



AYUDAS RAMÓN Y CAJAL CONVOCATORIA 2016

Turno de acceso general

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Título:

Microscopic dynamics of proteins from molecular simulations

Resumen de la Memoria:

My research focus is in the study of the conformational dynamics of proteins, the biomolecules that undertake most of the functions in living cells. Protein polypeptide chains typically need to fold into their three-dimensional (native) structures to undertake their functions. Since the start of my research career I have aimed at establishing connections between experiment, theory and molecular simulations.

My main research lines involve the use of atomistic or coarse-grained molecular dynamics (MD) simulations and a cutting edge method for deriving microscopic kinetic (Markov state) models (MSMs) from the data. Using atomistic MD I have investigated the dynamics of short peptides, that serve as model systems for full proteins with less computational burden, and also full enzymes. For the study of disordered peptides I use coarse-grained models, on which I acquired expertise during my PhD.

My main research lines are listed below.

(1) Folding kinetics of peptides: My strongest achievement in this area is the determination of kinetic rates for the fastest processes in protein folding @helix nucleation (JACS, 2011) and hairpin formation (JCTC, 2013) from molecular dynamics, MSMs and optimized force fields (Biophys J, 2012). With this work I solved important discrepancies between experiment and simulation.

(2) Internal friction in proteins: My main achievement in this area is the discovery of the molecular mechanism of "internal friction" (Nat. Commun., 2014). I run simulations of short peptides and model systems at different viscosities, recovering the experimental trends. Further work has confirmed and generalized our conclusions (JACS, 2015; JPCL, 2016). I currently follow this research path supported by a Plan Nacional Retos grant to me as a PI.

(3) Enzyme dynamics: My main achievement in this line is the derivation of MSMs from MD of gas diffusion in hydrogenases (Nat. Chem., 2016). I predicted mutations that reduce the inhibition of the enzyme by oxygen, as confirmed experimentally, opening new avenues for clean energy production. This work followed the determination of the rates of oxidation of the active site of the enzyme (Angew Chem Int Ed, 2014) and the development of the methodology for building the MSM (JCTC, 2015)

(4) Intrinsically disordered proteins (IDPs): My main achievement is establishing the use of coarse-grained models for explaining binding mechanisms of cancer related IDPs to their targets. I first studied the dependence of the binding dynamics of HIF1a to CBP in the simulations on model parameters (Mol. Biosys., 2012). My student V. Oleinikovas applied the model in a combined experimental-simulation study of the PUMA-Mcl1 (PNAS, 2014).

(5) Protein mechanics: I have recently started working on the dynamics of protein unfolding under a pulling force (JMB, 2016). I have conclusively addressed the discrepancy between two-state folding in bulk and multi-state folding upon pulling (JPCL, 2016). Currently I conduct work in close collaboration with experimental groups on mechanical unfolding of gpW, titin and Fim domains.

(6) Statistical mechanics models of protein folding: My main achievement in this area is determining the role of size scaling in the folding rates and stabilities of two-state folding proteins (JACS, 2009) and the development of an algorithm for the prediction of folding and unfolding rates (PCCP, 2011).

Resumen del Currículum Vitae:

The focus of my research career is in the conformational dynamics of proteins, which I approach using computational methods.

Since the start of my PhD I have contributed a total of 29 scientific publications, and have a steadily growing h-index of 11 (Google Scholar). I am the first (or co-first) author of 13 of these references and corresponding author of 4. I have published my work in some of the best journals of chemistry in the world: Nature Chemistry (1), J. Am. Chem. Soc., (3), Angew. Chem. Int. Ed. (1) and J. Phys. Chem. Lett. (2). Also I have published papers in two interdisciplinary high impact journals: Nature Communications (1) and Proc. Natl. Acad. Sci. USA (1).

During my PhD studies, supervised by Prof. Antonio Rey (Complutense University), my work focused on a family of very computationally tractable coarse-grained interaction models for proteins. In 2007 I moved to the CIB-CSIC to conduct post-doctoral work in Prof. Victor Muñoz's laboratory, funded by a Marie Curie Excellence Grant. My research focus shifted to the analysis and interpretation of folding experiments using simple statistical mechanical models. In Prof. Muñoz's lab I developed one of the key traits of all my work to come, the aim of explicitly connecting theory and simulation to experimental observables. In order to gain expertise in molecular dynamics (MD) simulations I moved to the University of Cambridge in 2009 to work in Robert Best's group, funded by the highly competitive FEBS Long Term Fellowship. During this period I studied small peptides using atomistic MD simulations, intrinsically disordered proteins (IDPs) and the functional dynamics of enzymes. While at Cambridge I supervised several research students (J. Carter, V. Oleinikovas), I was awarded a Wolfson College Junior Research Fellowship, I co-organized a CECAM workshop jointly with Robert Best and Prof. Benjamin Schuler (U. Zürich), and formed an extensive network of collaborations, including J. Blumberger (UCL), J. Clarke (U. Cambridge) and C. Leger (CNRS).



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In 2015 I started the tenure of a 5-year highly competitive Ikerbasque Fellowship at CIC nanoGUNE. During this period I have started work in the areas of protein conformational transitions induced by force as in single molecule experiments and protein misfolding. Currently I co-supervise two PhD students (R. Sharma, jointly with V. Muñoz, and A. Manteca, jointly with R. Pérez-Jiménez) and a Masters student (A. Aguirre). I have been awarded a Plan Nacional Retos grant as a PI and a supercomputing allocation of over 7 million hours from the PRACE research infrastructure.

The research students that have completed their work under my supervision have seen their work published in peer-reviewed journals and the two students I currently supervise have recently submitted their first manuscripts. I have given talks in national and international scientific meetings (CECAM, 2012, MolKin, 2013, GRS, 2011, Prodestech 2013 and 2015) and have also been invited to give seminars in research centers or universities (NIH-NIDDK, BIFI, King's College London, U. Cambridge, EBI-EMBL). Finally, I regularly conduct peer review for J. Chem. Phys., Biophys. J. and J. Phys. Chem., among others.



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Turno de acceso general

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Título:

From DNA constructs to superexcited ions: in silico decoding of the electronic structure and reactivity of complex systems

Resumen de la Memoria:

Son varias las líneas de investigación en las que podrían clasificarse los trabajos realizados por la candidata a lo largo de su trayectoria investigadora.

La primera se desarrolla durante su etapa predoctoral en la Universidad Autónoma de Madrid (UAM) y se resume en el estudio de la reactividad, el enlace y sus perturbaciones en complejos ion-molécula en fase gas. Estos resultados permiten racionalizar un gran número de resultados de espectrometría de masas, así como profundizar en la caracterización de enlaces agósticos en complejos metálicos.

La etapa postdoctoral de la candidata, desarrollada entre las Universidades Libre de Berlín y Friedrich Schiller en Jena, se centra en el estudio estático y dinámico de la fotofísica y fotorreactividad de cromóforos de interés biológico y médico. Durante esta etapa, cabe destacar las aportaciones de la candidata a la fotoquímica de los endoperóxidos, así como la completa caracterización y modelización de la dinámica a través del primer ejemplo en la literatura de un punto de degeneración a 8 estados, significativamente más eficiente para la relajación de sistemas excitados electrónicamente que las intersecciones cónicas a dos estados, frecuentes en compuestos orgánicos.

Apoyándose en la experiencia y metodologías aprendidas durante su doctorado y estancias postdoctorales, la candidata desarrolla desde su incorporación a la UAM dos conjuntos de líneas de investigación en las que pretende ir más allá de la caracterización estática de los sistemas de interés, monitorizando así su evolución en el tiempo, mediante simulaciones de dinámica molecular. El primer subconjunto lo constituyen tres líneas de investigación aplicadas que serán desarrolladas en el marco de cooperaciones con dos empresas pioneras en sus campos, como son la farmacéutica GlaxoSmithKline y la empresa biotecnológica especializada en láseres y tratamientos fotodinámicos Biolitec AG y cuyos objetivos se enfocan hacia (i) el estudio la fotoestabilidad y fototoxicidad de fármacos y excipientes farmacéuticos tras su interacción con luz UV y visible, (ii) el desarrollo y mejora de métodos para la caracterización estructural de metabolitos de fármacos basados en el cálculo de secciones eficaces colisionales y (iii) el diseño de nuevos fotosensibilizadores precursores de oxígeno singlete para su aplicación en terapia fotodinámica.

El segundo subconjunto lo componen otras tres líneas de orientación fundamental. La primera está enfocada al diseño de fotosensibilizadores metálicos y todo orgánicos para su aplicación en síntesis orgánica mediada por catálisis fotoredox. La segunda línea aspira a entender cómo la naturaleza y patrón de sustitución de los heterociclos de purina y pirimidina regulan la topología de las superficies de energía potencial fundamentales y excitadas y por tanto determinan la fotoestabilidad o fotorreactividad de los ladrillos de ADN y ARN, así como la de sus derivados. La última línea tiene como objeto la caracterización electrónica de especies superexcitadas procedentes de la ionización de los orbitales más internos, necesaria para la modelización de la dinámica acoplada de núcleos y electrones en procesos químicos elementales, como la autoionización o la migración de carga, iniciados por láseres ultracortos XUV/rayos X.

Resumen del Currículum Vitae:

Inés Corral se licencia en Químicas por la Universidad Autónoma de Madrid (UAM) en el año 2000, obteniendo el Premio Extraordinario de Licenciatura. Posteriormente, se incorpora al grupo de Estructura y Reactividad Molecular del Departamento de Química de la UAM donde realiza sus estudios de doctorado, bajo la dirección de los Profs. Manuel Yáñez y Otilia Mó. En 2005 obtiene el grado de Doctora con la calificación de Sobresaliente Cum Laude y mención de doctorado europeo, defendiendo la tesis "Enlace y Perturbaciones de Enlace en Reacciones Ion-Molécula en Fase Gas". La calidad de este trabajo de investigación le supone a la candidata los galardones de Premio a la Mejor Tesis Doctoral de la Comunidad de Madrid de 2005, concedido por la Real Sociedad Española de Química y Premio Extraordinario de Doctorado de la Facultad de Ciencias de la UAM. Entre 2005 y 2008 realiza dos estancias postdoctorales en las Universidades Freie Universität Berlin (FUB) y Friedrich Schiller en Jena (FSJ), financiadas por las fundaciones Ramón Areces y Alexander von Humboldt, y un contrato de investigación con la Universidad FSJ. En 2009, se incorpora al Departamento de Química de la UAM con un contrato Juan de la Cierva y al finalizar el mismo es contratada como investigadora a cargo de la Advanced Grant "XUV/X-ray lasers for ultrafast electronic control in chemistry" financiada por el ERC. En la actualidad es Prof. Ayudante Doctor en el mismo Departamento, donde dirige la línea de investigación de Estados Excitados del Grupo de Estructura y Reactividad Química. Fruto del trabajo desarrollado a lo largo de estos años son los 54 artículos publicados, varios de ellos, en revistas de gran prestigio internacional como Nature Comm., Angew. Chem. -Int. Ed, J. Am. Chem. Soc., Chem. Sci., Chem. Comm., Chem.-A Eur. J., y de mayor impacto en el área de Química Física como J. Phys. Chem. Lett., J. Chem. Theory Comp., J. Phys. Chem. B y C, los 4 capítulos de libro y un editorial de un número especial de la revista Computational and Theoretical Chemistry de los que es coautora. Conviene resaltar que la candidata es primera autora en 26 de las anteriores publicaciones, autora para correspondencia en 16 de ellas y que el promedio de autores en sus publicaciones es de 5. Estos resultados han sido asimismo presentados como ponencia oral en 17 conferencias internacionales. A todo esto, hay que añadir que la candidata ha dirigido, entre las Universidades FSJ y UAM, 2 tesis doctorales (1 de ellas como única supervisora y que ha sido premiada con el Premio Extraordinario de Doctorado de la Facultad de Ciencias de la UAM), 7 trabajos de fin de grado y 3 tesis de máster. En estos momentos dirige 6 tesis



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doctorales, 3 trabajos de fin de grado y 1 tesis de máster.

La candidata ha sido investigadora principal de la acción integrada hispano-alemana "Mecanismos para la generación de oxígeno molecular singlete" concedida en 2011. En la actualidad dirige dos proyectos de investigación con la empresa GlaxoSmithKline UK y uno con Biolitec AG y mantiene fructíferas colaboraciones con grupos experimentales y teóricos estadounidenses, europeos y nacionales. La candidata ha participado en más de 15 proyectos de investigación financiados por organismos públicos españoles (1.4 millones de euros) y extranjeros (6.4 millones de euros) y en dos COST Actions.



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Turno de acceso general

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Título:

Catálisis asimétrica

Resumen de la Memoria:

My research line during my scientific career has focused in different fields of catalysis (asymmetric, organocatalysis, metal (Zr, Hf, Cu, Pd, Au, Ag and Zn) and visible-light photoredox). My research can be divided into 5 stages with high mobility (5 groups in 4 countries) and scientific production (52 papers + 1 submitted) in only 12 years. In every research group that I have been I published 1 article as a minimum.

The first stage (Sep.2004-July2005) as an undergraduate student of Chemistry. My scientific career started in Sept. 2004 in the group of Prof. Pedro (Univ. of Valencia) doing my final research project in diastereoselective Michael additions, and continue with an Erasmus stay in Leiden Univ. (The Netherlands) in the group of Prof. Overkleeft working in the "synthesis of N-glycan labeled probes". This period has been resulted in 3 publications.

The second stage (Sep.2005-July2010) at the University of Valencia where I carried out my PhD studies. My PhD thesis was based in the development of new enantioselective Friedel-Crafts reactions using Zr(IV)-BINOL complexes (PhD Thesis with "Excellent cum laude") under the supervision of Prof. Pedro and Prof. Fernández. During this period I was supported by a PhD fellowship from the Valencian government. During this stage, I had the possibility to spend 4 months in the group of Prof. Jørgensen in Aarhus Univ. (Denmark) working in asymmetric organocatalysis. In this stage, I gained experience in asymmetric catalysis that resulted in 12 publications (10 from my PhD thesis and 2 from Aarhus Univ.).

The third stage (August2010-Sep.2012) corresponds to my first postdoc in the group of Prof.Rueping in RWTH Aachen Univ. (Germany). My research work was focused in visible-light photoredox catalysis and activation of allylic alcohols. In this period I have gained much more experience in photochemistry and organic synthesis, and resulted in 10 publications. I have worked in several projects that involved C-H functionalization of tertiary amines as well as asymmetric synthesis (synthesis of Vitamin E).

The fourth stage (Oct.2012-Sep.2014) I hold a Marie-Curie fellowship (FP7-PEOPLE-2011-IEF-300826) in the group of Prof.Feringa (Chemistry Nobel Prize 2016) in Groningen Univ. (The Netherlands). In this period I have completed an outstanding work in the field of catalysis. I worked in catalytic cross-coupling reactions using organolithium reagents as well as asymmetric copper catalysis. This period was very productive with 13 papers.

The last stage (Oct.2014-present) corresponds to my reincorporation to the Univ. of Valencia as a Juan de la Cierva in the group of Prof. Pedro working in asymmetric catalysis, both metal and organocatalysis. In this period, I have supervised undergraduate (6), master (3) and PhD students (1), and my production has resulted in 13 papers (+1 submitted).

During my short scientific career, I received several fellowships and stipendiums (Erasmus, Collaboration grant, PhD fellowship, Stipendium from RWTH Aachen Univ., Intra-European Marie-Curie fellowship and Juan de la Cierva). I have attended several conferences with 50 contributions (19 oral and 2 invited talk). I have participated in 7 research projects. My high international mobility, scientific production and supervision of students show my leadership and independent capabilities to perform an independent research.

Resumen del Currículum Vitae:

I received my degree in Chemistry from the Univ. of Valencia in 2005, with the best academic record. Still as an undergraduate student I started my research career performing the final degree project with Prof. J.R.Pedro and I.Fernández on diastereoselective Michael additions (2 publications). The same year, I joined the group of H. Overkleeft (Leiden Univ., The Netherlands) as an Erasmus Fellow (5 months) working on the synthesis of N-glycan labeled probes (1 publication).

In 2006, I obtained a pre-doctoral Grant from the Valencian Government to perform PhD studies in the group of Prof. J.R.Pedro working on the development of new asymmetric Friedel-Crafts reactions. The thesis, defended in July 2010, deserved the "Excellent cum Laude" qualification and produced 10 publications. During this period, I also carried out a 4 month stay with the group of Prof. K.A.Jørgensen (Aarhus Univ., Denmark) working on organocatalysis resulting in 2 publications.

In August 2010, I moved to RWTH Aachen Univ. (Germany) to carry out my first post-doctoral research stay in the group of Prof. M.Rueping for 26 months. My research focused on visible-light photoredox catalysis and the activation of allylic alcohols, and produced 10 publications. Moreover, I supervised a Canadian undergraduate student under UROP, an international program of the RWTH Aachen Univ.

In 2012, I was awarded an Intra-European Marie Curie Fellowship (FP7-PEOPLE-2011-IEF-300826) and started a 24 month post-doc, in the group of Prof. B.Feringa (Nobel Prize in Chemistry 2016) in the Univ. of Groningen (The Netherlands). In this second post-doc, I performed research on catalytic cross-coupling reactions with organolithium reagents as well as on enantioselective copper catalysis. This research provided 13 publications.

Since October 2014 I hold a research contract within the Spanish Government "Juan de la Cierva" program and I joined the group of Prof. J.R.Pedro (Univ. of Valencia) where I'm performing research on asymmetric catalysis, focused in organocatalysis and organometallic



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additions to cyclic imines, having already published 13 articles (+1 submitted).

As a summary, I have published 52 articles (+1 submitted) from which 28 correspond to research performed without my PhD supervisor. My research have been published in high impact peer reviewed journals which include: Angew.Chem.Int.Ed. (6), Chem.Sci. (2), ACS Catal. (4), Green.Chem. (1), Chem.Comm. (3), Chem.Eur.J. (7), Org.Lett. (8), Adv.Synth.Catal (4), Chem.Asian J. (1), ChemCatChem (1), J.Org.Chem. (2), Org.Biomol.Chem. (3), RSC Adv. (1), Tetrahedron (3), Eur.J.Org.Chem. (1), Beilstein J.Org.Chem. (1), Synthesis (2), Tetrahedron Lett. (1) and Anales RSEQ (1), which have received more than 1200 citations with an h-index=19. I am also co-authored a book chapter. I have presented 48 contributions in scientific meetings which include 19 oral communications and 2 invited lectures, and I participated in 7 funded research projects. My leadership qualities and independent thinking is demonstrated by the supervision of 3 bachelor and 2 master thesis. Currently, I'm supervising 3 bachelor, 1 master and 1 PhD students. Additionally, I collaborate with teaching activities in the Univ. of Valencia (238 hours), and I have been accredited by ANECA as a Prof. Contr. Dr. and Prof. Ayud. Dr. I have been examiner of 8 Bachelor Thesis.



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Turno de acceso general

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Título:

Química Organometálica y Catálisis Homogénea

Resumen de la Memoria:

Jesús Campos studied Chemistry at Universidad de Sevilla (First National Award, 2007), carrying out undergraduate research both at the departments of Organic (enantioselective catalysis) and Inorganic (olefin polymerization) chemistry under the umbrella of two competitive research grants. He moved to the University of Manchester to work with Prof. John D. Sutherland (MPhil, 2008) on prebiotic chemistry. Back to Spain he joined the group of Prof. E. Carmona to work on C-H activation and fundamental organometallic chemistry. He received two PhD Awards and an International PhD Distinction (2012) after spending a visiting stay (FPU) with Prof. M. Brookhart (Univ. of North Carolina, 2010). Dr. Campos' research on the rhodium-catalyzed isotopic labelling of organic molecules attracted the attention of Astra Zeneca (Dr. N. Bushby), Novartis (Prof. H. Andres) and RC Tritec (Dr. Nüeckel), with whom collaborations were established. These patented investigations were recognized with the Javier Benjumea Puigcerver Research Prize to Campos and Carmona (2013). In addition, Dr. Campos obtained a second Master Degree in Crystallography and Crystallization from the International University Menéndez Pelayo (2010).

He returned to the US as a postdoctoral researcher joining the group of Prof. R. H. Crabtree at Yale University (2013-2014), to work in green catalysis and energy-related transformations. Soon after, Dr. Campos became the only postdoctoral associate in a research group comprised of 11 junior co-workers, which placed him in a position of high responsibility. In particular, Dr. Campos directly led a project focused on the valorization of renewable materials by homogeneous catalysis (e. g. Nature Comm. 2014, as corresponding author). This triggered a collaboration with the industrial sector (Greenleaf Biofuels) and was recognized with the Premio Joven a la Cultura Científica (Sevilla City Council, 2015).

He was awarded with a competitive Talentia/Marie Curie Fellowship for a second postdoctoral period in the group of Prof. Simon Aldridge at University of Oxford (2014-2016), focusing on bond activation and catalysis with Main Group systems. Among the main achievements, Dr. Campos developed the first boron-version of the well-known Negishi cross-coupling protocol, a breakthrough in metal-catalyzed borylation chemistry. Besides, he was involved in several projects dealing with the activation of small molecules by group 14 elements and frustrated Lewis pairs.

He was recently awarded with a competitive Marie Curie IF (2016) under which he has pursued the establishment of his independent research career at Univ. of Sevilla. After a short time, Dr. Campos has secured one of the most competitive research projects at national level (BBVA Foundation, <5% success rate) as the Principal Investigator, and he is currently supervising 2 PhD, 1 master and 1 last-year undergraduate student. In particular, he is developing new ways of chemical cooperation based on intercluster compounds and transition metal frustrated Lewis pairs.

The applicant has demonstrated to have a wide background in the fields of organometallic chemistry and catalysis, which has provided him with leadership, management, problem-solving and project planning skills, essential to become a young research leader.

Resumen del Currículum Vitae:

The career progression of the candidate is outstanding. Dr. Campos has a strong publication record at this early stage, with 40 scientific articles in international top journals (37 in the first Quartile Q1), including Nature Chemistry (1), Nature Communications (1), JACS (7), Angew. Chem. (5) and Chem. Sci. (2). Moreover, Dr. Campos has signed as the first author in 19 of his 34 publications (in three of those first and second author equally contributed). Importantly, in five of his publications (Nat. Commun., 3 Angew. Chem. and Dalton Trans.) the Fellow signed as corresponding author, thus evidencing the leading role that he has been performing in his early career. Two of those Angew. Chem. corresponding author publications were highlighted as "Hot Paper" by the editor. Since his first publication in 2010 Dr. Campos has received 380 citations (source: Web of Science; 135 citations in 2016; 442 citations from GoogleScholar) and has reached an h-index of 13 in only six years from his first report.

The international profile of Dr. Campos is remarkable. After graduating at University of Sevilla with the highest marks (First National Award), he obtained his first master degree from University of Manchester (UK, 2008). During his PhD studies (FPU fellowship), the most prestigious PhD fellowship in Spain, he spent three months at the laboratories of Prof. Maurice Brookhart (University of North Carolina, USA). Furthermore, the applicant carried out his postdoctoral research within two of the top-5 ranked research institutions worldwide, namely Yale (USA) and Oxford (UK) universities.

He has actively participated in national and international conferences across Europe and USA, contributing with 8 oral presentations and 9 posters. Moreover, he has been invited to deliver scientific talks at the universities of Bath (UK), Oxford (UK) and Granada (Spain, to be given in March 2017).



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The applicant has secured two of the most competitive international fellowships at the postdoctoral level: Talentia/Marie Curie COFUND and Marie Curie IF. In both cases, he had the original ideas, wrote the scientific projects and acted as the coordinator, demonstrating his independent thinking and creativity. Importantly, he has recently been funded as the Principal Investigator from the BBVA Foundation (2016) within one of the most competitive and multidisciplinary funding programs across Spain (<5% rate success).

Dr. Campos has directly supervised and mentored a number of students in Carmona, Crabtree and Aldridge research groups and he is currently supervising and co-supervising 2 PhD, 1 master and 1 last-year undergraduate student working on diverse projects based on chemical cooperativity and catalysis.

The relevance of the scientific results achieved by the applicant led him to establish several industrial collaborations and deliver a patent. In view of these results he was also awarded with several research prizes that include X Premio a la Investigación Javier Benjumea Puigcerver (2013, shared with Prof. Carmona), Premio Joven a la Cultura Científica (2015, Sevilla City Council) and Premio Investigadores Jóvenes (2016, Real Maestranza de Caballería de Sevilla).

His career progression, scientific achievements and mentoring experience represent a convincing endorsement of Dr. Campos capacity to be a research leader at Ramón y Cajal level.



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Título:

Multiscale Modeling of Heterogeneous Catalytic Processes

Resumen de la Memoria:

The research activities of Dr. Aleix Comas-Vives focus on understanding complex catalytic processes by means of first principles simulations and multiscale modeling. His main research interests are in the field of energy, particularly on the CO₂/CO conversion to fuels catalyzed by oxide-supported nanoparticles. The ultimate goal of his research is to provide fundamental knowledge that help developing more active, selective and sustainable catalysts via rational design.

During his PhD at the Autonomous University of Barcelona (2009), he provided crucial atomistic understanding of metal-catalyzed homogeneous reactions; in particular of hydrogenation and oxidation reactions. By the end of this PhD he mastered the modeling of homogeneous catalysts by means of highly complex ab initio molecular dynamics simulations. For his PhD work, Dr. A. Comas-Vives was awarded the Extraordinary Award of Doctorate. In his first postdoctoral stay at the University of Ulm (Germany) he extended his area of expertise to surface science and electrochemistry. In 2012, he started as postdoctoral fellow in a highly prestigious institution (ETH Zürich, ranked top-4 in Europe) under the supervision of Prof. Christophe Copéret. Here, he moved to the field of surface chemistry and heterogeneous catalysis and studied the reactivity of hydrocarbons on metal oxide surfaces, the characterization of active sites in zeolites and the catalytic activity of well-defined metallic single-sites towards the upgrade and valorization of hydrocarbons.

Since 2014, he has been PI of three research projects and co-PI of an additional project in the field of computational heterogeneous catalysis, raising a total amount of more than 720.000 Eur. Among them, an SNF Ambizione Fellowship (2014-2016, 438.551 Eur.), which allowed him to start his independent carrier and also a research grant from ETH Zürich that currently hires a PhD student working under his supervision (2015-2018, 187.302 Eur.). During his scientific carrier, Dr. A. Comas-Vives has published several important contributions in the field of catalysis. He has co-authored 36 publications including one book chapter (21 publications within 2014-2017). Among them, he has published in PNAS (2), JACS (6), Angewandte Chemie (2), ACS Central Science, Chemical Reviews, and ACS Catalysis (2). He has an h-index equal to 16 and 724 citations. Dr. A. Comas-Vives has given 25 oral presentations in conferences and research centers, six of them upon invitation. He has active collaborations with several international group leaders in their respective fields: quantum chemistry (Prof. P. Sautet, UCLA), metadynamics simulations (Dr. M. Iannuzzi, University of Zürich), surface science and heterogeneous catalysis (Prof. C. Copéret, ETH Zürich), dry reforming of methane (Prof. C. Müller, ETH Zürich), NMR spectroscopy (L. Emsley, EPFL Lausanne), kinetic studies of heterogeneous catalysts (Prof. F. Ribeiro, University of Purdue) and zeolite synthesis (Prof. I. Hermans, University of Wisconsin-Madison). Overall, the detailed research carrier of the candidate proves the great leadership of Dr. A. Comas-Vives in order to successfully develop his own research lines in the field of computational heterogeneous catalysis.

Resumen del Currículum Vitae:

Dr. A. Comas-Vives obtained the bachelor degree in Chemistry at the Autonomous University of Barcelona in 2004. He did his PhD in Theoretical and Computational Chemistry at the Autonomous University of Barcelona under the supervision of Profs. A. Lledós and Gregori Ujaque. During this period he was awarded a Predoctoral FI grant from the Generalitat de Catalunya and an FPU Fellowship from the Spanish Government. For his work during the PhD in the field of computational homogeneous catalysis he received the Extraordinary Award of doctorate (2009).

Dr. A. Comas-Vives has 7 years of international experience abroad since he obtained the PhD degree. From 2010 to 2012 he did a postdoctoral stay in the field of theoretical electrochemistry under the supervision of Prof. T. Jacob. In 2012, he moved to Switzerland (ETH Zürich) and started working in the field of surface chemistry and heterogeneous catalysis under the supervision of Prof. C. Copéret.

In 2014, he started his independent carrier via an SNF Ambizione fellowship and started developing his own research line at ETH Zürich. His main research interests are focused on using and developing multiscale modeling approaches to the CO₂/CO conversion to fuels catalyzed by oxide-supported metal nanoparticles. He is also interested in the upgrade of hydrocarbons catalyzed by single-site catalysts supported on oxides. Within his main research line, he has been the only Principal Investigator of three research projects and co-Principal Investigator of an additional one and he has an extended list of international collaborators (see summary of the research carrier and the main research line).

During his scientific carrier (2005-2017), he has published 36 papers in scientific papers (including one book chapter) in high-impact journals such as PNAS (2), JACS (6), Angewandte Chemie (2), Chemical Reviews, ACS Central Science or ACS Catalysis (2). He is corresponding author of 11 papers and first author of 10 papers. He has given 25 oral presentations in conferences and research centers, six of them upon invitation and has been invited as keynote speaker in the next *II Biental de la Real Sociedad Espanola de Química* in the session devoted to Theory (Sitges, 25-29 June 2017). Dr. A. Comas-Vives has participated in a total of 22 funded research projects. His



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supervision experience can be summarized as follows: 3 postdoctoral fellows, one PhD student, one master thesis and five semester students. He has teaching experience in the Universitat Autònoma de Barcelona and in the Bachelor degree of chemistry at ETH Zürich. In summary, the candidate obtained his PhD only 7-8 years ago but he has an excellent research-track record, he has published very important contributions in the field of computational catalysis and has demonstrated a very high degree of independence in order to lead scientific research, being an excellent candidate in order to join the Spanish Research System via the Ramon y Cajal program.



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Nombre: ROMERO NIETO, CARLOS
Referencia: RYC-2016-19705
Área Científica: Química
Correo Electrónico: romero.nieto.carlos@gmail.com

Título:

Synthesis and Properties of New Organic Materials

Resumen de la Memoria:

I started as an undergraduate student preparing totally asymmetric PPV dendrimers at the Department of Organic Chemistry of the University of Castilla-La Mancha. I got my PhD degree from the same university on the synthesis of novel phosphorus-based architectures and made important contributions in the field of organophosphorus materials; i.e. I developed novel dendrimers with a dithienophosphole core and exploited their properties in fields such as photophysics, self-assembly, liquid crystals and sensors. During my PhD, I spent thirteen months in the group of Prof. Baumgartner in Calgary (Canada), a leading research group on phosphorus heterocycles chemistry. I highlight from my PhD the discovery of novel multifunctional organophosphorus gels and liquid crystals. This investigation was an important breakthrough in the field since it paved the way to a research line that is currently still under development.

After, I carried out a postdoc with the Prof. Guldi at the department of Physical Chemistry of the University of Erlangen during aprox. three years. There, my expertise was the study of the optoelectronic properties of novel materials and the preparation of prototype devices for photovoltaic applications. In particular, I investigated the electronic communication between organic/inorganic materials by means of ultrafast spectroscopic techniques; i.e. transient absorption spectroscopy, steady-state spectroscopy and electrochemical techniques. I focused my investigations on three types of materials: a) subphthalocyanine-based conjugates, b) carbon nanoforms and c) self-assembled materials. As a whole, I reported new strategies to obtain materials with efficient electron transfer events for photovoltaic applications. At the end of my postdoc, I published seventeen publications (see CV).

After, I formed my independent research group at the Institute of Organic Chemistry of the University of Heidelberg, Germany. I have currently two research lines: a) I develop novel phosphorus-based architectures as multifunctional materials for light-based applications. I discovered a new synthesis to access novel phosphaphenalenenes. Also, I reported for the first time the impact of embedding six-membered phosphorus heterocycles into polyaromatic systems. I described novel highly luminescent phosphorus heterocycles and successfully developed a new generation of organic light-emitting diodes. b) I investigate new boron-based materials for solid-state luminescence. I discovered a new protocol to switch on the solid-state luminescence of classically non-emitting aldehydes and enable piezochromism. Thus, with my independent research group, I have established robust bedrocks in two fields of research, which are currently under development. My independent research has led, among others, to two Angewandte Chemie and a patent. A JACS article and a second patent are currently under revision.

Resumen del Currículum Vitae:

I developed my skills in organic synthesis as an undergraduate student achieving the synthesis of asymmetric dendrimers at the Department of Organic Chemistry of the University of Castilla-La Mancha. I got my PhD from the same university on the synthesis of novel phosphorus-based dendrimeric structures. Also, I could teach practical courses in organic chemistry for third-year students during three semesters. To hone my skills on phosphorus chemistry, I spent two predoctoral stays, a total of thirteen months, in the Prof. Baumgartner group in Calgary, Canada, a renowned expert in phosphorus heterocycles chemistry. There, I supervised four-months summer projects for undergraduates. As a whole in my PhD, I exploited the properties of novel phosphorus-based molecules in fields of research such as photophysics, self-assembly and sensors.

After my PhD, to strengthen the multidisciplinary of my education, I carried out a postdoc with the Prof. Guldi at the Department of Physical Chemistry of the University of Erlangen, Germany, during more than three years. During that time, I touch practical courses on physical chemistry. I investigated a variety of novel organic/inorganic materials, their optoelectronic properties and the preparation of prototype devices for photovoltaic applications; I focused my investigations on: a) subphthalocyanine-based conjugates, b) carbon nanoforms and c) self-assembled materials. As a result, I published more than fifteen publications in journals of very high impact such as Nature Communications, Angewandte Chemie, Journal of the American Chemical Society, Advanced Materials, Advanced Functional Materials, Chemical Science.

In 2013, I began my independent research career at the Institute of Organic Chemistry of the University of Heidelberg, Germany, as Junior Group Leader and started the German Habilitation. To this end, I was awarded with a Liebig Fellowship, a prestigious research grant from the Association of the German Chemical Industry to build up my own research group. According to my background, I started my independent research career on the development of novel phosphorus-based architectures as multifunctional materials for light-based applications and I started a new field of research based on boron-based materials. My two research lines have led, among others, to two Angewandte Chemie articles (one of them hot); I also got a patent. I have presented my work in more than twenty national/international conferences and I will be given by February 2017 a total of seven invited talks in renowned universities from Spain,



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England and Germany.

Recently, I successfully passed the first evaluation of the German Habilitation and I was awarded by the University of Heidelberg with the prestigious Hengstberger Award. I also got a second project as P.I.

Since 2013, I am lecturer assistant of Prof. Bunz, teaching organic chemistry for third-year students and in 2017, I will teach my own specialized lecture: fundamentals and applications of phosphorus chemistry. To date, I have supervised in my group a total of five bachelor theses, six research interns, three theses, one master thesis, two PhD candidates and a postdoc.

Currently, I am organizing for the fourth semester a lecture series at the University of Heidelberg. In March 2017, I am organizing of the European Hengstberger Symposium New Horizons in Smart Materials.



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Nombre: BARRIO FERNANDEZ, PABLO

Referencia: RYC-2016-20951

Área Científica: Química

Correo Electrónico: pablo.barrio@uv.es

Título:

New Perspective in organometallic and asymmetric synthesis

Resumen de la Memoria:

My research career started in the group of Prof. Barluenga during the last year of my degree working on the application of Fischer carbene complexes (FCC) in asymmetric synthesis. I then continued my training by undertaking PhD studies in the same group. During this period my topic of research switched to the transmetallation reaction on FCC. Firstly, the qualitative modification of the reactivity of FCC by carbene transfer to nickel was reported for the first time. Unprecedented [3+2+2] and [2+2+2+1] cyclization reactions with terminal alkynes were observed (ACIE 2003). Then the reactivity towards allenes was studied. The complementarity exhibited by two transition metals (Ni, Rh) enabled the selective formation of up to four different products from the same starting materials by the careful choice of the catalyst and the reaction conditions (2xJACS 2004). Finally, the reaction of either FCC with internal alkynes afforded cyclopentane derivatives, respectively (JACS 2007, Tetrahedron 2006).

During this period I carried out two short stays working on the synthesis of cyclen based ligands and the corresponding terbium(III) complexes (CC 2007) and the low-valent iron catalyzed cross-coupling reaction, respectively.

I continued my career as a post-doctoral fellow in the group of Prof. Carreira at ETH Zurich. For several months, I worked in several asymmetric catalysis research projects. Finally, I also worked on the total synthesis of the natural product Microcin SF 608. An advanced intermediate bearing the core of the natural product was accomplished. However, the total synthesis could not be achieved before I finished my stay in Zurich.

During my current stage in Valencia, I have worked in several projects. Regarding tandem reactions including an intramolecular aza-Michael reaction (IMAMR), a CM/IMAMR tandem process has been reported on linear substrates (CEJ 2010); while a nucleophilic addition/IMAMR takes place with those bearing an aromatic tether (OL 2010). In the field of DOS, Ellman's imines derived from o-halobenzaldehydes were shown as versatile substrates for the asymmetric construction of a carbo- and heterocycles (OL 2011, 2xOL 2013, CEJ 2013, OL 2014, CEJ 2015, 2xOL 2016, JOC 2016). Recently, a new research line within the field of chiral Brønsted acid catalysis has been set up. First, a tandem allylation/RCM process was reported (ASC 2013). Then, the use of functionalized allylboronic esters in asymmetric catalysis has been reported for the first time (CC 2015 Emerging Investigators Special Issue). This year the Brønsted acid catalyzed allylboration of o-alkynylbenzaldehydes was studied (ACS Catal 2016). Finally, I have started working on a medicinal chemistry project (PCT Int. Appl. (2014), WO 2014128198 A1 20140828). My research articles have totally received 913 citations (212 of them, a 23% in 2016), an average of 141 citations per year during the last 5 years 2012-16. These data may be summarized in an H index = 15.

Currently, my two main research lines are related with asymmetric allylations and the use of o-substituted chiral sulfinimines in DOS. The first of them, has resulted in 4 publications and a PhD Thesis. Moreover, international collaborations with world-leading research groups (Profs. Akiyama and Houk) have been established. The second one has given rise to 10 publications, 3 MSc and 2 PhD Theses.

Resumen del Currículum Vitae:

My research career started in the group of Prof. Barluenga where I undertook PhD studies on the transmetallation reaction of Fischer Carbene Complexes (FCC). First, the qualitative modification of the reactivity of FCC by transmetallation to nickel was reported for the first time. Then, the reactivity towards allenes was studied. Finally, the reaction of FCC with internal alkynes afforded cyclopentane derivatives. These results were gathered in my PhD Thesis.

During my PhD, I carried out two stays at Trinity College Dublin and the Max Planck Institut für Kohlenforschung, respectively.

I continued my career as a post-doctoral fellow in the group of Prof. Carreira at ETH Zurich where I worked in several asymmetric catalysis projects as well as on the total synthesis of the natural product microcin SF608.

Then, I joined the group of Prof. Fustero in Valencia as a Juan the la Cierva fellow. During this time, besides collaborating in several ongoing projects such as the intramolecular aza-Michael reaction or the use of terphenyl compounds in medicinal chemistry, I have been given the opportunity to set up my own research lines dealing with the use of Ellman's imines derived from o-halobenzaldehydes in DOS and the chiral Brønsted acid-catalyzed allylboration reaction. I have also co-tutored four (4) Master and three (3) PhD Theses (two more are underway, one scheduled for March 2018) and written two reviews and a Personal Account, by invitation. In order to improve the international profile of my CV as well as to establish scientific collaboration with leading research groups in several fields of my current interest, during the last years I have performed three (3) short post-doctoral stays abroad working in the groups of Prof. Akiyama (Gakushuin University-Japan), Prof. Prakash (University of Southern California-USA) and Prof. Hammond (University of Louisville-USA). Two (2) publications have already derived from those stays, two more are under preparation and several students have been exchanged.

The results obtained along my career have given rise to 29 publications in international journals (24 Q1: 2CR, 3 JACS, 1ACIE, 1 ACS Cat, 7 OL, 2CC, 1ASC, 4CEJ, 1 JOC, 1 OM, 1 Chem. Rec.), an international patent and 8 communications to national and international conferences



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highlighting my participation as speaker in a COST action and in two International workshops and 5 invited lectures in the US and Japan. In addition, I would like to highlight several recent international recognitions to my incipient career: the invitation to the CC²s 2015 Emerging Investigators Special Issue and the Thieme Chemistry Journals Award 2015; as well as invitation to write reviews for The Chemical Record and Synthesis and an interview in Synform (Young Career Focus, Synform 2016 A15-17). Finally, I have acted as Main Proposer in a COST Action (CO-2016-2-21214) and as a Secondary Proposer in a Marie Skłodowska Curie Innovative Training Network (FLUROVAL-H2020-MSCA-ITN 2017) applications, both currently under evaluation, and I am currently preparing my application for an ERC Consolidator Grant (deadline February 8th).



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Nombre: GARCIA LOPEZ, JOSE ANTONIO
Referencia: RYC-2016-20137
Área Científica: Química
Correo Electrónico: joangalo@um.es

Título:

Organometallic, coordination chemistry and catalysis

Resumen de la Memoria:

For the last 12 years I have focused my research on two complementary topics: organometallic chemistry and its application in catalysis. During my PhD and initial postdoctoral experience I studied the synthesis and reactivity of novel palladacycles. This period gave rise to 12 articles in *Organometallics*, one in *Chem. Commun.* (featured as front cover) and a patent application on the preparation of Buchwald type precatalysts for amination reactions. I acquired a large experience in several synthetic and purification techniques of different types of compounds (coordination, organometallic and organic) as well as their structural characterization. During my predoctoral stay in Glasgow (U. K.), I also learned the basis of DFT calculations, a useful tool that I have later applied in several of my publications. In my postdoctoral stay in Manchester (30 months), I explored: i) transition metal catalyzed reactions involving C-H activation steps, ii) trapping of reactive intermediates such as arynes, and iii) oxidative couplings. From these topics, I published two articles in *Angew. Chem. Int. Ed.* and two in *Org. Lett.* This postdoctoral experience conferred me additional skills to design more complex organic transformations and perform mechanistic experiments. Since my re-incorporation to the University of Murcia in 2015, I have developed my own research line focused on transition metal catalysis in cascade reactions, a topic of high interest because these transformations are the key for the development of more sustainable processes. So far, this research line has given rise to one *Angew. Chem. Int. Ed.*, one *Adv. Synth. Catal.* and one *Chem. Commun.* (just accepted with revision). In addition I have established international collaborations with Prof. Michael Greaney (U.K) and Dr. V. Metha (India) to write interesting reviews on topics such as the synthesis of biaryls (*Chem. Soc. Rev.*) and Pd-catalyzed remote C-H activation (*Chem. Cat. Chem.*), and further experimental collaborations are currently underway.

Resumen del Currículum Vitae:

I completed the B.Sc. in Chemistry in the University of Murcia (UMU) in 2004. I joined the PhD program in the same University, working on the synthesis and reactivity of cyclopalladated complexes. In 2010, I obtained my PhD degree with an European mention, since I performed a predoctoral stay at the University of Glasgow (U.K.) to study DFT calculations. I continued working as a postdoctoral researcher at the UMU for nearly 2 years. During this period I gained insight into organopalladium chemistry. In 2012, I moved to the University of Manchester (U.K.) because I got a postdoctoral research associate contract for 18 months. Later on, I got a postdoctoral fellowship from the Séneca Foundation to remain in Manchester for another 12 months. In that period, I worked on projects involving transition metal-catalyzed reactions and trapping of reactive intermediates, such as arynes. In April 2015, I got a two years postdoctoral contract at the UMU. Since then, I have implemented a new research line devoted to the discovery of new synthetic methods based on transition metal catalysis. Along all these years I have acquired a strong background in both organometallic chemistry and catalysis, which is reflected in one patent and 21 publications, all of them in the first quartile (Q1; 1 *Chem. Soc. Rev.*, 3 *Angew. Chem. Int. Ed.*, 1 *Adv. Synth. Catal.*, 1 *Chem. Commun.*, 2 *Org. Lett.*, 1 *Chem. Cat. Chem.*, and 12 *Organometallics*). I am the corresponding author in five of them (H index 12, total citations 366). I have participated in 8 research projects funded by regional (2), national (8) and international (1) programmes. I participated in 12 national and international conferences, including an oral communication in the last EuChems. Additionally, I have been referee of international journals such as *Org. Lett.*, *Chem. Eur. J.*, *Dalton Trans.*, *J. Organomet. Chem.*, *RSC Adv.* I have also been involved in the teaching of several subjects in the area of Inorganic Chemistry within the Chemistry degree at the University of Murcia. Moreover, I have co-directed the final year project (TFG) of two students (other two TFG are in progress), one master thesis (TFM), and currently I am the co-supervisor of a PhD student. Additionally, I have the "Profesor contratado doctor" certificate by the ANECA.



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Nombre: CARRILLO FUMERO, ROMEN

Referencia: RYC-2016-20296

Área Científica: Química

Correo Electrónico: rocarril@ull.es

Título:

Supramolecular Chemistry, Green Chemistry and Drug Delivery

Resumen de la Memoria:

During my entire career, I have acquired a strong background in organic chemistry, with a broad interdisciplinary training. Indeed, in all these years of research, I have designed and synthesized molecular responsive systems, I have studied and quantified non-covalent interactions, I have developed greener synthetic methodologies and I have envisioned novel strategies for targeted drug delivery.

In my PhD years, supported by a FPU fellowship, I started developing receptors where intermolecular non-covalent interaction between host and guest were vital for the chiral discrimination displayed by the whole system. Such interactions could be detected and quantified by instrumental techniques (Angew Chem 2009). More recently, as an independent researcher, I have also evaluated a completely different mechanism of cooperativity, which although it is usual in proteins, it is still scarcely reported in synthetic receptors (Angew Chem 2011, Chem Eur J 2013, JOC 2014).

During my post-doc in David Leigh's group, supported by the prestigious Ramón Areces fellowship, I took advantage of non-covalent and organometallic interactions for the control of molecular shuttles and walkers (Chem Sci 2011, JACS 2014). Such an experience in supramolecular organometallic chemistry made possible a collaboration with the Universidad de Valladolid, to create a chiroptical switch (Chem Comm 2011).

Worth to mention, I have also been involved in several projects of synthetic methodology during my PhD and afterwards. Indeed I have lately started a novel research project that looks for greener synthetic methodologies. This research line has been very fruitful leading to the discovery of direct C-H arylation reactions and also a metal-free oxidation with air at room temperature and atmospheric pressure (Angew Chem 2014, Chem Comm 2015 & 2016, Green Chem 2016).

Finally I am also developing an innovative method for targeted drug delivery, based on conceptually novel stimulus-responsive molecular capsules and/or pro-drugs. It is worth to mention that this research line has been economically supported by MINECO (CTQ2015-7324-JIN, 204490), acting as PI) and by Asociación Española contra el Cáncer (aecc 2016, 135000), acting as PI) and it has passed to the 2nd step of the ERC Starting Grant.

Resumen del Currículum Vitae:

I completed my Chemistry Degree at Universidad de La Laguna (best grade of my promotion), and then I was awarded a FPU fellowship to carry out my PhD degree, which I got in 2007.

During my PhD, I mainly worked in supramolecular chemistry and in the synthesis of bioactive compounds and methodology. Furthermore, during my PhD studies, I carried out a 6-month predoctoral stay in Columbia University, under the supervision of Colin Nuckolls, working on conductive polymers and conductive self-assembled aromatic columns. My PhD research led to nine international peer-reviewed publications, most of them as first author. In 2007, I joined the research group of Prof David Leigh, as a postdoctoral research associate at the University of Edinburgh. I was awarded a Fundación Ramón Areces 2-year-long Postdoctoral fellowship and later on, I was hired by the University of Edinburgh. My main task there was making synthetic analogues of the linear molecular motor actin (molecular walker) consisting of two orthogonal switches based on organometallic complexes. I also developed novel sulfur redox shuttles. In January 2010 I came back to Spain and I joined the group of Tomás

Martín at the Instituto de Productos Naturales y Agrobiología (CSIC), where we studied novel cooperative guest binding mechanisms mimicking those found in some enzymes. In 2011

I was hired as a Torres Quevedo Resercher in SIELTEC Canarias, where I developed bio-degradable self-assembled peptidic nanotubes for the entrapment of atmospheric carbon dioxide. Then, in 2013 I joined Instituto Universitario de Bio-orgánica (IUBO) since I obtained a grant from the REGPOT call of the 7th framework programme of the EU (FP7-REGPOT-2012-CT2012-316137-IMBRAIN) which provided me with funding for my research lines and for hiring a postdoc. Additionally, I have got funding from MINECO (CTQ2015-73234-JIN) and from Asociación Española contra el Cáncer aecc (Ayuda a Investigadores en Oncología 2016), in all cases as PI. Worth to mention, one project proposal inspired in one of such research lines, made it to the second step of the highly competitive ERC-Starting Grant. In summary, I have participated in 7 projects, two of them as PI; I have attended to several national



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and international congresses and I was part of the organizing committee in 3 international symposia; I have been hired as Torres Quevedo Researcher; and I have 26 publications in indexed journals, including: 3 Angewandte, 1 JACS, 1 Chem. Sci., 4 Chem. Commun., 3 Chem. Eur. J., 2 Org. Lett., 1 Green Chem, 3 JOC. Remarkably I have published 7 papers as corresponding author in top rated chemical Journals: 2 Angew (one of them highlighted in SYNFACTS and SYNFORM), 2 Chem. Commun. (One of them invited to the Emerging Investigator Issue), 1 Chem. Eur. J., 1 Green Chem. and 1 JOC (selected as featured article and cover). I have also performed reviewer tasks for several journals (JACS, Chem Eur J, etc). Moreover I have got funding for my research lines from public and private national institutions and from the european comission, and I reached the second step of the ERC-Starting Grant 2014. I am currently supervising 4 PhD students and one master student. All of the above prove my scientific and leadership abilities.



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Nombre: TATAY AGUILAR, SERGIO

Referencia: RYC-2016-19817

Área Científica: Química

Correo Electrónico: sergio.tatay@uv.es

Título:

Synthesis and Deposition over Surfaces of new Materials with Interest for Molecular Electronics and Spintronics

Resumen de la Memoria:

I have more than 12 years of professional experience. In 2004, I started working on the synthesis of different ligands, especially oligopyridine conjugates, and their metals complexes for the development of new metallosupramolecular architectures and molecular machines (Inorg. Chem. 47 (2008) 5197, Chem. Commun. 47 (2011) 8235). I also used these molecules as active components of sensing devices (Org. Lett. 8 (2006) 3857), photovoltaic solar cells (J. Mater. Chem. 17 (2007) 3037) and light emitting electrochemical cells (Inorg. Chem. 48 (2009) 3907). In collaboration with Prof. R. García (Microelectronic Institute of Madrid) I combined bottom-up (surface functionalization with Self-assembled Monolayers) and top-down (Local Oxidation Lithography) approaches to deposit target molecular nanoobjects over nanopatterned areas of a silicon surface. This led to the organization over surfaces, with unprecedented accuracy, of Mn₁₂ Single-molecule Magnets (Adv. Mater. 19 (2007) 291), Ferritin biomolecules (Adv. Mater. 22 (2010) 588) and Prussian Blue Analogue nanoparticles (Adv. Funct. Mater. 22 (2012) 3625). By the end of my pre-doctoral period I joined the group of Prof. H. Vos (Dublin City University, Ireland) to improve my knowledge on polypyridine photophysics (Inorg. Chem. 49 (2010) 6897).

In 2008, I defended a European PhD entitled: Bistable Metallic Complexes for Organic electronics: Synthesis and Surface Organization of Rotaxanes and Single Molecule Magnets. Next, he joined the Unité Mixte de Physique CNRS/THALES (UMR137) under the supervision of Dr. P. Seneor as a post-doctoral researcher. In the UMR137 I worked in the group of Prof. A. Fert (Nobel laureate 2007) on the integration of organic materials into spintronic devices. There, I was able to deposit Self-assembled Monolayers into organic magnetic tunnel junctions (*ACS Nano 6 (2012) 8753), showed that these hybrid devices are capable of working at high voltages in future spintronic applications (Adv. Mater. 24 (2012) 6429) and filled a patent (WO/2012/113898). During this part of my career, I became very familiar with UHV deposition techniques (Appl. Phys. Lett. 106 (2015) 082408), advanced surface characterization techniques like VASE (Small 10 (2014) 1594), XRR (Inorg. Chem. 52 (2013) 6214), SAES (Adv. Funct. Mater. 22 (2012) 3625) and CT-AFM (Appl. Phys. Lett. 108 (2016) 243101). I was also well trained in optical and AFM lithography techniques and got all the background necessary to perform ultralow noise (magneto)transport measurements at room and low temperature (J. Phys. Chem. Condens. Matter. 28 (2016) 094010).

In January 2013, I re-joined the ICMol and set a new line of research based on the development of new materials with interests for molecular electronics and spintronics. Within this line of research, I developed new coordination complexes (*Chem. Eur. J. 20 (2014) 6939, *Org. Biomol. Chem. 12 (2014) 7572, *Eur. J. Inorg. Chem. (2016) 1851) and worked on the deposition of self-assembled monolayers over ferromagnetic substrates (*AIP Adv. 5 (2015) 057131 and *Langmuir 31 (2015) 5311). Besides, I have integrated some of those systems into molecular/organic junctions (J. Am. Chem. Soc. (2014) 8314 and J. Am. Chem. Soc. (2016) 2576). During this period, I have co-supervised 1 PhD and 5 Master Students.

Resumen del Currículum Vitae:

I work at the Instituto de Ciencia Molecular (ICMol, María de Maeztu excellence unit since 2016) at the Universitat de València (UV, excellence campus since 2010). In 2003, I gained my Degree in Chemistry from the UV (Extraordinary Award to the best graded), shortly afterwards I obtained a FPU Grant and joined Coronado's group as a pre-doctoral student. Moreover, I gained expertise in the fields of nanotechnology, molecular magnetism and the chemistry of supramolecular materials, obtaining deep skills in organic, coordination and surface chemistry. During my doctoral period, I was also able to obtain knowledge in other areas like molecular sensing or molecular photophysics. In 2008, I completed my PhD in Chemistry on the design of Bistable Metallic Complexes for Organic Electronics with the highest mark "Cum Laude" along with the Best Thesis in Chemistry award from the UV.

After obtaining my PhD degree I joined the Unité Mixte de Physique CNRS/THALES (UMR137) as a post-doctoral researcher shortly after becoming a Marie Curie (MC) IEF Fellow. There, I worked for four years in the area of molecular spintronics, more precisely on the integration of organic materials into spintronic devices mastering lithographic techniques and magnetotransport measurements.

At the beginning of 2013, I re-joined the ICMol as a Juan de la Cierva-MC CIG Fellow and set a new line of research dealing with the development of different materials with interests for molecular electronics and spintronics. I am specially attracted by the possibilities offered by Bistable Metallic Complexes. Within this line of research, I have co-supervised M. Mattera (2014), J. Gomez (2015), P. Hirchenhahn (2015), M. Gavara (2016) and E. Miguel (2016) Master thesis. Moreover, I completed the supervision of Dr. J. Ponce PhD thesis (2014) and I am currently supervising M. Mattera (to be completed in 2017) and M. Gavara and E. Miguel PhD thesis (to be completed 2020).



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Turno de acceso general

On top of that, I have combined my research with Chemistry teaching at the UV and in 2016 I was appointed Assistant Professor of Inorganic Chemistry at the Faculty of Chemistry in Valencia.

My ability to develop an independent research and to self-finance my research, both at the UMR137 physics and at the ICMol, is illustrated by the obtaining of two consecutive Marie Curie Actions (NANOCON and SAMESFERE), the publishing of 7 articles as corresponding author and the granting of 3 synchrotron proposals as main proposer. During my career, I have worked with a number of collaborators in many different areas, showing my capacity to work in a high-level collaborative and multidisciplinary environments, and have published 1 patent and 34 "peer-reviewed" papers with 99 co-authors (24 in the 1st quartile, in half of these papers Prof. Coronado is not among the authors list) in primary Materials Science, Physics and Chemistry journals. I accumulate more than > 700 citations (avg. citations 2012-2016 >95 cit /year) and an h-index of 14. I have directly participated in different international conferences (13 of them as oral communications, 4 as an invited speaker), European Projects (7) and seminars.

Moreover, I peer-reviews Royal Society of Chemistry (RSC), American Chemical Society (ACS), Elsevier and Institute of Physics (IOP) Journals and I am a Member the Real Sociedad Española de Química (RSEQ, from 2005).



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Turno de acceso general

Nombre: GARCIA FANDIÑO, REBECA
Referencia: RYC-2016-20335
Área Científica: Química
Correo Electrónico: rebecca.garcia.fandino@usc.es

Título:

Computational study of supramolecular systems at the interface between Chemistry and Biology

Resumen de la Memoria:

My PhD (FPI-MCINN) was focused on the experimental and computational evaluation of metal-catalyzed cycloadditions (6 papers, 1 patent). During my PhD I became interested in computational simulations applied to chemical supramolecular systems, which led to focus my career in that field.

In my 1st postdoc I joined the group of Prof M Orozco (IRBB-PCB,MECD-Fulbright) where I acquired valuable expertise in Molecular Dynamics simulations of large macromolecular architectures (nanotubes & proteins in solution). As a result of this period, 4 papers were published in recognized journals (JACS, JMB, PLOS Comput Biol, OBC).

During my 2nd postdoc with Prof MSP Samson (Oxford University-UK, MECD-JCastillejo) I was involved in a project related with the simulation of nanopores in lipid bilayers, resulting in the publication of 2 important manuscripts:PNAS-where I am the only author besides supervisor, and ACS Nano-first&corresponding author.

After 4 years of postdoctoral experience I moved back to Spain associated to the group of Prof JR Granja (CIQUS-USC) with a Juan de la Cierva contract, where I started my own research line on the simulation of supramolecular systems in different environments. I have also maintained a secondary research line based on the computational study of organometallic reactions. As a result, 14 publications (1 more submitted) and 4 Book Chapters were published in some of the best journals in the area (ACS Nano, JACS, OL, Chem Sci, CEJ, etc), besides a registered database transferred to industry. I got my own funding as PI from different projects, i.e. Xunta de Galicia-Emergentes (2012-2015,55.000€) and MINECO-Proyecto Jóvenes Investigadores-Retos (2016-2019, 204.490€). During this time I have also performed 380 hours of teaching duties and supervised several students: 3PhD-in supervision, 2TFM, 6TFG, 2STSM (H2020), 3industrial fellowships.

Recently, I was awarded with a FCT Investigator Grant (IF/01133/2015) from Ministerio da Ciência, Tecnologia e Ensino Superior de Portugal), and I am currently PI at Faculdade de Ciências, Universidade do Porto. This grant has allowed me to continue my research line focused on the design of new and improved antibacterial agents based on understanding their action mechanism at the level of membranes.

I have enhanced my academic research with a complementary industrial approach. As main founder & CEO of MD.USE Innovations SL, I lead a team that develops commercial scientific software & apps for molecule visualization & simulation based on state-of-the art technologies, such as Virtual/Augmented Reality. Currently supporting 3 salaries, it has won several autonomic and national awards and has allowed the funding of a PhD student (Doctorado Industrial 2015-2019, MICINN) and my participation in European calls as PI.

From the point of view of internationality, apart from my actual position as FCT Investigator Grant in Portugal, I have recently obtained international funded contracts as PI (membrane transporting proteins-INP México) and I have been partner in different International Training Network (MC-ITN) proposals focused on antimicrobials. I am collaborator in a European grant proposal to BBSRC, in the framework of the nanopore studies. I also participate in the Management committee of a H2020 COST action (CM1306), aiming to integrate static and dynamic aspects of biomolecules.

Resumen del Currículum Vitae:

I obtained my PhD(FPI-MCINN) at the University of Santiago de Compostela (2006, Cum Laude, Extraordinary Prize). I performed 2 predoctoral stays in Madrid (UAM) and Germany (Philipps-Universität Marburg).

I have an extensive postdoctoral experience of more than 4 years in 2 groups: For my 1st postdoc with Prof M Orozco at IRBB-PCB (~3 years) I obtained a MECD/Fulbright fellowship. For my 2nd postdoc I joined Prof MSP Sansom in Oxford University-UK(~1.5 years,Xunta de Galicia/Alvariño & MECD/JCastillejo).

A Juan de la Cierva contract (2010) allowed my temporal return to the Spanish academic system. I associated to Prof JR Granja (CIQUS-USC) where I obtained funding for my own research as an independent PI from a competitive grant aimed to support brilliant young researchers (Xunta de Galicia-Emergentes, 2012-2015, 55.000€) and from Proyecto Jóvenes Investigadores sin vinculación o con vinculación permanente (MINECO-Retos, 2016-2019, 204.490€). I also achieved > 7 million hours of computing time competing to BSC-RES calls.



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ADMINISTRATIVA

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Turno de acceso general

I was recently awarded with the highly competitive FCT Investigator Grant (IF/01133/2015) from Ministerio da Ciência, Tecnologia e Ensino Superior de Portugal), and I am currently PI in Facultade de Ciencias, Universidade do Porto (Portugal).

I have supervised several students: 3PhD-in supervision, 2TFM, 6TFG-1 interexchange German student, 2 STSM (Short Term Scientific Missions, under H2020 COST CM1306), 3 industrial fellowships. I have also performed 380 hours of teaching duties.

My scientific productivity is reflected by 26 published articles in high impact journals and 1 more submitted paper (J Mat Chem B): ACS Nano (x2), PNAS, JACS (x2), Chem Sci (x4), ACS Catal, OL (x2), CEJ (x3), JOC, JPCC, JPCB, PCCP, Plos Comput Biol, JMB, OBC, Dalton Trans(x2), Curr Top Med Chem, Bioinformatics, being first or corresponding author in 14 of them. Furthermore, I have also published 4 book chapters in Wiley, Elsevier (x2), Springer Nature, the last 2 ones to be published in 2017 as corresponding author. I am also author of an internationally extended patent (WO2005/002496) and of a registered public database (<http://cyclo-lib.mduse.com/>) transferred to industry.

The international projection of my career has been recognized with my incorporation into the Management Committee of European COST Action (CM1306-H2020). Furthermore, I am collaborator in a European grant proposal to BBSRC (BB/K01644X/1) and have been partner in several MC-ITN proposals (Marie Curie Action in H2020, i.e. MSCA-ITN-2016, MSCA-ITN-2017). I have recently accomplished 2 international contracts with INP-Mexico as an independent PI and have led a European proposal (Fortissimo-2) with the participation of industries of the size of Janssen(J&J).

The transversal profile of my research and its real projection into society benefits is reflected by the recent launching of the enterprise MD.USE Innovations SL (www.mduse.com), a University start-up in which I am the main founder and CEO. It has been distinguished with (2.000), winner of GOF-Telefonica (25.000) and Seklab Awards II. Currently it supports 3 workers on staff and it is co-funding a PhD student through a Doctorado Industrial grant (MINECO, 2015-2018, 64.620) and has been selected to participate in the internationalization program ICEX-Next (MINECO).



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Turno de acceso general

Nombre: PEREZ CUADRADO, CRISTOBAL

Referencia: RYC-2016-19881

Área Científica: Química

Correo Electrónico: cpcuadrado@gmail.com

Título:

Instrument development. Water Clusters and microolvation of organic molecules from broadband rotational spectroscopy. Novel techniques for chiral analysis by microwave spectroscopy.

Resumen de la Memoria:

I have more than ten years of active research experience working in leading international laboratories in Spain, the USA (3 years) and currently in Germany (2 years). Relevant publications from this period comprise two studies published in Science, three in Angewandte Chemie International Edition, and four in The Journal of Physical Chemistry Letters among others. Additionally, The relevance of my research has been acknowledged with several invited contributions to international conferences. Among then, last September I was invited as plenary speaker to The 24th International Conference on High Resolution Molecular Spectroscopy hosted in Pague, Czech Republic to present my results on water clusters and microsolvation by means of broadband rotational spectroscopy. I was also invited to present my research at the Gordon Research Seminar in Ventura, California in January 2016. My scientific career can be divided in the three following periods:

I obtained my PhD from the Universidad de Valladolid under the supervision of Prof. Jose Luis Alonso. My PhD work, "Rotational Spectra of Natural Aminoacids", focused on structural studies of biologically relevant molecules using molecular rotational spectroscopy and novel laser ablation techniques (2006-2011).

After graduation, I moved to Charlottesville, Virginia, USA. Here, I had the opportunity to work with Prof. Brooks H. Pate as postdoctoral research associate (2011-2014). This 3-year period was extremely fruitful as I was responsible for designing, developing and building several experimental setups for broadband rotational spectroscopy. In addition, I was responsible for implementing a new research line in water clusters and microsolvated organic molecules. As a result, we were able to push the current limits of rotational spectroscopy and perform pioneering works, two of which were published in Science, on water clusters.

After this fruitful three-year period, I was hired in October 2014 as postdoctoral researcher at the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg, Germany, working with Prof. Melanie Schnell. During this period I was directly responsible as senior person of the chirality research line, which I led in the last two years. In November 2015, my research was promoted with a Research fellowship from the Alexander von Humboldt Foundation to continue in the development of new experimental approaches to study chiral systems using rotational spectroscopy. I presently pursue this research line to explore new applications of these techniques.

I have been involved in three main research lines throughout my career in which we have been able to perform pioneering work that has contributed to usher into a new era for rotational spectroscopy. These research lines are:

- New and Novel instrument development for microwave Spectroscopy.
- The study of pure water clusters and microsolvation effects
- New experimental methods for chiral analysis.

Resumen del Currículum Vitae:

Pérez Cuadrado, Cristóbal

ORCID: 0000-0001-5248-5212

Date of birth: 05-06-1979

Nationality: Spanish

EDUCATION

2011 PhD in Chemistry. Department of Chemistry. University of Valladolid, Spain.

Thesis advisors: Prof. Dr. Jose Luis Alonso and Prof. Dr. Juan Carlos Lopez.

2005 Master in Chemistry. Department of Chemistry. University of Valladolid, Spain.

Advisor: Prof. Dr. Celia Andres

2004 Chemistry Degree. Department of Chemistry. University of Valladolid, Spain.

CURRENT POSITION

2015 -2016 Postdoctoral Senior Researcher at the Max Planck Institute for the Structure and Dynamics of Matter. Hamburg, Germany.

PREVIOUS POSITIONS

2015 -2016 Alexander von Humboldt postdoctoral fellow at the Max Planck Institute for the Structure and Dynamics of Matter. Hamburg, Germany.

2014 -2015 Postdoctoral researcher at the Max Planck Institute for the Structure and Dynamics of Matter. Hamburg, Germany.

2011 -2014 Posdoctoral Research Associate in the Department of Chemistry at University of Virginia. Charlottesville, USA.

FELLOWSHIPS & AWARDS

2016 Juan de la Cierva-incorporacion. Spanish National Programme for the Promotion of Talent and Its Employability. Declined.

2015 -2016 Posdoctoral research fellowship from the Alexander von Humboldt Foundation at Max Planck Institute for the Structure and



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Turno de acceso general

Dynamics of Matter. Hamburg, Germany.

2005 - 2009 National Spanish training programme for research (FPI, Formación de personal investigador). Department of Chemistry at University of Valladolid, Spain.

- SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2011 - 2014 2 PhD Students. Department of Chemistry at University of Virginia, USA.

2014 - 2016 3 PhD Students. Max Planck Institute for the Structure and Dynamics of Matter. Hamburg, Germany.

- TEACHING ACTIVITIES

2011 - 2014 Teaching Assistant - Molecular Spectroscopy, at University of Virginia, USA.

2006 - 2010 Laboratory Classes. Universidad de Valladolid

- ORGANIZATION OF SCIENTIFIC MEETINGS

2008 Member of the organizing committee. Isolated Biomolecules and Biomolecular Interactions (IBBI 2008). Valladolid, Spain.

- COMMISSIONS OF TRUST

Since 2016 - Reviewer for international peer-reviewed scientific journals

- MEMBERSHIPS OF SCIENTIFIC SOCIETIES

2016 Member of the Royal Spanish Society of Chemistry. RSEQ, Real Sociedad Española de Química.

2016 Member of the Jóvenes Investigadores Químicos (JIQ).

- SCIENTIFIC PUBLICATIONS

I have coauthored 26 articles throughout my career in international peer-reviewed journals: Science (2), Angew. Chem. Int. Ed. (3), Journal of Physical Chemistry Letters(4), Chemistry European Journal (1), PCCP (6) among others. These papers have received more than 500 citations. In most of them I am first or second author showing that I was close responsible for the project.

- RESEARCH INTEREST

Instrument development. Broadband Rotational Spectroscopy. Structural studies of pure water clusters and microsolvated organic molecules. New techniques for chiral analysis using microwave spectroscopy.

- COLLABORATIONS

- Prof. Dr. Brooks H. Pate. Chemistry Department, University of Virginia, USA.

- Dr. Melanie Schnell. Max Planck Institute for the Structure and Dynamics of Matter. Hamburg, Germany.

- BrightSpec Inc. Instrument development for chiral applications. Charlottesville, Virginia, USA.