johnson Matthey. El grupo del Dr. Mayoral consta actualmente de 5 estudiantes de doctorado.





Turno de acceso general

Nombre:FRANCAS FORCADA, LAIAReferencia:RYC2018-025394-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:laia.francas@gmail.com

Título:

Catalytic Processes for Solar Fuels Production

Resumen de la Memoria:

Dr. Laia Francàs career has been focused on the study of redox catalytic reactions for solar fuels production. The aim of this research field is to use solar energy, water and CO2 to produce a fuel. One key process is the water oxidation to yield the electrons to produce a fuel. This is an energetically and kinetically demanding process since it involves the formation of an oxygen-oxygen double bound from two water molecules. However in order to efficiently achieve the fuel generation, several processes need to take place in a simultaneous and harmonious manner. Such as: (1) Light harvesting and charge separation; (2) Water oxidation; (3) Fuel production through a reductive process.

During her career Dr. Francàs had the unique opportunity to work in each of the above-mentioned processes yielding 28 published scientific articles, 2 reviews (one of them being cited over 236 times), 2 published book chapter, 1 article under review in Nature Chemistry another one in Nature Catalysis and 5 more works in preparation. Her articles have been cited over 712 times, resulting in an h-index of 11 (WoS).

Her PhD (2006-2011, Universitat Autònoma de Barcelona) was based in the design, synthesis and characterization of ruthenium catalysts for oxidative transformations both for water oxidation and alkene epoxidation (process 2). Consequently she became an expert on NMR spectroscopy and electrochemical techniques. She then moved to Institute of Chemical Research of Catalonia (2012-2014), where she further developed her skills in the design of oxidation catalysts and mechanistic study trough different analytic techniques such as, EPR, Raman, IR, UV-Vis spectroscopies. Her other main research line during this period was the preparation of supported molecular catalysts (process 2). In addition, she started studying light-driven water oxidation processes (Process 1). Since 2015 she works in Imperial College London (ranked in the top 3 European research institutions) using pump-probe optical techniques to study the charge generation, charge transfer and accumulation in light-driven reactions both in homogenous and in heterogeneous phase (process 1). Her main role during this period has been to apply her molecular knowledge to depict mechanisms in metal oxides catalysts. In addition, she also had the opportunity to work in the design and study of photocathodes for hydrogen evolution and she is currently supervising a master project on CO2 reduction (Process 3).

In the future she will expand her acquired knowledge to design and prepare hybrid molecular-metal oxides catalysts. Her aim is to obtain more robust catalysts by rationally designing their reactivity, tuning steric and electronic properties. The new catalysts will be test towards important industrial processes such as: water oxidation, alkene epoxidation, alcohol oxidation and glycerol transformations. These processes will also lead to a more efficient fuel production due to the more facile electron extraction from these substrates. Their mechanism will be studied using different spectroscopic techniques in order to determine the rate limiting step of the reaction. This will allow the design and preparation of a more efficient next generation of catalysts for solar fuels production.

Resumen del Currículum Vitae:

Dr. Laia Francàs has a wide experience in the study of catalytic reactions for solar fuels production: From the catalyst design to the mechanistic study of light-driven reactions.

During her career she has demonstrated to be a valuable young researcher by being awarded several grants and fellowships during her PhD (in the Universitat Autònoma de Barcelona, UAB) and her 2nd postdoc. Highlighting that she was awarded with a Marie Skłodowska-Curie Individual Fellowship (2015-2017, total 183.455) which is one of the most challenging postdoctoral European fellowships. This allowed her to develop the project Water Oxidation for Solar Fuels Production at Imperial College London (ICL, ranked 3rd in European Research Institutions, The Times) in James Durrant s group.

In addition she has participated in 11 research projects. Her more important contribution has been in the FET-PROACT A-LEAF European project. She has been involved in the preparation and development of this project for the ICL participation. This project was awarded with a total of 8 million (488.522, for Imperial College London).

During her career she has mentored 6 master, 7 PhD and 4 visiting students (ICIQ and ICL), co-supervised three master projects (ICL) and one final degree project in collaboration between ICL and UAB.

From the academic point of view Dr. Francas has been accredited as a lecturer by AQU (Catalan Agency for University Quality). She has been developing her academic teaching skills in practical laboratories in UAB and performing inorganic chemistry tutorials for 1st and 2nd year chemistry degree students in Imperial College London.

She has a wide experience in organizing dissemination activities such as: conferences (2015, Early Career Researchers Symposium Solar Fuels: moving from materials to devices), outreach activities (Annually from 2015, Artificial photosynthesis project in Joves i Ciencia and





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participation in several editions of imperial festival) and seminars (2015-2018 seminars in Photochemical Energy Conversion).

Dr. Francàs career has led to 32 important publications in the solar fuels field, with 712 citations and h-index of 11: Chemical Society Reviews, Energy Advanced Materials, JACS (3), ACS Energy Letters, Nature Communications, ACS Catalysis (4), and Chemical Science, ChemSusChem Chemistry European Journal, Inorganic Chemistry (6), Dalton transactions, Journal of Physical Chemistry C, Catalysis Science and Technology (2). Currently, she has a paper under revision in Nature Chemistry and another one in Nature Catalysis.

She has given oral presentations in 19 international and national conferences, one of them as a Keynote speaker (International Solid State Ionics -21, 2017) and another one as invited speaker (CPE summer symposium, 2018). In addition she has presented 11 posters.

She has an international network as demonstrated by her publications with collaborators in different fields, such as: DFT calculations (Prof. V. Batista, Yale University and Dr. Albert Poater, Universitat de Girona), metal oxides sample preparation (Prof. K-S. Choi, Wisconsin University), molecular catalysts synthesis (Prof. Franc Meyer, Göttingen University).

In summary, as detailed in the other sections of this CV Dr. Francàs has demonstrated to be a leader fully capable to develop her own research projects on solar fuels catalysis.





Turno de acceso general

Nombre:FERNANDEZ MOREIRA, VANESAReferencia:RYC2018-025872-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:vanefm78@gmail.com

Título:

Metallodrug as theranostic agents

Resumen de la Memoria:

Al finalizar la licenciatura en Ciencias Químicas en la Universidad de Vigo (2003) decidí realizar la tesis de licenciatura (tesina) y el D.E.A. en esa misma universidad. A continuación en 2005 me trasladé a la Universidad de Cardiff en Reino Unido donde realicé el doctorado bajo la supervisión del Dr. M.P. Coogan y Dr. A. J. Amoroso gracias a una beca EPSRC del gobierno inglés. El proyecto que desarrollé se basaba en el diseño de COMPLEJOS LUMINISCENTES DE METALES d6 con aplicaciones como SENSORES para sistemas HOST-GUEST y en BIOIMAGEN. Motivada por este campo decidí ampliar mis conocimientos en el área incorporando a los complejos lantánidos, el otro grupo de compuestos metálicos que con sus propiedades luminiscentes singulares, los hacen complementarios a los que ya había estudiado. Para ello realicé mi primera etapa postdoctoral en el grupo del Prof. J.-C-Bünzli en el Ecolé Polytechnique Federale de Lausanne EPFL en Suiza, grupo reconocido por sus aportaciones en la química de los lantánidos. El proyecto que realicé estaba financiado por la Swiss National Science Foundation (SNSF) y enmarcado dentro de una acción COST (COST-D38). Allí no solo adquirí conocimientos sobre la química de los LANTANIDOS sino que también aprendí diferentes estrategias de BIOCONJUGACION, múltiples ENSAYOS BIOQUIMICOS, y a trabajar utilizando tecnologías LAB-ON-A-CHIP. A continuación en el 2009, me trasladé al Trinity College Dublin al grupo de la Prof. S. Draper, donde me adentré en el campo de la QUIMICA SUPRAMOLECULAR, sus aplicaciones en MATERIALES LUMINISCENTES. Esta segunda etapa posdoctoral estuvo financiada por una beca MARIE CURIE ToK y ha sido tremendamente útil para diseñar nuevos ligandos que cumplan unas características fotofísicas específicas. Cabe resaltar, que a pesar de las exigencias y el desafío planteado durante estos periodos investigadores, al ir cambiando el tipo de química en cada uno de proyectos que desarrollé, todos se han completado satisfactoriamente. Prueba de ello son las publicaciones que han derivado.

En el 2011 me incorporé como investigadora postdoctoral en el grupo de la Prof. M.C. Gimeno en Universidad de Zaragoza (UZ) y con posterioridad al Instituto de Síntesis Química y Catálisis Homogénea (ISQCH) donde me encuentro en la actualidad. Desde entonces mis capacidades y responsabilidades han ido creciendo progresivamente hasta el punto de conseguir desarrollar e implantar una línea nueva de investigación METALOFARMACOS EN TERAGNOSIS que colidero junto con Prof. Gimeno. Mi experiencia en el desarrollo de agentes de VISUALIZACION CELULAR, manejo de distintas técnicas de MICROSCOPIA Y ESPECTROSCOPIA DE FLUORESCENCIA, así como en distintos ENSAYOS BIOLOGICOS (MTT, ELISA, SDS-page, etc.) han sido claves para su rápida implantación en el grupo de investigación. Resultados de esta línea han sido publicados en revistas de gran calidad científica donde SOY AUTORA DE CORRESPONDENCIA. Chem. Sci., Chem. Eur. J, Inorg. Chem. o Organometallics entre otros son algunos ejemplos que demuestran su futuro prometedor. En lo que respecta a responsabilidades institucionales, soy representante del colectivo de doctores no permanentes en el departamento de química Inorgánica y en el ISQCH. He coordinado el dossier de bienvenida en relación a PRL del Instituto y participo periodicamente en actividades de supervisión, diseminación y difusion.

Resumen del Currículum Vitae:

Research ID: M-2772-2014 ORCID: 0000-0002-1218-7218

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- 33 artículos en Journal Citation Reports[®]. Publicaciones: (2) predoctorales, (8) doctorales, (1) 1er postdoctoral, (1) 2do postdoctoral, (21) Periodo UZ-ISQCH.

- Artículos en revistas de gran impacto como Angew. Chem. Int. Ed., Chem. Sci., Small, Chem. Commun., Chem. Eur. J., Adv. Funct. Mater., Pure & Appl. Chem., etc.

- 1 Capítulo de libro: Advances in Organometallic Chemistry, en prensa.

- 1 Newsletter article: EPA, 2018.

- Más de 1400 citaciones.

- 24 de las contribuciones sin mi supervisior de tesis.

- 7 articulos como autora de correspondencia (Chem. Sci., Chem. Eur. J., Chem. Commun., Inorg chem., Dalton Trans., Organometallics y Inorg. Chim. Acta).

- Primera autora en 18 artículos (incluyendo aquellos que por política de grupo están en orden alfabético)

- Acred. Aneca: Profesora Ayudante Doctora.

SELECTED PUBLICATIONS (total 33)

1) Progress with, and prospects for, metal complexes in cell imaging. M. P. Coogan* and V. Fernández-Moreira* Chem. Commun., 2014, 50, 384-399.





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2) Luminescent Re(I) and Re(I)/Au(I) complexes as cooperative partners in cell imaging and cancer therapy. V. Fernández-Moreira,* I. Marzo and M. C. Gimeno* Chem. Sci., 2014, 5, 4434-4446. 3) Heterobimetallic Complexes for Theranostic Applications. V. Fernández- Moreira* and M. Concepción Gimeno* Chem. Eur. J., 2018, 24, 3345-3353. FORMACIÓN 2008: Ph.D.: Synthesis of ligands-organic conjugates for biological imaging applications. Cardiff University, UK. Dr. M.P.Coogan y Dr. A. Amororso. 2003 -2005: Tesis y D.E.A.: Universidad de Vigo. Dr. E. Freijanes Rivas y Dr. M. D. Couce Fortúnez. 2003: Licenciatura en C. Químicas, Doble especialidad: Orgánica e Inorgánica, Universidad de Vigo **EXP. PROFESIONAL** 2011: Investigador asociado: Universidad de Zaragoza/ISQCH. IP: Prof M.C. Gimeno 2009-2010 Investigador postdoctoral: Trinity College Dublin, Irlanda. IP. Prof. S. Draper 2008-2009 Investigador postdoctoral: Ecole Polytechnique Féderalé de Laussane, Switzerland. IP: Prof. J.-C. Bünzli EXP. DOCENTE y SUPERVISIÓN (TOTAL: 5 Erasmus, 1 TAD, 2TFM, 5TFG) En los 3 último años: 2018-2019: Dirección de Tesis Doctoral en curso de Marta Redrado y Andrés luengo (que sera defendida en 2019) 2017-2018: Dirección de TFM: Marta Redrado. Dirección Tesis Doctoral: Andrés Luengo 2016-2017: Dirección de TFG: Marta Redrado y Adrián Torguet CONGRESOS: SELECCIÓN (Total: 33) COMITÉ ORGANIZADOR Y CIENTÍFICO: GEQO2018-Zaragoza CONTRIBUCIÓN ORAL: IX Reunión Científica de Bioinorgánica. Cadiz, Spain, Junio, 2015. Compuestos de Re(I) y Re(I)/Au(I): Agentes de visualización celular y anticancerígenos. CONTRIBUCIÓN INVITADA: 7th International Conference on f Elements (7ICfE). Colonge, Germany, 2009. Bioconjugation of Lumininescent Lanthanide Helicates and its Applications. CONTRATOS Y BECAS DISFRUTADAS: SELECCIÓN 2009 2010: Beca Postdoctoral: Marie Curie ToK Fellowship 2008 2009: Contrato Postdoctoral: Swiss Office for Science and Education Foundation 2005 2008: Beca Doctoral: Engineering and Physical Sciences Research Council (EPSRC) PARTICIPACION EN PROYECTOS: SELECCION:(TOTAL 10) Nacionales:CTQ2016-75816-C2-1-P, CTQ2015, 70371- REDT, INNPACTO:IPT-2012-0067-060000, FECYT:FCT-15-10128). Europeos: Marie Curie FP6-14472, COST Action D38

PARÓN LABORAL: Baja por maternidad: 28/04/2014-15/09/2014





Turno de acceso general

Nombre:CIRERA FERNANDEZ, JORDIReferencia:RYC2018-024692-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:jorcire@gmail.com

Título:

Computational Modeling of Spin-Crossover systems: From molecules to Metal-Organic Frameworks

Resumen de la Memoria:

Dr. Cirera main research framework evolves from the study of the interplay between the local electronic structure of a transition metal center and its implications in the stereochemistry, magnetic and spectroscopic properties of the whole molecule. This research allows for a rational design of new molecules and materials with tailored properties based on their local and global electronic structure. Within this framework, several research lines have been developed on the course of the last 10 years, which has provided with major contributions in the field of inorganic, physical and theoretical chemistry. His central research line is the study of spin-crossover (SCO) processes in inorganic systems of different complexity, from molecules, to clusters, to Metal-Organic Frameworks (MOFs), with emphasis in the computational modeling of the transition temperature (T1/2). Due to the accuracy of these calculations, and the understanding of the experimental trends in terms of the underlying electronic structure, major advances in the rational design of new SCO molecules with tailored T1/2 has been outlined. He is author and co-author of 11 publications in such field (8 as first author, 4 as a corresponding), all in first quartile peer reviews journals, and has directed 3 final degree projects under this research line. He has also been 6 times invited speaker on this topic in different conferences. Dr. Cirera has worked in the development and implementation of non-standard computational approaches to study MOF type materials, research line in which he has 4 papers and one final master project. Some highlight from this research line are the development of a fully polarizable force field for the MIL-53(Cr) MOF, which allows to correctly describe the water microstructure within the pores and its implications in the breathing behavior of the material, and the development and implementation of a hybrid Molecular Dynamics / Monte Carlo scheme to study spin-crossover behavior in the [Fe(pz)2Pt(CN)4]-MOF. The later uses ab initio-based ligand-field force fields to compute the T1/2, in excellent agreement with the experimental data. Moreover, the methodology was used to study the water loading effect on the T1/2 tuning, allowing for the very first time to get insight into the physical process controlling such behavior. More recently, a combination of classical molecular dynamic simulations and periodic electronic structure calculations has been used to study the only known MOF material exhibiting stimuli-controlled single-crystal reversible phase transition. This process can be used to encapsulate guest molecules that could not fit through the pores, and the calculations provided with the energetic profile responsible for such behavior. This work was published in Advanced Materials. Other projects involve the use of electronic structure calculations to study magnetic exchange pathways in inorganic molecules, allowing for a full characterization of the different type of interactions between metal centers. He has also works in the field of bioinorganic chemistry (mechanistic and spectroscopic studies) and in the computational study of organic probes of relevance for the early detection of neurodegenerative diseases. He has been also instrumental in the development of the SHAPE code for Continuous Shape Measures analysis, as well as some of its basic tools.

Resumen del Currículum Vitae:

Jordi Cirera (Barcelona, 1979) graduated in Chemistry from the University of Barcelona (2002) and received his doctorate with honors from the same university in 2006. His first postdoctoral stage was at Stanford University (2007-2010) working on spectroscopic studies and theoretical modeling of copper mediated biogenesis in metalloproteins, under the supervision of Prof. Edward I. Solomon. Later, he moved to the University of California, San Diego (UCSD), for a second postdoctoral stage with Prof. Francesco Paesani (2012-2014), working in the development and implementation of novel methodologies for the computational modeling of spin-crossover processes in Metal-Organic Frameworks (MOFs). He has been visiting researcher at the Max-Planck Institute für Festkörperforschung (MPG-FKF) in Stuttgart, and the Institut de Physique et Chimie des Matériaux (ICPMS) in Strasbourg, under the supervision of Prof. Jens Kortus, developing new methodologies for the calculation of zero-field splitting parameters in transition metal complexes, key parameters in the study of Single-Molecule Magnets. Dr. Cirera has been awarded with several grants, including a PhD grant from the Spanish government (AP2002-2236), a grant for his first postdoctoral stage (2006 BP-A 10041), a Hellmann Fellowship Foundation grant for his second postdoctoral stage, and a Beatriu de Pinos/Marie Curie COFUND fellowship grant (2013 BP-B 00155). He has also been co-PI in the European Prace project SPINMOLSURF (15th Prace Call, project ID: 2016163898), awarded with 17.2 millions of CPU computer hours. He has been speaker at 32 conferences (6 invited) at national and international conferences and research centers, and is co-author of 36 publications in peer review journals (h-index 21, total citations 2381, 6 as a corresponding author, one as a single author) and two book chapters (one as a single author). During the period 2002-2007 and 2014 to date he has conducted different teaching assignments within the Inorganic Chemistry area at the University of Barcelona (around 1000h). Such teaching activities include both regular lectures in the chemistry, pharmacy and chemical engineering degrees, and advanced inorganic laboratory practices (given in English) in the chemistry degree. He has directed six





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final degree projects, three of them in his major research line (i.e, computational modeling of Spin-Crossover systems), one of them already published, and one master project. He is also responsible for different scientific outreach activities, being the most recent one a collaboration with the visyon360 virtual reality company to develop a set of augmented reality molecular models. The prototype deck as well as the cellphone application will be ready during the 2019 summer. He is co-organizer of the IQTC-UB annual Symposium since 2014 (4 editions, last one awarded with 2370 for funding) and co-organizer of the upcoming FHI-AIMS workshop, that will be held in Barcelona during the summer of 2019 (currently awarded with 32400 from CECAM and PSI-K networks) Currently he is a research scientist at the University of Barcelona, and is part of the Materials Networking project, partially funded within the EU Horizon 2020 research and innovation program (grant 692146). He took a volunteer paternity leave of absence between 2011-2012, to allow his wife to continue with her academic career.





Turno de acceso general

Nombre:SANCHEZ NAVARRO, MACARENAReferencia:RYC2018-024759-IÁrea Temática:Ciencias y tecnologías químicasCorreo Electrónico:macasn@hotmail.com

Título:

Synthesis of bioactive compounds to understand and influence biological systems of interest

Resumen de la Memoria:

My research career has always been focused in understanding biological problems by taking advantage of chemical tools.

In 2006 I got a fellowship to do my PhD at the Instituto de Investigaciones Químicas, working on the chemical synthesis of glycodendrimers. This research work provided training in viable synthetic strategies for these complex molecules, in the chromatographic procedures for their purification and the appropriate techniques to their structural elucidation. I also adquired extensive knowledge in carbohydrate and dendrimer chemistry, protecting group manipulations, microwave reactions, and analytical techniques. In addition, I did several stages in other laboraries (Universita degli studi de Milano, Universidad Complutense de Madrid and University of Oxford). After defending my PhD thesis I did a short postdoc in Universidad complutense de Madrid where I worked on the synthesis of fullerene modified with sugars. In this case, we also studied the capability of this compounds of inhibit viral infection processes. Afterwards I got awarded with a fellowship from the fundación Ramón Areces to do a postdoctoral stay in the University of Oxford. I was involded in several projects of chemical modification of proteins. The interdisciplinary nature and scientific relevance/quality of the projects remarkably contributed to increase my technical skills and scientific knowledge. As shown, all the results outlined lead to interesting publications. It is worth to mention, that this work provided training in protein design, expression and modification and other relevant aspects of Chemical Biology. This postdoctoral stay also helped me in developing my teamwork, discipline, and communication (report writing and presentations) skills, which are essential for the work to be successfully conducted within an interdisciplinary environment.

In 2012 I joined professor Ernest Giralt¿s group at IRB Barcelona to work on the modification of protein with BBB peptide shuttles to increase their transport across the BBB. One year after I got awarded with a Juan de la Cierva fellowship. In 2016 I got promoted to research associate. In this period I have learnt about peptide synthesis and its therapeutic applications as well as molecular biology techniques. At present I am in charge of some of the cellular experiments that complement our research. My position in the laboratory has been gaining weight. Currently I am involved in grant application processes in different aspects since design of the scientific project to the distribution of the budget. In addition, I am supervising PhD and master students in the lab.

The beginning of my career was focused in understanding a very relevant phenomenon in nature, multivalency, especially in the interaction of carbohydrates with their receptors. I was able to apply the key concepts learnt to the design of new families of compounds, glycodendrifullerens and glycodendriproteins. After getting in touch with proteins I got engaged by the potential of selectively modifying them to question several biological problems. This is why I have been able to implement the tools to modify a given protein with a selected peptide in order to adjust its features in the laboratory of Prof. Giralt.

This natural path has allowed me to learn the key aspects for using chemical tools to interrogate biological systems.

Resumen del Currículum Vitae:

My reseach career shows a natural evolution in the Chemical Biology area:

1. During my PhD training (CSIC, 2006-2009), I was engaged in the development of relevant synthetic chemical methodology for accessing glycodendrimers, allowing for the preparation of different glycodendrons, with natural glycans and surrogates. These structures were used to study the interaction against the innate immune receptor DC-SIGN. The results were published in peer reviewed journals (Bioconjugate Chem. 2011, 22, 1354; ACS Chem. Biol. 2010, 5, 301) and a patent (N° EP09380127). In addition, I participated in two review articles about carbohydrate multivalent systems targeting DC-SIGN (Drug News Perspect. 2010, 23, 557) and about dendrimer synthesis (In Frontiers of Nanoscience; Elsevier: 2012; Vol. 4, p 143).

2. Postdoctoral stay at Universidad Complutense of Madrid (2010). During this period, I carried out a scientific project involving the preparation of water soluble fullerenes and the evaluation of their physicochemical properties. Two families of compounds were prepared, dendrofullerenes and glycodendrofullerenes (Biomacromolecules 2013, 14, 431; J. Am. Chem. Soc. 2011, 133, 16758; Chem.-Eur. J. 2011, 17, 766; Chem. Commun. 2010, 46, 3860).

3. Postdoctoral stay at University of Oxford (2010-2012). During this time, I worked on site-selective modification of proteins with different ligands of interest (carbohydrates, fluorophores or spin labels). A brief summary of the major accomplishments are the following: (1) development of hydrothiolation of alkynes by two thiol fragments across the carbon-carbon triple bond to give a dithioether derivative with exclusive 1,2-addition (Chem. Commun. 2011, 47, 11086); (2) development of a tag-and-modify strategy for the practical synthesis of homogeneous fluorinated glyco-amino acids, peptides and proteins carrying a fluorine label in the sugar, allowing access to first examples of directly radiolabeled ([18F]-glyco)proteins (Chem. Commun. 2010, 46, 8142); (3) Synthesis of multivalent glycodendriprotein constructs (bearing up to 1,620 glycans) (Nat. Commun. 2012, 3, 1303).





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4. Postdoctoral stay at IRB Barcelona (2012-present): First as a Juan de la Cierva (2013-2016) fellow and later as a Research Associate, in Prof. Ernest Giralt¿s laboratory I have been mainly involved in the development and use of peptides able to cross the Blood-Brain barrier (BBB), named BBB-shuttles. The main results can be summarised as: (1) implementation of methodologies to modify proteins with selected BBB-shuttles (Chem. Sci. 2018, 9, 8409; Pept. Sci. 2017, 108:e22928) with special focus on monoclonal antibodies in order to increase their transport towards the brain parenchyma. (2) Development of a new BBB-shuttles derived venoms (MiniCTX-3: Chem. Comm. 2018, 54, 12738; MiniAp-4: Angew. Chem. Int. Ed. 2016, 55, 572); (3) study of the complexation between lipopeptides and insulin to increase its transport across the intestinal barrier (ChemMedChem 2018, 13, 2045); (4) development of cellular assays to evaluate the ability of nanobodies or peptides to inhibit EGF/EGFR interaction (Angew. Chem. Int. Ed. 2017, 50, 1847; Curr. Opin. Chem. Biol. 2017, 38, 134; Chem. Soc. Rev. 2016, 45, 4690).