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AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2020

Turno de acceso general

Nombre: RIVADA WHEELAGHAN, ORESTES
Referencia: RYC2020-028851-I
Área Temática: **Ciencias y tecnologías químicas**
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Título:

Molecular Organometallic Chemistry for Electrochemical Energy Storage

Resumen de la Memoria:

I specialized in organometallic chemistry at the IIQ, Seville (Spain) and obtained my PhD in 2013 under the supervision of Dr. Salvador Conejero. As Dr. Conejero s first PhD student, I started the research line concerning well-defined electrophilic Pt(II)-complexes, stabilized with N-heterocyclic carbene (NHC) ligands and their reactivity towards small molecules activation. Consequently, my work laid the foundations for future PhD candidates at Dr. Salvador Conejero s lab and has generated 8 scientific publications. Besides, during my PhD I worked in collaborative research projects developing 13-C enriched NHC ligands to stabilize Ru-nano particles and stayed for 4 months under the guidance of Prof. David Milstein at the Weizmann Institute of Science (Israel) working on Metal-Ligand cooperation reactions.
Later, I continued for two more years as a postdoc fellow working with Prof. David Milstein on sustainable homogeneous catalysis using well-definded Fe-complexes. The catalysts developed were used for carbon dioxide hydrogenation and organic transformations (2 works published). Also, working in close collaboration with other postdoctoral researchers, because of the inherent difficulties and high-risk nature of this research, a well-defined Fe-complex active in catalytic olefin metathesis was developed. These results remain confidential and under revision (re-submitted in 2020, Nature, 2017-09-11803A-Z).
From 2015 till 2018 I worked at the Okinawa Institute of Science and Technology (Japan) with independence, thanks to 2 highly competitive, international fellowships secured form the Japan Society for the Promotion of Science: JSPS Short Fellowship (1 year) and JSPS Standard Fellowship (2 years), including a 2 years JSPS-Kakenhi-grant (9,000 /year). I organized my project and supervised students. Here, I matured as a synthetic molecular inorganic chemist and created a new research line for the group related to multimetallic systems and their metal-metal cooperative reactivity. I have published 5 works (1 co-corresponding author) and another will be soon submitted.
Acknowledging the implications that electrocatalysis have in energy transition, I shifted to learn the electrochemical theory and experimental techniques to develop molecular electrocatalysts towards energy storage application.
Thus, I secured a Juan de la Cierva Incorporación fellowship with Prof. Antoni Llobet to develop molecular water oxidation electrocatalysts. However, I declined to accept my current position as principal investigator, MOPGA Team Leader at the Laboratoire d Electrochimie Moléculaire, Université de Paris, France.
MOPGA stands for Make Our Planet Great Again, an international competitive and multidisciplinary funding program created by the President of the Republic of France E. Macron to attract scientific talent to France. In 2018, I was awarded PI of a project grant worth 1,270 k (no overhead costs included). Thanks to this, I have created a small research team (2 postdoctoral researchers) which I managed and led (https://oresteschem.wixsite.com/home). We have successfully published in Dalton Trans (featured as HOT Article and Cover) our first contribution in molecular electrochemistry and electrocatalysis. Currently, my team targets molecular bimetallic complexes with short metal-metal distance to promote electrocatalytic C2-product formation from CO2
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Resumen del Currículum Vitae:

I did my B.S. chemistry studies at the University of Oviedo (2008) and later moved to Seville to perform my MSc. in Advance Studies in Chemistry (2009) and European PhD in inorganic chemistry (2013, with honors). I secured 2 fellowships to perform my PhD, declining the PhD-fellowship from the university to accept an FPU. From this period, I published 8 scientific papers 6 as 1st author, including JACS and ACIE. For the work reported in JACS I received the Primer Accesit-Investigación CicCartuja-Ebro Foods Award. I also published 2 scientific works from collaborating with Prof. B. Chaudret (ACIE and ChemSciTech, with 141 and 94 citations respectively in Scopus). The work from this period was presented in 12 national/international conferences.
I have a high level of international mobility (92 months), starting with a 4-month research stay in Israel working with Prof. Misltein during my PhD. This, secured me a postdoctoral contract for 2 years to work in homogeneous catalysis. Here, I published 3 papers in Organometallics (62 citations), InorgChem (82 citations) and ACIE (56 citations). This work has been presented at 3 international conferences (2 posters and Oral). Another article remains under review (re-submitted in 2020, Nature, 2017-09-11803A-Z), from an ambitious project performed in collaboration with other postdocs in the group.
After 2 years in Israel, I moved to Okinawa (Japan) to work with Assist. Prof. Julia Khusnutdinova. Being the most senior postdoc and thanks to two secured Japan Society for the Promotion of Science fellowships, including a 2 years JSPS-Kakenhi-grant (9,000 /year), I explored my scientific ideas with independence and created a new research line in the group related to metal-metal cooperative reactivity. I have published 5 scientific works: 2 1st author (ACIE and ChemEurJ with Cover Feature), 1 2nd author with equal contribution in DaltonTrans (1st author supervised), and 1 as corresponding author in ChemSci (1st author supervised). Part of the work developed in Japan has been presented orally in 6 national/international conferences. At the 98th Annual Meeting of the Chemical Society of Japan (8000 attendees), I

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obtained the CSJ presentation award.
Before I finalized my postdoctoral research in Japan, I secured a Juan de la Cierva Incorporación fellowship which I declined in favour of the awarded Make Our Planet Great Again grant (1270k), an international competitive and multidisciplinary funding program. This grant allowed me to build an organometallic lab from scratch including the purchase of a wide range of equipment and to create a small team (2 postdoctoral researchers hired) (https://oresteschem.wixsite.com/home). Since summer 2019, my lab has been operative and one piece of work been successfully published in Dalton Trans (featured as HOT Article and Cover) and presented in an online poster competition in Twitter (CIC). The MOPGA funding spans till December 2022.
Besides my scientific obligations, I reviewed for ChemCatChem, AsianJOrgChem and CoordChemRev. I acted as external examiner at the PhD defense of Juan José Moreno díaz (2018) and Praxedes Sáncez Mellado (2019). I am have submitted 3 projects in the past 6 months: 1 JCJC (Agence Nationale de la Reherche), and 1 EMERGIA (Junta de Andalucía) and 1 JIN (Ministerio de Ciencia e Innovación) as PI. I participate in COST call (under evaluation).

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Turno de acceso general

Nombre: CARNE SANCHEZ, ARNAU
Referencia: RYC2020-029749-I
Área Temática: **Ciencias y tecnologías químicas**
Correo Electrónico: arnau.carne@icn2.cat

Título:

Síntesis de materiales porosos metal-orgánicos

Resumen de la Memoria:

My research career has been focused in the synthesis of functional molecular materials, which properties can be modulated through the principles of Supramolecular Chemistry. I have pursued the development of extended 3D Metal-Organic Frameworks (MOFs) and molecular 0D Metal-Organic Polyhedra (MOPs) from a fundamental and applied point of view.
I was introduced in the field of MOFs during my PhD. The first period of my research career was dedicated to two important challenges that MOFs were facing: i) their scale up production; and ii) the synthesis of MOFs in the form of nanoparticles (nanoMOFs) (Chem. Soc. Rev 2011). These challenges were faced together by implementing the spray-drying technique as a novel methodology for the mass production of nanoMOFs and their related composites (Nature Chemistry 2013 & Adv. Mater. 2015 & Adv. Funct. Mater. 2015). This new methodology was patented (EP20110183773) and licensed to MOFapps (http://www.mofapps.com/). The availability of a broad range of nanoMOFs made it possible performing cytotoxic studies to evaluate the biocompatibility of the most representative MOF structures and start using them as contrast agents for magnetic resonance imaging (JACS 2013 & Chem. Eur. J. 2015).The results of the PhD thesis were recognized with the extraordinary doctorate award issued by the UAB.

My experience in porous materials was further increased during my post-doctoral studies in Kitagawa s group at Kyoto University (Japan) thanks to the financial support of the 2-years JSPS fellowship granted in 2014. We developed novel post-synthetic methods to endow MOFs with CO photo-releasing properties for biomedical applications (Chem. Sci. 2017). During this postdoctoral stage, I was also introduced to an alternative family of porous materials: the Metal-Organic Polyhedral molecules (MOPs). We made an important contribution to the field by synthesizing the first robust MOPs based on Rh(II) (Rh-MOPs) (Inorg. Chem. 2016 & Chem 2017). I took advantage of the robustness and solubility of Rh-MOPs to assemble MOPs into amorphous supramolecular polymers that display the intrinsic porosity of the MOP units (Nat. Commun. 2018).

The new concepts learned in Kitagawa s group were in line with the research conducted in Maspoch s group when I returned to ICN2 in 2017 thanks to the Juan de la Cierva fellowship (incorporación - 2018). In these past years, we have developed a new method to control the assembly of nanoMOF particles into colloidal crystals exhibiting photonic properties (Nature Chemistry 2018 & Chem. Soc. Rev 2019) and into self-folding films (Angew. Chem. Int. Ed. 2018 & Adv. Mater. 2019). Most importantly, in 2018, I have established my independent research line focused on the synthesis of porous materials based on MOPs. As main responsible of this line, I have supervised 1 PhD thesis and 2 Master Thesis, and I m currently supervising 2 postdoctoral researchers, and 2 PhD and 1 master students. In this research line, we have demonstrated that Rh-MOPs behave as nanoscopic molecules amenable to stoichiometric reactivity through coordination and covalent chemistry (JACS 2019 (X2) & Chem Commun 2019 & Angew. Chem. Int. Ed. 2019 & 2020 corresponding author). This scientific background and experience has allowed me to be awarded LaCaixa Junior Leader Fellowship in 2020 enhancing my independent scientific career.
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Resumen del Currículum Vitae:

Name: Arnau Carné Sánchez
ORCID: 0000-0002-8569-6208 / Google Scholar: Arnau Carné-Sánchez / Researcher ID: B-3979-2019
Date of birth: 17/07/1985
Nationality: Spanish

Education:

2014 PhD in Chemistry at the Catalan Institute of Nanoscience and Nanotechnology (ICN2) / Universitat Autònoma de Barcelona (UAB), Spain.
Thesis: New synthetic method for nanoscale metal-organic frameworks and their application as contrast agents for magnetic resonance imaging
Honours and awards: Cum laude, Extraordinary Doctorate Award (UAB)

2009 Master in Environmental Diagnosis and Management at the School of Applied Sciences of Cranfield

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University, United Kingdom

2008 Bachelor in Chemistry at the Universitat Autònoma de Barcelona (UAB), Spain.

Current position:

2020 - present: "La Caixa" Junior Group Leader at ICN2

Previous positions:

2018 - 2020: Juan de la Cierva (Incorporation) Research Fellow at ICN2

2016 - 2018: Senior postdoctoral researcher at ICN2

2014 - 2016: Postdoctoral Researcher at the Institute for Integrated Cell-Material Sciences (iCeMS) at Kyoto University, Japan / PI: Prof. Susumu Kitagawa

Fellowship and awards:

2010 FI PhD Fellowship granted by the Generalitat de Catalunya

2014 2-year Postdoctoral Fellowship granted by Japan Society for the Promotion of Science (JSPS).
Amount of subsidy: 8.888.000 yen (73.000) / Research budget: 2.400.000 yen (19.700).

2018 Juan de la Cierva (Incorporación) postdoctoral fellowship granted by Spanish Ministry of Science, Innovation and Universities. Amount of Subsidy: 64.000 .

2020 La Caixa Junior Group Leader fellowship Junior Leader retaining granted by La Caixa foundation.
Amount of Subsidy: 177000 / research Budget: 115500

Indicators of Quality in scientific production:

Articles:
Articles published: 32

Publications in Q1: 32

Average impact factor for published articles: 13

Publications in journals with Impact factor higher than 10: 18 [Chemical Society Reviews (2), Nature Chemistry (2), Nature Communications, Advanced Materials (2), Advanced Functional Materials, Chem, Angewandte Chemie International Edition (4), Journal of American Chemical Society (3), Journal of Materials Chemistry A and Accounts of Chemical Research].

Articles as corresponding author: 5 [Journal of American Chemical Society (2), Angewandte Chemie International Edition (2) and Chemical Communications].

Citations (Des 2019 google scholar):

h-index: 22
Total citations: 2351
Articles with more than 100 citations: 7 / Average citation per paper: 73
Yearly increasing number of citations
2014: 95 / 2015: 148 / 2016: 197 / 2017: 295 / 2018: 377 / 2019: 455 / 2020: 622

Selected oral contributions at international conferences:

EuroMOF Young Investigator Symposium. October 2019. Paris, FRANCE. INVITED

21st Iranian Inorganic Chemistry Conference (IICC21). August 2019. Arak, Iran. INVITED

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MOF Young Investigator Symposium. September 2016. San Diego, USA. INVITED

Patents:

Patent: Method for the preparation of metalorganic frameworks (EP 2 764 004 B1 and US 9,352.489 B2)
Publication date: 10/04/2013 (granted)
Inventors: D. Maspoch, I. Imaz, A. Carné-Sánchez and A. María Cano Sarabia
Currently the patent is licensed to the European company, MOFapps (http://www.mofapps.com/).

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Turno de acceso general

Nombre: CRIADO FERNANDEZ, ALEJANDRO
Referencia: RYC2020-030183-I
Área Temática: **Ciencias y tecnologías químicas**
Correo Electrónico: alejandro.criado@gmail.com

Título:

Preparation, modification and biomedical applications of carbon-based nanostructures and related materials

Resumen de la Memoria:

The candidate has focused his entire research career on the chemistry of carbon-based/metaldichalcogenide nanostructures. He showed during this period how this chemistry emerges from the synthesis of carbon nanoforms, ending up in device applications, passing through the tailoring of their properties to accomplish a beneficial role. For instance, new synthetic strategies allowed the generation of aromatic molecules with potential applications in molecular electronics because of their interesting optoelectronic properties. The candidate also developed new modification methods to overcome limitations and to implement new capacities on carbon nanostructures (CNTs) such as graphene derivatives, carbon nanotubes and molybdenum disulfide. As a matter of fact, he developed a functionalization method of (CNTs) towards achieving molecular paddle-wheels and water-dispersible CNTs. By radical reactions, improved CNTs were created and, at the same time, specific anchoring moieties were incorporated. Additionally, the candidate explored non-conventional methods for the covalent functionalization of graphene with high efficiency in short times under solvent-free conditions. He also addressed a systematic study about the effect of solvents in the reactivity of graphenide intercalated with potassium cations, providing the fundamental principles of graphenide reactivity. Recently, he modulated the conductivity and spectroscopic properties of layered molybdenum disulfide by highly effective chemical phase engineering.

His motivation on carbon nanostructures and related materials led him to explore their applications in different areas. Due to his knowledge about chemical modification of these materials, he was able to implement lacking features that are particularly required in some fields. For instance, he manufactured a biosensor based on CNTs for the detection of prostate cancer for early diagnosis, achieving results that exceed that of state-of-the-art. By modification of chemical vapor deposited graphene (CVDG) he designed biosensors exploiting its electronic properties. On one hand, he explored the conductive properties of modified CVDG as a matrix-free platform in a laser desorption/ionization mass spectrometer for glycomic analysis. On the other hand, he implemented the sensing ability to an array of 50 microtransistors based on CVDG as potential devices for in vivo sensing in neural tissues. Recently, he designed an extremely sensitive Surface-Enhanced Raman Scattering immunosensor based on the MoS2/Au@Ag core shell nanoparticle hybrid nanomaterial for the detection of liver, testicle, ovary, and gastric cancer biomarkers.

At present time, the candidate is developing other research topics, such as wearable graphene-based sensors for monitoring sweat, new chemical approaches on Carbon nanotube-based nanofibers and novel synthetic methods of nanographene for bioelectronics, among others.

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Resumen del Currículum Vitae:

Dr. A. Criado has mainly focused on the synthesis, functionalization and bioapplication of carbon nanotubes, graphene, and related materials. In particular, he has deeply explored the preparation and characterization of well-defined nanographenes by bottom-up approaches. Regarding carbon nanotubes, he has developed new strategies for its chemical modification. Concerning 2D materials as exfoliated graphene and MoS2, he addressed new and alternative covalent modifications, to optimize efficiency, selectivity, and functionality. He has also worked on the biomedical application of these nanomaterials, mainly in biosensing for the early diagnosis of diseases.

Dr. Criado recently joined CICA research centre (Universidade da Coruña, UDC) as distinguished researcher through the Atracción de Talento Xunta de Galicia program, where he has started his own research group. In 2015-2020 he was a JdlC Incorporación researcher and senior postdoc in the Carbon Bionanotechnology laboratory at CICbiomaGUNE, where actively managed the daily activity of the group, developing his own research lines and supervising 7 postdocs and 2 PhD students. In 2013-2015 he was a fellow postdoc in the group of Prof. Prato at Trieste University (Italy). In 2013, he received his PhD at the Universidad de Santiago de Compostela (USC) being awarded the Extraordinary Award. In 2006, he was graduated in Chemistry at the Universidad de Santiago de Compostela (USC) being awarded with the Extraordinary Prize in Chemistry Degree.

The candidate s potential has also been acknowledged by the achievement of different awards. The most remarkable has been in 2013, he was awarded among 20.000 young scientists as one of the 550 most qualified young researchers to participate in 63rd Lindau Nobel Laureate Meeting (Germany). He has published 31 research articles in high-impact journals such as Science (IF: 41.85), Science Adv. (IF: 13.12), ACIE (IF: 12.96) and CheM (IF: 11.53). 87% of his published papers are in the first quartile (Q1) of their fields. He is corresponding author in 11 publications being last author in 1 of them. He has received more than 1153 citations with an average of 245 citations per year in the last 3 years. His h-index is 14 (WoS). He has participated as Principal Investigator in 3 projects and as Co-Principal Investigator in 4

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international research projects, including the Graphene Flagship and some other projects of the EU s framework programs (FP7 and H2020).
The candidate also has teaching experience with 363h of training for a Higher education training cycle (Ciclo formativo de grado superior) at CICbiomaGUNE and Centro Educativo CIFP Don Bosco LHII (Spain, 2018), and with 120h as teaching assistant at USC (Spain, 2010). Additionally, he has been teaching, mentoring, and hosting of 14 visiting students in University of Trieste and CIC biomaGUNE. He participated in 28 national and international research congresses with 12 oral contributions and 2 invited talks. He is Thesis advisor of two PhD students (2016-2020, 2020-2023) at Universidad del País Vasco (Spain) and supervisor of one Master thesis (2019) at Università di Bologna (Italy).
His current independent research is focused on new preparation and modification methods of carbon nanostructures and other 2D materials to tailor their properties and their applications, mainly in biosensing.

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Turno de acceso general

Nombre: DONGIL DE PEDRO, ANA BELEN
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Área Temática: **Ciencias y tecnologías químicas**
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Título:

Supported nanoparticles on carbon materials for biomass conversion

Resumen de la Memoria:

My research career has been always linked to heterogeneous catalysis, specially the development of carbon supported catalysis. One of the limitations of carbon materials is derived from their inertness, so that its functionalization and dispersion of small nanoparticles is challenging. So, my research has also been dedicated to improve the dispersion of nanoparticles. In this respect I acquired a strong expertise during my postdoctoral period at U.Concepción regarding organometallic synthesis of nanoparticles.
My first contact with heterogeneous catalysis was during my end of career project at Complutense University. The project was related to the synthesis of catalysts based on TS-1. I used the materials for the enantioselective epoxidation of alkenes.
After a period working in industry, I started my PhD at the end of 2006 at the Institute of Catalysis and Petroleochemistry with an FPI Grant from the Ministry of Education. As a result, I obtained Outstanding Cum Laude, European Mention and the extraordinary doctoral degree.
I have personally performed all the catalysts synthesis, characterization and reaction tests and the corresponding data treatment of all the techniques including XPS, Raman, thermal analysis, Solid-State NMR, among others during my PhD.
In this context I can organize my research on the following lines:
a) Immobilization of homogeneous complexes on carbon supports and its catalytic performance on enantio and chemo selective reactions. This corresponds to my PhD period. I studied functionalization of carbon materials with amine ligands and anchoring of Ru complexes for the chemoselective hydrogenation of C=O bond.
b) Supported metal nanoparticles applied as catalysts on enantio and chemoselective reactions. This corresponds to my PhD and postdoctoral experience. I evaluated the synthesis by industrial methods (flame spray pyrolysis) and other non-traditional methods (polyol) of metal nanoparticles to apply them in enantioselective hydrogenation of ethyl pyruvate and chemoselective hydrogenation of nitroarenes.
c) Bifunctional catalysts applied on the selective purification of H2. Postdoctoral period. I studied Ni/CeO2 and Cu/CeO2 systems supported on carbon nanotubes and graphene and its application on WGS and PROX reactions, and evaluated the effect of alkali dopants.
d) Heterogeneous catalysts for biomass transformations. Postdoctoral experience. I tested Ni and bimetallic NiCu nanoparticles on hydrodeoxygenation of guaiacol (lignocellulosic compound). I studied the influence of chemical surface and morphology of the support and shape selectivity.
e) CO2 valorisation. Postdoctoral period. NiZrO2 systems supported on carbon nanotubes and the effect of the synthesis method on CO2 methanation were evaluated.
Also, within this line I am now PI of a project related to the study of transition metal carbides in methanol synthesis from CO2 hydrogenation.
f) Hydrogenation of lignin molecules using formic acid as hydrogen source. This is my future research line for which the expertise acquired during my postdoctoral stage on lignin transformations and nanoparticles synthesis will be put in place. Also, I will lead and coordinate a H2020 project during 2021-2025 on this topic. Thanks to this project I will collaborate and do secondments in top of the class facilities related to Operando and in situ characterization.

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Resumen del Currículum Vitae:

Dr. Dongil has extensive experience in the synthesis and characterization of carbon materials and nanoparticles applied in heterogeneous catalysis. She obtained an FPI grant from the Ministry of Education and finished her PhD in 2011, for which she won the extraordinary doctoral award with European mention. During her PhD she studied the modification and functionalization of carbon surfaces with organic molecules and organometallic complexes, starting a new research line in her group in a topic with few works until that date. She enjoyed two secondments at the ETH Zürich and the Chimie Physique Electronique institute in Lyon where she acquired in-depth knowledge of the in situ study of catalytic reactions by infrared, and techniques for anchoring organometallic complexes. Subsequently, she completed a postdoctoral period at the ETH in Zurich where she was responsible for the acquisition and set-up of equipment such as fixed bed reactors, adsorption equipment and in situ infrared. Then, she won a Fondecyt project as Principal Investigator funded by the Chilean Ministry of Education to work at the University of Concepción, obtaining 14 manuscripts. During this period, she participated as a co-researcher in 2 projects of the U. Concepción and has collaborated with the University of Chile and University of Alicante. She acquired a strong background on organometallic nanoparticles synthesis and lignin conversion from which 6 manuscript resulted. These practical and theoretical skills will be relevant in her future line as a Ramón y Cajal researcher.

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Her curriculum includes 28 articles, of which 21 are Q1 of Chemistry or Materials Science of the JCR, and 4 more articles are under review. She has presented contributions at 26 congresses (19 international and 9 oral). As a measure of the quality and her contribution to the work, it should be noted that she is first author of 85% of her articles being the corresponding author in 10. She has contributions in high impact journals in Materials (Carbon), and more specialized journals (Journal of Catalysis, Applied Catalysis B, Catal.Sci.Techn.).
She has acted as reviewer of general chemistry (Carbon, Chemical Communications) or catalysis (Appl. Catal. B: Env, Catal. Comm.) and has supervised 1 doctoral Thesis and 4 Master Theses of which 4 SCI articles and 5 oral presentations in congresses resulted.
She participated in the organization of an in-situ spectroscopy course at the U.Concepción and is member of the organising committee of the IX international congress of Carbon for Catalysis. She has been professor of chemical engineering at the U.Concepción and at UNED in teaching activities related to heterogeneous catalysis in the Master of Science and Chemical Technology.
She has so far obtained funded as PI of 1.1 million .
Her current interests include CO2 valorisation and biomass transformations to fuels and chemicals and in the following years the candidate will lead and be coordinator of one collaborative European project funded within the H2020 programme and two international collaborative projects funded by CSIC in those research fields. Within the frame of this H2020 project she will do secondments at LIKAT to work on Operando spectroscopy and will also get hands on experience on in situ TEM and near atmosphere pressure XPS that she will apply during her independent research lines.

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Turno de acceso general

Nombre: BREA FERNANDEZ, ROBERTO JAVIER
Referencia: RYC2020-030065-I
Área Temática: **Ciencias y tecnologías químicas**
Correo Electrónico: qorjbrea78@gmail.com

Título:

In situ lipid and peptide synthesis: biomimetic construction of functional self-assembled systems and chemoselective modification of proteins

Resumen de la Memoria:

My career goal is to become a renowned academic research scientist working on high-impact approaches to solving biological and biomedical problems using a core background in chemistry. More specifically, my primary interest involves the development of chemical strategies to control lipid and peptide formation, generate functional self-assembled systems and modulate protein modification in living cells and organisms. Such approaches are extremely useful both as therapeutics and as tools for understanding key biological processes. My previous training in organic supramolecular chemistry, biomimetic chemistry, biochemistry and chemical biology has prepared me ideally to transfer my knowledge and expertise to novel and exciting multi- and interdisciplinary scientific areas.

I began my research career as an undergraduate student at USC in Prof. Juan R. Granja s lab (MEC Fellowship), working on the synthesis of non-natural amino acids and the covalent modification of peptides. During my PhD (FPU and Xunta fellowships), my main efforts were focused on the design, synthesis, characterization and applications of self-assembling cyclic peptide nanotubes [15 publications (10 as first author), 1 patent]. My most relevant finding was the fabrication of a new class of highly stable heterodimeric tubular assemblies. Interestingly, I showed their efficiency as biosensors, photoactive bioinspired devices, molecular switches and MRI agent contrasts. I also had three opportunities to expand my chemical expertise with Profs. M. Reza Ghadiri (TSRI), Nazario Martín (UCM) and Dirk M. Guldi (FAUEN). My PhD thesis got the best possible qualification (Cum laude). Additionally, I was awarded with the V Lilly Prize of investigation for PhD students and the USC Extraordinary Doctorate Award.

As a postdoctoral fellow in Prof. Neal K. Devaraj s lab (UCSD), my research was focused on the development of chemoselective strategies for the construction of artificial cellular systems [22 publications (11 as first author), 6 patents]. I also won the highly competitive HFSP Cross Disciplinary Fellowship to continue my studies on synthetic cells. Moreover, I developed a powerful technology for the reconstitution of proteins driven by the in situ synthesis of phospholipids. Remarkably, I was selected as a finalist for the Career Awards at the Scientific Interface (Burroughs Wellcome Fund).

Since December 2018, I m an Assistant Project Scientist at UCSD, expanding the range of chemical reactions to generate self-assembled structures, trigger in situ lipid formation and control protein depalmitoylation in living cells and organisms [10 publications, 3 patents].

It is worth mentioning my participation in 25 research projects. I have secured $161K in funding and assisted in acquiring $7.1 million in grants. Moreover, my research work was presented in 48 scientific meetings (22 oral and 26 poster) and published as 33 original papers (18 as first author) in high-impact journals (6 JACS, 3 ACIE, 3 PNAS, 3 Nat. Commun.,), 4 book chapters and 7 patents. I also mentored 28 investigators. Additionally, I received several academic and research awards (12 Prizes/Honors). This experience has given me the opportunity to get a top-level training in multiple fields, allowing me to have the criteria and critical mindset to begin projects that combine chemical, biological and biomedical sciences.

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Resumen del Currículum Vitae:

My research career began as an undergraduate student (MEC Fellowship) in Prof. Juan R. Granja s lab (Universidad de Santiago de Compostela). Afterwards, I was awarded with several prestigious fellowships (FPU, Xunta de Galicia) and started my PhD studies on the construction of functional self-assembling cyclic peptide nanotubes [15 publications, 1 patent]. During my predoctoral research, I also had three opportunities to expand my chemical expertise with stays in the labs of Profs. M. Reza Ghadiri (TSRI), Nazario Martín (UCM) and Dirk M. Guldi (FAUEN). In 2013, I defended my PhD Thesis (Cum Laude).

After my PhD, I joined (December 2013) Prof. Neal K. Devaraj lab at the University of California, San Diego, working on the fabrication of self-assembled non-natural cellular systems [22 publications, 6 patents]. Only a couple of months later, I won the highly competitive Human Frontier Science Program (HFSP) Cross Disciplinary Fellowship (CDF) to continue my studies on artificial life forms.

Since December 2018, I have worked as an Assistant Project Scientist at UCSD, focusing my independent research on the development of chemical strategies to generate self-assembled structures, control in situ lipid formation and modulate modification of proteins in living cells and organisms [10 publications, 3 patents].

During the course of my research career, I have gained top-level training in diverse areas of chemistry (organic, supramolecular, biomimetic, biochemistry, chemical biology) and proven to be productive in all of them. This fact is reflected in 33 peer-reviewed articles (31 in Q1; 18 as first author) in high-impact journals (including 6 JACS, 3 ACIE, 3 PNAS, 3 Nat. Commun., 2 Chem. Soc. Rev., 2 Chem. Eur. J., 2 J. Phys. Chem. B, 1 ACS Cent. Sci.,). These publications have been highlighted with 2 covers and 4 concentrates in Chem. Eng. News. Moreover, they are highly cited articles, receiving a total of 1409 citations. I have an h-index of 18. I have also published 4 book chapters (2

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as corresponding author). Additionally, I am author of 7 patents (6 international, 1 Spanish).
It is worth mentioning my participation in 25 research projects (15 in USA, 10 in Spain). I have secured $161K in funding and assisted in acquiring $7.1 million in grants. Moreover, my research work has been presented in 48 scientific meetings (22 oral communications, 26 posters) and 2 invited talks. I have been collaborating with industry (Palm Therapeutics, ONO, Janssen) and other academic research groups (>15). I have mentored 28 investigators (6 postdocs, 18 PhD students, 1 MSc candidate and 3 visiting scholars). Moreover, I am a member of several scientific associations (AACR, RSC, ACS, RSEQ) and the Editorial Board (Topic Editor) of Biomolecules (MDPI). I have also served as a PhD committee member and regular reviewer for numerous journals (JACS, ACIE, Chem. Soc. Rev,).
I have been awarded with prestigious and highly competitive fellowships during my entire career [MEC (Collaboration), FPU, Xunta de Galicia (Predoctoral), Xunta de Galicia (Postdoctoral), HFSP CDF]. Additionally, I have been recognized with numerous academic and research awards [V Lilly Prize of Investigation, Special Mention EYCA, Medichem Prize, USC Extraordinary Doctorate Award, Nanoscale Horizons (RSC) Prize, Finalist CASI (BWF), Hijos de Rivera Award (Best Professional Trajectory)].

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Turno de acceso general

Nombre: SWIDEREK , KATARZYNA PATRYCJA
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Área Temática: **Ciencias y tecnologías químicas**
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Título:

Theoretical studies of reactivity in cellular processes

Resumen de la Memoria:

The professional activity and the main research line of Dr. Swiderek is focused on theoretical studies of chemical transformations that occur in cellular processes. In general, three closely connected areas to this mainline of interest can be distinguished in her recent career path i.e., inhibition and drug design, the origin of biocatalysis, and design of biocatalysts. In particular, most of Dr Swiderek s studies are based on MD simulations using hybrid QM/MM potentials. The results obtained from the computational studies of biological catalysts can provide information to be widely exploited on pharmacological, medical and industrial areas.

Up to now, the main goal was to study mechanisms of different chemical processes, crucial for the functioning of living cells but also pathogenic processes. These have included peptide bond formation and cleavage, phosphodiester bond cleavage and formation, adenyl transfer etc. Nevertheless, due to the recent success in obtaining the financial support for her StopProt research project from Spanish Ministerio de Ciencia, Innovación y Universidades and Generalitat Valenciana, now Dr Swiderek s work is mostly focused on the chemistry of C-N bond in enzymatic processes. Here the main target is to understand, using theoretical tools, the reaction mechanisms of C-N bond cleavage catalyzed by proteases involved in viral replication like those from HIV or COVID, or those involved in other disease-causing processes, such as 20S Proteasome and Rhomboid protease. Consequently, the possibility of inhibition of these harmful for human health biological systems is explored, including the design of new potential molecular blockers.

Finally, the hydrolysis mechanisms of C-N bond in the promiscuous enzymes, like CALB and Bs2, is also under investigation. Studies on C-N bond cleavage chemistry in these systems (that have not been evolved to catalyze this reaction by Nature), is especially vital in order to understand the origin of biocatalysis and future design of biocatalysts.

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Resumen del Currículum Vitae:

Dr Swiderek, researcher and mother of 2 girls (11 and 7 years old), studied Chemistry and obtained her BsC (2007) and PhD (2011) at the Lodz University of Technology (Poland). Her PhD, supervised by Prof. P. Paneth, was based on theoretical studies on binding isotope effects in LDH. In 2008 she stayed 3 months in the Helmholtz Centre for Environmental Research (Leipzig, Germany), funded by an AXIOM - Marie Curie Host Fellowship under the supervision of Dr H. Richnow. In 2011, she moved to the University of Valencia (Spain) for her first postdoctoral stay under the supervision of Prof. I. Tuñón, where her work was focused on peptide bond formation studies. From 2015, she was contracted in an NIH project (USA) as a postdoctoral researcher at University Jaume I under the supervision of Prof. V. Moliner (UJI) and Prof. A. Kohen (University of Iowa, USA), where her work was focused on quantum tunneling and dynamics effects in enzyme-catalyzed reactions. At the same time, as a PI of the project entitled "Mechanism of formation and breaking of peptide and phosphodiester bonds based on theoretical studies of the reaction catalyzed by Ribosome 70S and Protease and Integrase of HIV-1" funded by the Polish Ministry of Science and Higher Education, she supervised a PhD student at Lodz University of Technology (Poland), thesis defended in 2019. In 2017 she moved for 6 months to the lab of Prof. I. H. Williams at University of Bath (UK), working on the methyl transfer mechanism reaction in GNMT enzyme, kinetic isotope effects and heat capacities. In 2018 she obtained a 2-years Juan de la Cierva Incorporation contract from Spanish Ministerio de Economía y Competitividad at University Jaume I. Recently, (1/10/2020), she obtained a 3-years contract as a PI and researcher in a JIN project funded by the Spanish Ministry of Science, Innovation and Universities at the same University, and her research is funded by a SEJI 2020 grant (Scientific Excellence Junior Researchers Grants program of Valencian Government) and a grant funded by University Jaume I, in which she is also PI. Her professional activity is focused on theoretical studies of reactivity in cellular processes based on a molecular dynamics (MD) simulation using hybrid quantum mechanics/molecular mechanics (QM/MM) potentials. This methodology allows providing results such as Gibbs free energy barriers, binding free energies, kinetic and binding isotope effects (KIE and BIE), etc... of enzymatic systems that can be directly compared with experimental data. The main target of Dr Swiderek is to study the fundamentals of enzyme reactivity and its potential applications on designing inhibitors and new biocatalysts. Results of these studies provide new information and a powerful tool to be widely exploited on pharmacological, medical, and industrial areas. Dr Swiderek is a co-author of 55 publications (50 scientific papers, 4 reviews and 1 book chapter). She is the corresponding author in 14 scientific articles. She has co-supervised 1 PhD thesis, 4 MsC thesis, 3 Bachelor s Thesis, and she is co-supervising 3 PhD students. She has received several awards and scholarships. She participated in more than 25 international conferences. She is member of the Spanish Royal Society of Chemistry (RSEQ), its Specialized Group of Chemistry and Computation (GEQC) and of the Sociedad Española de Bioquímica y Biología Molecular (SEBBM). In 2021 she joined the editorial board of BioChem.

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Turno de acceso general

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Área Temática: **Ciencias y tecnologías químicas**
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Título:

From metal catalysis to chemical biology

Resumen de la Memoria:

I carried out the Thesis in Univ. of Oviedo (2007-11; FPU grant; mentors: Prof. Barluenga/Valdés; "excellent cum laude", PhD extraordinary award). I implemented the use of tosylhydrazones as carbonyl surrogates in metal-catalyzed and novel metal-free synthetic methodologies. This research was recognized by 9 original publications in top journals (1 NatChem, 2 ACIE, 2 CEJ, 1 ASC, 3 EJOC, first author in 7/9 articles, 681citations, 3 papers with>100 citations, average IF =7.8). This research line has produced 5 more thesis and 18 papers so far. The NatChem 2009 received the prestigious SUSCHEM PREDOC2010 prize (RSEQ).

During this period, I carried out two international stays of 6 months in top research groups (Prof. Aggarwal, 2008 Bristol; Prof. Charette, 2010 Montreal).

I moved to LMU München for the postdoctoral studies (Prof. Carell, 2011-14; MEC and AvH grants). During this period, I headed the subgroup of synthetic biology and worked on the field of DNA modifications and nanotechnology with the goal of expanding the genetic code. The work crystallized on the implementation of a new design principle for DNA base pairing, based on the concept of reversible imine chemistry, used to stabilize DNA duplexes and nanostructures. Recognition of this research: 1 ACIE, 2 CC, 1 ChemSci, 78 citations, average IF=8.6. Furthermore, 2 theses resulted by continuing this research.

In 2015 I joined the Mascareñas group CIQUS, (JdC grant) which permitted me to further develop my multidisciplinary formation and get immerse in the fascinating field of cell Biology. There I led the research focused on translating non-natural metal catalyzed transformations to biological habitats, including living cells. Based on this project, several high impact papers have been reported. In all cases I have been either the first/main author (2 NatCommun, 1 ChemSci, 1 JACS, 1 Nano Lett, 1 Cell Rep. Phys. Sci.) or the corresponding author (1 ChemBioChem, 1 ACIE VIP, 1 Nat. Chem. submitted).

In addition, I have recently received funding for independent research (I+D+I RETOS-JIN) and initiate work on photochemical catalysis with 1TFM and 1TFG students. We have obtained very promising results on bioorthogonal photocatalysis, which were presented in a symposium conference and are now being refined for publication. This has been delayed because of the COVID outbreak.

During all the periods I have secured funding through competitive fellowships (FPU, postdoctoral MEC and AvH, JdC Formación/Incorporación). Overall, during my career I got a top-tier and impacting scientific production in multidisciplinary research, with a high authorship proportion, and I demonstrated also a high international mobility (5 groups/universities). I have already supervised the research of a number of students (5 TFM/2 TFG) and currently, 3 PhD ongoing (2 just started,) 1 TFM and 2 TFG ongoing), and I am starting my fully independent work.

I have been accredited as Profesor Contratado Doctor and received the I3 certification. This application aims to start a completely independent career facing novel goals defined by an innovative cross-disciplinary approach, working at the interface of nanomaterials science, supramolecular chemistry, catalysis and cell biology. I would finally like to emphasize that I was ranked 1º and 3º in the reserve list of R&C calls of 2018 and 2019.

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Resumen del Currículum Vitae:

After graduating in Chemistry (2006) I was awarded a FPU grant and joined the group of Prof. Barluenga/Valdés (2007-11). The research Thesis was focused on the development of metal-catalyzed and novel metal-free synthetic methodologies (Recognitions: Best Thesis in Chemistry, U. Oviedo, and SUSCHEM2010 PREDOC prize, RSEQ). I also performed 2 stays with Prof. Aggarwal (Bristol, 2008) and Prof. Charette (Montreal, 2010).

The postdoctoral career (Spanish Postdoctoral and German Humboldt Fellowships) was undertaken under the supervision of Prof. Carell (LMU Munich, 2011-14). During this period, I developed independent research leading the subgroup of synthetic biology.

In 2015, I joined the group of Prof. Mascareñas (USC, CIQUS Institute) (JdC Formación and Incorporation grants). Recently I have started a new interdisciplinary and innovative research line at the between chemistry/biology frontier in the area of photochemical catalysis in biological scenarios, funded by the Programa I+D+I RETOS-JIN (181.5 k).

I have been very productive in all the stages of my career, with most of the articles published in top-tier journals (average IF: 7.8 (2008-2012); 8.6 (2013-2014); 10.4 (2015-2020). My publications received 927 citations (897 without self-citations, 641 documents) (>100cit/year since 2016; >48cit/paper with 3 articles with >100 citations). As a result of this activity, I have a steadily growing h-index of 15 (Scopus). I have published: 2 NatCommun, 1 JACS; 1 NatChem, 4 Angew, 2 ChemSci, 2 CC, 2 CEJ, 1 ASC, 3 EJOC, 1 Nanolett, 1 Cell. Rep. Phys.Sci. and 1 ChemBioChem. Moreover, 1 ACS nano has been accepted provided a major revision is made. I am first author of 9 out of the 10 most cited

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papers and first or corresponding author in 70% of the articles published during my postdoctoral stays, and co-corresponding author in the 2 more recent contributions, demonstrating my leading role in the research. In addition, I am the sole author of a book chapter of Science of Synthesis. I have also a patent application.

I have delivered 12 invited/oral presentations in national/international conferences. I have participated in 14 competitive national and international research projects (Spain/Germany). Furthermore, I have obtained funding for my research through competitive fellowships (Humboldt fellowship=19.2k , JdC Incorporación grant=6k).

I have had teaching duties during all the different stages of my career. I have taught experimental courses of organic chemistry in Chemistry, Pharmacy and Biotechnology degrees. On the other hand, I have officially directed 5 TFM students (LMU Munich and USC). Currently I am responsible for the co-direction of 3PhD (2 just started), a TFM and 2TFG student. I have been accredited as Profesor Contratado Doctor and received the I3 certification.

Summarizing, during my career, I have worked in top research groups in Spain, England, Canada and Germany which shows my capacity to work in interdisciplinary and international environments. I have been very productive during all the research periods. I have been also very active in mentoring and supervising, and I am right now starting my fully independent work. Obtaining the Ramón y Cajal grant is essential for further progressing.

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Turno de acceso general

Nombre: KHEZRI KHEZRI, BAHAREH
Referencia: RYC2020-029990-I
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Título:

Experimental studies on microrobots and electrocatalysis

Resumen de la Memoria:

I have spent my career in globally recognized research institutes and universities. I have worked at Nanyang Technological University, Cambridge Centre for Advanced Research and Education (Singapore), University of Cambridge (UK) and the University of Chemistry and Technology, in Prague, Czech Republic. I have spent the past twelve years involved in science and engineering outreach in the fields of nanorobots and electrocatalysis.

In the nanorobot field, my research involves the fabrication and characterization of programmable functional nano/microrobots for environmental and biomedical applications, mainly via proof-of-concept projects. I construct drug-delivery vehicles capable of smart encapsulation, self-navigation, and releasing substances in a rapid and controlled manner (e.g. electrochemical triggers). In addition, these microscale machines add a new dimension based on motion to decontamination processes, resulting in new on-the-fly remediation protocols, with higher efficiency, shorter cleanup time and potentially lower costs. In electrocatalysis, I focus on designing, engineering, and fabricating electrocatalysts for CO2 reduction (ERCO2). ERCO2 using renewable (solar or wind) energies produces value-added chemicals and fuels and simultaneously reduces our carbon footprint. Developing an effective catalyst is vital, as there are currently no industrial-scale operations utilizing this technology in view of its low energetic efficiency. My recent progress in ERCO2 shows that structural and compositional modulations are promising to regulate the accessible surface area and promote the activity for the selective production of value-added chemicals.

I have coauthored ~50 articles, which have received more than 1500 citations and my h-index is 24. My work has been published in top-ranked journals such as Nature Machine intelligence, Chem, Advanced Materials, Advanced Functional Materials, ACS Nano, Angewandte Chemie, and JACS. I received in 2019 and currently hold a grant (400.000 euros) from GACR (The Czech Science Foundation) to start my own research group.

Beyond my successes as a researcher, I have teaching experience as it was one of my commitments to my scholarship during my Ph.D. As a graduate student at NTU, I served as a teaching assistant in labs as well as lectures in courses on physical, analytic, and electrochemistry.

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Resumen del Currículum Vitae:

I am currently a senior scientist at the Advanced Functional Nanorobots center in Prague, Czech Republic. I have completed my bachelor's and master's at Isfahan University of Technology and Isfahan University, Iran, respectively where I attained a strong academic foundation of chemistry-related subjects through my undergraduate and graduate courses. I did my Ph.D. at Nanyang Technological University as a top-ranked university under AStar international prestigious scholarship started in August 2008. During my Ph.D. program, I gained valuable experiences in analytical environmental chemistry. My Ph.D. research was focused on the development of analysis methods for air pollutants using diverse analytical instruments including GC, HPLC, IC and ICP. After Ph.D. completion, I was fortunate to receive AStar Postdoctoral Fellow (2012-2014) to pursue research in the field of electrochemistry and electroanalysis. In January 2015, I joined the Cambridge Centre for Advanced Research and Education in Singapore (CARES). I involved in the Electrochemical Multi-scale Science, Engineering and Technology subprogram and worked on multiscale electrochemical characterization and analysis. Our research targeted the development of multi-scale electroanalytical tools for the investigation of catalytic reactions and the adoption of electro-synthesis as a potential source for clean and selective routes for chemical production. I had this opportunity to work under the supervision of Prof Martin Pumera (NTU), Prof Richard D. Webster (NTU), Prof Adrian Fisher (Cambridge) and Markus Kraft (Cambridge) as director of CARES. At the same time, I have also gained additional knowledge and experience in material science (especially 2D-materials, synthesis and exfoliation), water splitting, 3D-printing and synthetic micro-nanorobots from my post-doctoral stay at Prof Martin Pumera research group. Doing postdoctoral research in different environments and research areas made it possible for me to receive as much lab experience and I realized my research interests. In summary, I have spent the past twelve years heavily involved in science and engineering outreach mainly in nanorobot field and electrocatalysis. In nanorobot field, my research projects involve fabrication and characterization of programmable functional nano/microrobot towards environmental and biomedical applications mainly as proof-of-concept projects. We were able to construct drug-delivery vehicles capable of smart encapsulation, self-navigation, and releasing substances in a rapid and controlled manner. In addition, these microscale machines have added a new dimension based on motion to decontamination processes, resulting in new on-the-fly remediation protocols, with higher efficiency, shorter cleanup time, and potentially lower costs. In the electrocatalysis field, I focused on designing, engineering, and fabricating electrocatalysts for CO2 reduction (ERCO2). My recent progress in ERCO2 shows that the morphological structure modulations and tailoring of surface chemical compositions are a promising approach to

AYUDAS RAMÓN Y CAJAL
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regulating the accessible surface area and promoting the activity for selective chemical production from CO2. My work has been published in journals such as Nature Machine intelligence, The Chem, Advanced Materials, Advanced Functional Materials, Angewandte Chemie, and JACS. I received it in December 2019 and currently, I am holding a grant (400.000 euros) from GACR (The Czech Science Foundati

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Turno de acceso general

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Área Temática: **Ciencias y tecnologías químicas**
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Título:

Design and development of metal based catalysts and their application in organic chemistry

Resumen de la Memoria:

My main research line is focused on the development of catalysts for making organic transformations with higher levels of efficiency and sustainability. Moreover, throughout my career I have also made significant contributions in fields such as organic or supramolecular chemistry. The experience in these parallel topics has certainly enriched my current research line in catalysis, owing the great multidisciplinarity of the field.

During my PhD studies in the group of Professors Belén Abarca and Rafael Ballesteros in the Organic Chemistry department at Universitat de València, funded by the competitive FPI program of Generalitat Valenciana, my work was focused in the study of the chemistry and the applications of nitrogenated heterocycles. Moreover, in this period I had the first contact with the heterogeneous catalysis field developing a new protocol for transfer hydrogenation of N-heteroarenes with alcohols. I achieved the doctoral degree in 2013 with excellent cum laude mark and international mention, due to a research stay of 4 months that I performed at Université de Strasbourg. The work performed in this period was reflected in 20 publications.

Then, from October 2014 I worked in the Leibniz Institute for Catalysis (LIKAT) at Rostock (Germany) in the group of Professor Matthias Beller, a worldwide reference in homogeneous and heterogeneous catalysis, with a fellowship granted by Fundación Ramón Areces. During this period, I developed homogeneous catalysts for performing simple hydrogenations and further hydrogenative functionalizations. Remarkably, I could develop the first non-noble metal based homogeneous catalyst for the hydrogenation of carbon dioxide to methanol. The results fulfilled at LIKAT were published in 12 papers.

In 2017, I joined the group of Professor Avelino Corma and Dr. Antonio Leyva at Instituto de Tecnología Quimica (ITQ at UPV-CSIC) in València, where I worked in the development of MOF materials hosting in their channels single atoms or well defined supramolecular complexes, for their application as heterogeneous catalysts in redox and coupling reactions. This work was reflected in 2 publications in top rated journals. During this period, I could also actively participate in a project with a chemical company.

Since September 2018, I started my own research line in the ITQ funded by a Junior Leader postdoctoral grant awarded by Fundación La Caixa (I renounced to the Juan de la Cierva contract 2017 call in favour of La Caixa program). Furthermore, I recently obtained more funds to follow my research, being granted with a SEJI project (Subvencions a l excel·lència juniors investigadors) by Generalitat Valenciana. Thus, I am currently supervising 3 PhD students and I have recently supervised 2 master students. My current research interests are based on the development of solid materials with well-defined catalytic centers for their application as catalysts in coupling reactions, CO and CO2 activation and industrially demanded hydrogenative and oxygenative transformations.

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Resumen del Currículum Vitae:

I am currently Junior Leader Postdoctoral fellow of Fundación La Caixa at Instituto de Tecnología Química (ITQ, Universitat Politècnica de València - CSIC) where I conduct my own research line inside the group of Prof. Fernando Rey.

My research career started in 2008, when I concluded my Bachelor studies in Pharmacy at Universitat de València with distinction (extraordinary prize of the Pharmacy Faculty). Since then, I have been awarded with 5 competitive predoctoral and postdoctoral grants (GVA FPI predoc, GVA predoc stays, Fundación Ramón Areces postdoc, UPV postdoc and Fundación La Caixa postoc) being hired for 7 years and 11 months with funds captured by myself.

My career can be divided in four main periods: i) at the Organic Chemistry Department of Universitat de València as PhD student in the group of Prof. Belén Abarca and Prof. Rafael Ballesteros, ii) at LIKAT (University of Rostock) as Ramón Areces postdoctoral fellow in the group of Prof. Matthias Beller, iii) at ITQ (UPV-CSIC) as UPV postdoctoral researcher in the group of Prof. Avelino Corma and Dr. Antonio Leyva, and iv) at ITQ as Junior Leader La Caixa fellow developing a different research line with my own project. I have worked in different research groups, demonstrating in all the periods a high productivity and independence.

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I have actively participated in 36 publications (44% without my PhD supervisors), including top-rated journals in general science (Nature Commun.) and multidisciplinary chemistry (4 Angew. Chem. Int. Ed., J. Am. Chem. Soc., 2 Chem. Sci., ChemSusChem), reaching a h-index of 15. In the last 5 years, I have published 20 papers with an average impact factor of 8 and, at this moment, I have two publications under preparation. Throughout my career, I have made 27 contributions in congresses and workshops, being 3, oral communications. In addition, I have participated in 8 projects corresponding to public calls and, currently, I am PI of two projects, one of 305.700 0 funded by Fundación La Caixa and another of 205.867 7 funded by Generalitat Valenciana. Remarkably, I have also participated as a researcher in two contracts with chemical companies.

I accumulate 34 months of international mobility: 4 months at Université de Strasbourg as predoctoral stay, and 2 years and 6 months of postdoctoral experience at LIKAT, in the group of Professor Matthias Beller with whom I maintain a collaboration.

I am currently directing three PhD students, two of them hired with funds captured by myself. Recently, I have also supervised two master students. Moreover, I have been involved in teaching activities in two universities (Universitat de València and Universitat Politècnica de València) where I have taught 171 hours in Chemistry and Industrial Engineering degrees, as well as in Chemical Engineering master. I am accredited as Assistant Professor by Agència Valenciana d Avaluació i Prospectiva (AVAP). I am also actively involved in science dissemination tasks, giving talks to high school students in the event of 11 F Día Internacional de la Mujer y la Niña en la Ciencia in the 2019 and 2020 editions.

Currently, and since my postdoctoral stay in LIKAT, my main research interest is centered in developing new catalysts for making organic processes more sustainable. From my previous experience in homogeneous catalysis, now I am working in the accurate design of reusable materials whose structure is adapted to the needed features of the catalyst.

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Turno de acceso general

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Título:

Computational chemistry for the discovery, characterization and design of new biocatalytic activities

Resumen de la Memoria:

Dr. Marc Garcia-Borràs is a Beatriu de Pinós Researcher at the Institute of Computational Chemistry and Catalysis (IQCC) at the University of Girona (UdG).
During his PhD under the supervision of Prof. M. Solà and Dr. J. M. Luis (UdG, 2012-2015, Extraordinary PhD Award), he worked on the computational study of the structure and reactivity of endohedral (metallo-)fullerenes, and he visited the groups of Prof. K. N. Houk (UCLA, USA, 3 months, 2014) and Prof. W. Thiel (Max-Planck-Institut Mülheim, Germany, 2 months, 2015). Then, he did a short (6 months) postdoc stay in the group of Dr. Osuna (UdG, Spain) working on the development of computational tools and protocols for characterizing the conformational heterogeneity of laboratory evolved enzymes. After, he joined the group of Prof. K. N. Houk at UCLA (USA) as a postdoc for 3 years (Jan. 2016 Jan. 2019), to work on the application of computational tools to understand important biocatalytic processes where both Natural and artificially designed enzymes are involved, acquiring large experience on the use of a large variety of computational techniques to solve chemical biology problems. He was supported by a Ramón Areces Postdoctoral Fellowship (2-years) to specifically work on the computational modelling and design of new (metallo-)enzyme catalyzed reactions, and he was awarded the 2018 UCLA Department of Chemistry and Biochemistry Postdoctoral Research Award for his scientific achievements.
In February 2019 he returned to Spain as a JdC-I fellow (UdG) to start his independent career. His research program is mainly focused on the application of computational methods to understand and design new biocatalytic processes. He is proposing new computational protocols for the characterization of enzymatic reactive intermediates, and developing and applying new mechanistically-driven rational enzyme design strategies to funnel these biocatalytic intermediates towards desired chemical transformations with specific selectivities. In Nov.-2019 he spent 1 month visiting the group of Prof. S. Flitsch (Univ. Manchester) to carry out enzymology wet lab work, in order to expand his skills and complement his approach to biocatalysis and enzyme design.
In Feb.-2020, he was awarded a MSCA-COFUND Beatriu the Pinós grant, and since July-2020 he is also PI of a MICINN Generación de Conocimiento project (PID2019-111300GA-I00) that supports his research program on biocatalysis. In Nov.-2020, he was appointed as a new independent PI of the IQCC.
He is currently supervising 3 PhD students and one master student, and he has established collaborations with world-leading groups in the biocatalysis and protein engineering fields (including Prof. F. Arnold, Prof. M. Reetz, among others).
At all stages of his scientific career he has secured funding for his research (including his salary) and his work has been recognized by the different awards and fellowships he has received. He has demonstrated an outstanding capacity to carry out high quality research, publishing 58 (54 Q1) high impact papers (6 as corresponding author), and he has been invited to give seminars and lectures in national and international events. His scientific outcome gives enough evidences of independent leadership and international recognition, highlighting his capacity to successfully design, develop, participate and lead research projects.
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Resumen del Currículum Vitae:

Dr. Garcia-Borràs (b. 1988) is a Beatriu de Pinós Researcher at the IQCC (UdG). He coursed the Master in Theoretical and Computational Chemistry coordinated by Universitat Rovira i Virgili (2020-2011, Extraordinary Master Award). Then, he started his PhD in Chemistry (2011-2015, FPU fellowship; 2015 Extraordinary PhD Thesis Award) at the IQCC (UdG) under the supervision of Prof. M. Solà and Dr. J. M. Luis. He visited the groups of Prof. K. N. Houk (UCLA, USA, 3 months in 2014) and Prof. W. Thiel (Max Planck Institute, Germany, 2 months in 2015). Upon graduation, Marc did a short post-doc stay (6 months) in the group of Dr. S. Osuna at UdG. In January 2016 Dr. Garcia-Borràs joined the group of Prof. K. N. Houk at UCLA as a postdoctoral researcher for a total of 3 years. He was awarded a Ramón Areces Postdoctoral Fellowship (2 years) to support his research project Multiscale Modelling Strategies for designing Functional Redox (Metallo)enzymes at Prof. Houk s lab (PI: Garcia-Borràs). During his postdoc with Houk, Marc worked on the application of computational tools to understand important (bio-)catalytic processes. He has collaborated with world-leading groups in the biocatalysis and directed evolution of proteins fields including the groups of Prof. F. Arnold (Caltech), Prof. M. Reetz (Max-Planck-Institute), Prof. D. Sherman (U. Michigan), among others. At UCLA, he was awarded the 2018 UCLA Department of Chemistry and Biochemistry Postdoctoral Research Award .
In February 2019 Marc moved back to Spain as a recipient of a JdC Incorporación Fellowship, that allowed him to start his independent career as a junior researcher at the IQCC (UdG) working on the computational modelling of biocatalytic intermediates for the discovery and design of new enzymatic activities. In Nov-2019, he spent 1 month vising the group of Prof. S. Flitsch (U. Manchester) to carry out wet lab experimental enzymology work funded by his JdC grant. In Feb.-2020 he awarded a MSCA-H2020-COFUND Beatriu the Pinós project, and

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since July-2020 he is PI of a MICINN I+D Generación de Conocimiento Tipo A project (PID2019-111300GA-I00). He is also PI of several computational projects (in 2019, 2020, and 2021-under evaluation) at the Red Española de Supercomputación (BSC-RES) that provide the necessary computational resources to carry out his research projects. In Nov.-2020 he was appointed as an independent PI at the IQCC, and he was finalist at the European Young Chemist Award (EYCA) 2020 - Early Career Researcher level by the EuCheMS.

He has published 58 papers (+2 book chapters) in top journals (54 Q1) including: 1 Nat. Chem., 2 PNAS, 2 Nat. Commun (+1 accepted), 1 Chem, 2 Nat. Chem. Biol., 1 ACS Cent. Sci., 10 JACS, 24 ACIE, 3 ACS Catal., 1 Chem. Soc. Rev., 7 Chem. Commun., 10 Chem. Eur.-J., 4 JCTC, among others; being first or second author in 37 publications, corresponding author in 6, and accumulating a total of 1087 citations (Scopus, 20 Jan. 2021), with an h index of 21. He has mentored and supervised several undergraduate students during their final degree projects, has supervised one Master s Thesis. He is currently supervising three PhD Students and one Master Student. He has contributed in several national and international conferences as coauthor, being presenting author of 7 invited talks and 16 oral communications. He is also reviewer for different international peer reviewed journals.

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Turno de acceso general

Nombre: MOLINUEVO SALCES, BEATRIZ
Referencia: RYC2020-029030-I
Área Temática: **Ciencias y tecnologías químicas**
Correo Electrónico: beatriz.molinuevo.salces@gmail.com

Título:

Sustainable valorization of livestock and agricultural waste following a circular economy approach.

Resumen de la Memoria:

Dr. Molinuevo-Salces has developed her activity in the area of chemical-environmental engineering, focused on agricultural and livestock waste management and treatment. She has mainly developed her research activities in two lines, namely anaerobic digestion (AD) and nutrient-recycling technologies. During her PhD studies (2007 - 2011) at the Technological Agricultural Institute of Castilla y León (ITACyL), she focused on studying the effect of the addition of vegetable wastes on the AD of livestock wastes and evaluating anammox and microalgae-based systems to treat the anaerobic digestates. The objective was to provide technological support to the livestock sector. She completed her knowledge and experience with two research stays (DTU-Denmark and WUR-The Netherlands), where she worked on anammox and microalgae-based systems, respectively. Her postdoctoral experience includes three research institutions. First, in 2011 at Aalborg University Copenhagen (AAU-CPH), working on AD of catch crops. Catch crops are mandatory to cultivate in Denmark and intended to avoid nitrogen leaching to the groundwater. The resultant biomass was evaluated as a co-substrate for agricultural AD plants in Denmark. After that, she joined a project to develop a biorefinery concept within organic farming. In this context, an organic protein concentrate (obtained by a biological fermentation) together with bioenergy were obtained from fresh green biomass. In 2015, she obtained a Marie-Curie postdoctoral fellowship at IMDEA Energy Institute in Madrid, Spain. In this case, she was Principal Investigator of an AMAROUT II research project on enhancing methane production from microalgae biomass (grown in livestock wastewater) by means of bioaugmentation. Third, in 2017 she joined ITACyL, to develop the gas-permeable membrane technology for ammonia recovery from livestock wastes (LIFE Ammonia Trapping). Nowadays, Dr. Molinuevo-Salces is a Researcher at ITACyL, focused on nutrient-recovery technology transfer and AD process optimization, as a Principal Investigator of the project LACTOCYL. Through her work experience at different international projects, she has worked in collaboration with industry and academia. She is a result-oriented person; able to conduct independently high quality research and technology transfer within the agro-food sector.
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Resumen del Currículum Vitae:

Dr. Molinuevo-Salces performed her PhD, funded by INIA, at the Technological Agricultural Institute of Castilla y León (ITACyL). She got the PhD with International Mention from the University of Valladolid in 2011. Her postdoctoral experience includes three postdoctoral contracts, first at Aalborg University Copenhagen (AAU-CPH), second at IMDEA Energy Institute (awarded with a MARIE Curie-AMAROUT fellowship) and third at ITACyL. In 2020, she got a position as a Researcher at the Livestock and Agricultural Waste Treatment Research Line at ITACyL, mainly focused on the optimization of anaerobic digestion (AD) and the development of nutrient-recovery technologies. Her research work resulted in 28 scientific articles, 1 e-book, 3 book chapters, 26 contributions to conferences (18 oral), 4 invited conferences and a variety of scientific reports for companies. She is first or corresponding author of 19 papers. The quality of her research is demonstrated since 80% of the articles are in Q1 journals. She is co-inventor of 1 patent. Her work has received 1081 citations (h-index: 17). Concerning the technology transfer, she has been involved in projects with companies, in the organization of workshops on livestock waste treatment and in the implementation of nutrient recovery technologies. Her team has been awarded with the FLC Award for Excellence in Technology Transfer in 2020.

International activity: The research trajectory of the applicant has a clear international character, including 2 predoctoral research stays of 4 and 3 months (DTU-Denmark and WUR-The Netherlands) and 4 years of postdoctoral experience at AAU-CPH. Moreover, she has been a lecturer and fulfilled the course for University Teaching for Assistant Professors, based on the Problem Based Learning method at AAU-CPH. A research stay at the United States Department of Agriculture (USDA) was planned for March 2020, but due to COVID-19 restrictions the stay has been postponed to the end of 2021.

Research independence: She was principal investigator of AMAROUT II and she currently leads LACTOCyL project (FEADER 2020-2023). She is supervising a PhD thesis, has supervised 15 Master thesis, 1 Bachelor thesis and several laboratory projects. She has been a member of the Evaluation Committee in 3 PhD defenses, been invited to work as an evaluator of 4 Scientific Projects and to a PhD International Expert Assessment. She presents an experience of 12 years as referee with 31 verified reviews for 18 international scientific journals.

Other CV merits: She has worked as a lecturer for the courses of Energy and Resources , Biomass conversion process and Bioenergy at AAU-CPH. She has worked as a lecturer at the European University Miguel de Cervantes (UEMC) and, from 2019, at the International University of La Rioja (UNIR).

Her mid term-to-long research objectives include continuing with the two research lines she has developed for the last 14 years (i.e. AD and nutrient recycling technologies). Specifically, she will focus on the extraction and purification of AD by-products as volatile fatty acids (VFAs) and the scale-up of the AD process. Regarding nutrient recovery, she will continue with the transfer of the membrane-based

technology at a commercial level with the ultimate objective of considering this technology as a Best Available Technique (BAT) for swine manure management.

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Turno de acceso general

Nombre: MARTINEZ PRIETO, LUIS MIGUEL
Referencia: RYC2020-030031-I
Área Temática: **Ciencias y tecnologías químicas**
Correo Electrónico: luismiguel.martinez@csic.es

Título:

Organometallic Nanoparticle Catalysis

Resumen de la Memoria:

I carried out my PhD thesis at the IIQ under the supervision of Prof. Cámpora (2007-2012). During these years, I synthesized, characterized and studied the reactivity of a great number of new organometallic complexes (Chem. Commun. 2010; EurJIC 2013; Chem. A Eur. J. 2015; Inor. Chem. 2017; Dalton Trans. 2019), including a novel NMR study (Organometallics 2012) and a review (Isr. J. Chem. 2020).
During a first postdoctoral stay at LCC in the group of Prof. Chaudret, in Toulouse (France), I focused my research on the synthesis, characterization and study of the surface chemistry of metal nanoparticles (MNPs). We developed the use of typical organometallic ligands such as N-heterocyclic carbenes (Chem. A Eur. J. 2015; Chem. Commun. 2016; NanoSO 2016; Chem. Commun. 2017; Chem. -A Eur. J. 2017; Chem. Commun. 2018; Nanoscale 2019) or secondary phosphine oxides (Catal. Sci. & Tech. 2016; Chem. -A Eur. J. 2017; PCCP 2017) for the stabilization of MNPs. In addition, we designed and synthesized some specific ligands for MNP stabilization, such as imidazolium-amidinate ligands (Chem. Commun. 2015; Chem. Sci. 2017; Catal. Sci. Tech. 2020). A second postdoctoral stay in Toulouse (LPCNO), allowed me to explore new MNPs as efficient catalysts in the lab of Prof. Van Leeuwen. During this 2° postdoc, my independence started to be notorious, publishing a review (Acc. Chem. Res. 2018) and three papers as corresponding author (NanoSO 2016, Chem. Sci. 2017; Chem. Commun. 2017), creating a network between different groups of various countries, and supervising and mentoring several PhD and master students.
In 2017 I achieved a Juan de la Cierva fellowship, which allowed me to start my independent career and to work with new supported/confined metal catalysts and magnetic catalysis at the ITQ in the team of Prof. Corma (Valencia, Spain). During this time, I have been Principal Investigator (PI) of two projects: Intramurales (42.222) and Primeros Proyectos de Investigación (PAID-06-18; 7.250). I have also participated in an important industrial project (Saudi Aramco; 298.000) and I am work-package leader in an international partnership ERC project (LAURELIN; 4.853.053). Moreover, during 2019 I supervised an MSc student and I am currently supervising a PhD and a MSc student as single director. The scientific production during this last stage of my career clearly denotes my independency; I have been invited to give three seminars, to write two books chapters and three reviews (Isr. J. Chem 2020, Catalyst 2020, Perspectives Catal. Sci. Tech. 2021). In addition, I have published five papers as corresponding author (Nanoscale 2019, Cat. Sci. Tech. 2020, J. Catal. 2019, Catalysts 2020, Cat. Sci. Tech. 2021).
In sum, I made significant advances during the last years concerning the synthesis, catalytic applications and surface chemistry of MNPs. I have also studied the importance of ligand-stabilized MNPs or confined/supported metal catalysts to control the reactivity/stability of a given reaction. This work led to publications in the best journals and allowed me to work side by side with top researchers on different disciplines.
Therefore, my main research line is based on metal nanoparticle catalysis, but always from the perspective of organometallic chemistry. More specifically, it is focused on Organometallic Nanoparticle Catalysis .

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Resumen del Currículum Vitae:

Research activity: January 2007- Present: 14 years
Stays abroad: 4 years and 6 months as postdoctoral researcher (Toulouse, France) and 3 months as predoctoral researcher (St Andrews, Scotland)
Articles in peer-reviewed journals: 35 (31 in Q1, 4 reviews, 18 as first author and 9 as corresponding author)
Books chapters: 2
Citations: 689
h-index: 17
i10-index: 20
Web sites: https://scholar.google.fr/citations?user=1k-MjAgAAAAJ&hl=en&oi=pll
https://www.scopus.com/authid/detail.uri?origin=resultslist&authorId=32667943600&zone=
I received my PhD degree in Organometallic Chemistry from the University of Seville in 2012 at the IIQ (CSIC-US), under the supervision of Prof. J. Cámpora. After doctorate, I moved to the group of Prof. B. Chaudret at LCC (CNRS-UPS) (Toulouse, France), for a postdoctoral stay. During this period, my research was centered on the synthesis, characterization and study of the surface chemistry of metal nanoparticles (MNPs). In July 2015 I joined the lab of Prof. P. Van Leeuwen at LPCNO (INSA-UPS) also in Toulouse, and I worked exploring new metal nanoparticles as efficient catalysts. In 2017, I achieved a Juan de la Cierva fellowship, which allowed me to start my independent career and to work with new supported/confined metal catalysts and magnetic catalysis at the ITQ (CSIC-UPV) in the team of Prof. Avelino Corma

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(Valencia, Spain).
During my scientific career, I have participated in numerous national and international projects, highlighting two projects as Principal Investigator (PI): Intramurales (42.222), which gave me the opportunity to start the supervision of my first PhD student (Christian Cerezo-Navarrete) as single director, and Primeros Proyectos de Investigación (PAID-06-18; 7.250), and an international partnership ERC project as work-package leader (LAURELIN; 4.853.053). Moreover, during the last years I have supervised two MSc students (Cristina Morales and Adrián García Zaragoza). In the course of my postdoctoral stage I also mentored 2 MSc and 6 PhD students.
I have published 35 papers (+ 1 under revision) in refereed journals, including 18 as first author and 9 as corresponding author. 31 of them were published in the first quartile (Q1: 1 Acc. Chem. Res., 1 Angew. Chem. Int. Ed., 1 Chem. Sci., 1 ACS Catal., 2 Nanoscale, 1 J. Catal., 6 Chem. Commun., 4 Chem. -A Eur. J., 5 Catal. Sci. Tech., 1 ChemCatChem, 1 Inorg. Chem., 1 Organometallics, 1 ACS Appl. NanoMat. 1 NanoSO, 2 Dalton Trans., 1 PCCP and 1 Eur. J. Inorg. Chem.).
I have been invited to give 3 seminars in research centres and universities (Universitat Rovira i Virgili, Universitat Jaume I and IIQ), to write two book chapters and four reviews. I have also participated in numerous international scientific conferences (ACS National Meeting, NanoTech, EUChemS, SILQCOM7th, etc.), specifically with 9 oral communications (imparted by myself) and 8 posters.
During my research career, I have been involved in different teaching (14.7 ECTS = 147 hours) and dissemination activities: (i) Feria of Science (2010-2012); (ii) Week of Science and Technology (2008-2012); (iii) Informative scientific article published in www.eldiario.es. Moreover, I am guest editor of a special number in Catalysts (MDPI) about Metal Nanoparticle Catalysis and an official reviewer for high impact journals (Chem. Sci., ChemCatChem, etc.).

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Turno de acceso general

Nombre: FEIXAS GERONES, FERRAN
Referencia: RYC2020-029552-I
Área Temática: **Ciencias y tecnologías químicas**
Correo Electrónico: ferran.feixas@gmail.com

Título:

Accelerating (Bio)molecular Recognition and (Bio)Catalysis with Computational Methods

Resumen de la Memoria:

Dr. Ferran Feixas is currently a Principal Investigator at the Institute of Computational Chemistry and Catalysis (IQCC) at the University of Girona (UdG) and co-Principal Investigator of the Computational Biochemistry Lab (CompBioLab) research group. In 2011, Dr. Feixas obtained his PhD in Chemistry with academic honors at the University of Girona under the supervision of Prof. Miquel Solà, Prof. Jordi Poater, and Dr. Eduard Matito. During the PhD thesis, he worked on the application and development of computational chemistry tools for the analysis of chemical bonding and aromaticity. In this period, he carried out short research stays on these research topics in France (Prof. B. Silvi), Czech Republic (Prof. R. Ponec), Germany (Prof. L. González). During the PhD, he also collaborated with Dr. L. Blancafort (UdG) and Prof. L. González (Universität Wien) to elucidate the mechanism of excited state hydrogen transfer in ortho-nitro benzaldehyde. Upon graduation, he moved to the University of California, San Diego (UCSD, United States), for a two-year postdoctoral position with a Beatriu de Pinós fellowship at the Prof. J. Andrew McCammon group. During this period, he worked on computer-aided drug discovery projects and exploring the role of protein flexibility by means of molecular dynamics and accelerated molecular dynamics simulations. In particular, he focused on the discovery of multi-target antibacterial drug leads for Mycobacterium tuberculosis in collaboration with Prof. E. Oldfield (University of Illinois-at-Urbana, USA) and protein folding studies with Dr. Miao (UCSD). In 2014, he joined the IQCC for the reintegration phase of the Beatriu de Pinós fellowship and subsequently in 2015 was awarded both Juan de a Cierva Incorporación (renounced) and the Marie Curie Individual Fellowship (IF-EF, MetAccembly) to study the processes of protein folding, biomolecular recognition, and assembly with accelerated molecular dynamics (aMD). In 2018, he became a Senior Researcher and co-Principal Investigator of the CompBioLab research group together with Prof. S. Osuna (ICREA/UdG) working in the field of biocatalysis.

In 2019, was awarded as Principal Investigator with a Programa Estatal de I+D+i Retos de la Sociedad project (RTI2018-101032-J-I00). The goal of the project is to develop computational tools to gain insight into the detailed molecular mechanisms of relevant (bio)chemical processes and, then, harness this information to enhance the discovery and rational design of novel drugs, supramolecular complexes, and/or (bio)catalysts. In this period at the IQCC, he has collaborated with world-leading groups to work in enzyme evolution (Prof. Osuna (UdG) and Prof. N. Tokuriki (British Columbia)), host-guest recognition (Dr. X. Ribas (UdG) and Prof. J. Jiménez-Barbero (CICbioGUNE)), excited-state aromaticity (Prof. Ottosson (Uppsala) and Prof. K. Mouth-Poulsen (Chalmers)), protein-fullerene assemblies (Prof. N. Martín (UCM), Prof. A. Cortajarena (CICbiomaGUNE)), liver cancer drug targets (Dr. G. Sabio (CNIC)), micromotor self-propulsion (Prof. S. Sánchez (IBEC)). Thanks to the MICINN contribution, Dr. Feixas started a research team (2 PhD students and 2 Master Students (2020)) with an independent research line as Principal Investigator at the IQCC (UdG). He has cosupervised the PhD thesis of Ouissam El Bakouri (PhD thesis defended 2017).

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Resumen del Currículum Vitae:

Dr. Ferran Feixas is currently a Principal Investigator at the Institute of Computational Chemistry and Catalysis (IQCC) at the University of Girona (UdG) and co-Principal Investigator of the Computational Biochemistry Lab research group. His scientific production includes 2 book chapters and 47 publications (+3 submitted) in international peer-reviewed journals ((among them, Nature, Nat. Commun, Chem. Soc. Rev., WIREs Comp. Mol. Sci, Adv. Funct. Mat., J. Am. Chem. Soc., Angew. Chem. Int. Ed., J. Mat. Chem. A., Nanoscale, Chem. Commun., J. Med. Chem., J. Chem. Theory. Comput., Chem. Eur. J., Adv. Synth. Catal.). In 33 out of 47 publications he is first, second author or corresponding author (11 as corresponding author). His publications accumulate 1700 citations (Web of Science), providing an h index of 23. The average citation per item is 36. In addition to that he has published 19 papers with neither PhD nor postdoc supervisors. He obtained his PhD in February 2011 with the maximum qualification excellent cum laude from the University of Girona. In 2015, he was invited together with his PhD advisors to write a review that summarizes most of the achievements of his PhD thesis (Chem. Soc. Rev. 2015, 44, 6434). He was awarded with the poster prize in the 9th Triennial Congress of the WATOC (July 2011). In the course of his research career, he has received several fellowships (FPU PhD fellowship, Beatriu de Pinós outgoing and reintegration grants, Juan de la Cierva Incorporación (renounced), and Marie Curie Individual Fellowship (MetAccembly project). During the postdoctoral stay at the UCSD, Dr. Feixas and coworkers explored the application of a tailored version of accelerated molecular dynamics (aMD) to study protein folding (J. Comp. Chem. 2015, 36, 1536). As independent researcher, Dr. Feixas have focused on understanding the molecular mechanisms of inhibitor selectivity in protein kinases (Nature 2019, 568, 557), substrate specificity in biocatalysis (Angew. Chem. Int. Ed. 2019, 58, 3097), and selective encapsulation of fullerenes in supramolecular capsules (J. Am. Chem. Soc. 2020, 142, 16051) among others.

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He has participated in 20 national and international research projects including three projects funded by the European Framework Programme H2020: Marie Curie MSCA-IF-2014-EF-661160 project as principal investigator and COST action ECOSTBio (CM1305) and Starting Grant ERC-2015-StG-679001 project as a participant. In 2019, was awarded as Principal Investigator with a Programa Estatal de I+D+i Orientada a los Retos de la Sociedad project (RTI2018-101032-J-I00) to establish his own research group at the IQCC. Ferran also established collaboration with Fundació Jaume Vicens Vives (2019-2023, 12,400 /year, PI: Feixas) and obtained computing hours from Red Española de Supercomputación and Partnership for Advanced Computing in Europe as PI. In the 2015-2020 period, he collected a total of 350.000 in funding as Principal Investigator. He has has participated in more than 70 conferences, 26 oral communications, in 11 of which as an invited speaker. He has presented his work at Pacifichem, WATOC, ACS National Meetings, and EuChemS conferences among others. He will be one of the main organizers of Girona Seminar 2022 on Biocatalysis. He has supervised the thesis of Dr. El Bakouri and the research project of 3 master students.

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Turno de acceso general

Nombre: MOONSHIRAM , DOOSHAYE
Referencia: RYC2020-029863-I
Área Temática: **Ciencias y tecnologías químicas**
Correo Electrónico: dooshaye.moonshiram@imdea.org

Título:

Inorganic Chemistry and Spectroscopy

Resumen de la Memoria:

I am currently a group leader at IMDEA Nanociencia working on time-resolved X-ray absorption in biological and chemical catalysis (http://nanociencia.imdea.org/home-en/people/item/moonshiram). I received my Ph.D from Purdue University, U.S.A, (2008-2013). After my thesis, I worked in 3 world-wide leading centres for artificial photosynthesis, and X-ray spectroscopy applied to photocatalytic complexes at Argonne National Laboratory, U.S.A (ANL, 2013-2016), Institute of Chemical Research of Catalonia (ICIQ, 2017), and at the Max Planck Institute for Chemical Energy Conversion (MPI-CEC, 2017-2018) as an Alexander Von Humboldt fellow.

During my career, I worked in a range of research areas in the development and application of synchrotron-based X-ray spectroscopies as probes of electronic and geometric structure in chemical catalysis for energy applications. I am interested in novel spectroscopic methods enabling the characterization of catalytic intermediates in solar fuel catalysts, and providing insights into metal oxidation, spins, and structural configurations. I have 27 peer-reviewed articles, 25 of which are in Q1, including 8 JACS, 1 PNAS, 1 Angew.Chem, 1 Nat.Commun, 1 Adv.Energy.Mater. 1 IScience, 1 Nat.Chem, and 1 Optica journals. Among these works, I was corresponding author in 7 journals, published 8 articles during my group leader position, and has led the first ultrafast X-ray spectroscopy study on a cobalt catalyst down to the picosecond (10-12 s) time resolution. This work revealed a complete mechanistic pathway followed by a hydrogen-evolving catalyst with spectroscopic characterization of the intermediates towards H-H bond formation step (J. Am. Chem. Soc., 2016, 138). The learning for these studies led us to investigate water oxidation photosynthetic complexes enabling the publication of a Nature Chemistry (Nat.Chem, 2020,12, 1060), where the role of X-ray spectroscopy by my group was disseminated on the front page of ICIQ news, MPI Institute for Eisenforschung, and ALBA.

I have established an international collaborative network of researchers in the synthesis of chemical catalysis, and have written and successfully led ~38 peer-reviewed proposals to obtain synchrotron time for X-ray based experiments. I received 16 invited talks in various international workshops and conferences well-recognized in my research field. Recently I have also reviewing European projects as an expert evaluator for the Horizon 2020 INEA - Energy Research and Innovation Fund projects.

I have been granted ~125.000 funding for a national Retos de la Sociedad grant, an Acciones de Dinamizacion Europa Investigacion project, and a research assistant grant through Communidad de Madrid during my group leadership. Aside from my research work, I received the ANECA certificate for profesor contratado doctor , and mentored Ph.D and undergraduate students allowing us to publish in Chem. Comm, Materials, JACS, Chem.Eur.J (Chem.Eur.J.2020, 26, 9527, Chem.Eur.J. 2020, 26,1), ChemSci, Angew.Chem, and PCCP (Under review). I was also teaching assistant in Mathematical Methods, General Physics, and Engineering Circuit courses and have in total 760 of teaching hours.

Such research and teaching opportunities awarded me with the H.Y Fan and Lijuan Wang Purdue distinction awards at Purdue, the Juan de la Cierva, and the Humboldt fellowships.

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Resumen del Currículum Vitae:

Currently group leader at IMDEA Nanociencia
ORCID: 0000-0002-6142-3440
Researcher ID: J-5138-2014
h-index = 15 (Google Scholar, January 2021)

Publications:
I have 27 peer-reviewed publications, 25 in the first quartile (Q1) of Multidisciplinary Chemistry and Physical Chemistry and 3 currently under review in Angew.Chem and Chem.Sci. I was the main contributor in most publications: 1st author in 8 publications, 2nd author in 7 publications, Corresponding author in 7 publications. - High-impact publications include 8 J. Am. Chem. Soc. (3 1st authored), 1 PNAS (1st

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authored), 1 Angew. Chem., 1 Nature Commun., 1 Adv.Energy Mater, 1 IScience, 1 Nat.Chem., and 1 Optica.

Scientific Seminars Contributions:
I have 32 presentations in international conferences and research centers, including 20 oral and 12 poster presentations. I have 16 invited talks out of the 20 oral presentations.

International Research Stays:
- 3 years at Argonne National Laboratory (ANL, USA)
~1 year at Max Planck Institute for Chemical Energy Conversion (MPI-CEC, Germany)

Competitive Awarded Fellowships:
- Alexander Von Humboldt postdoctoral fellowship (2017)
- Juan de la Cierva postdoctoral fellowship (2015)

- H.Y. Fan Award for Outstanding Research in Experimental Biophysics, Physics Departmental Awards Ceremony, Purdue University, Indiana, U.S.A (2013)
- Lijuan Wang Memorial Award for Women in Physics, Physics Departmental Awards Ceremony, Purdue University, Indiana, U.S.A (2013)

Research Projects:
-Awarded with National project from the Ministerio de Ciencias, Innovacion y Universidades (72.600), Acciones de Dinamizacion Europa Investigacion (6.875) and two year research assistant grant (45.000) through the comunidad de Madrid during group leadership.
- I have participated in a funding grant from the Department of Energy (DOE, USA) during my postdoctoral work at ANL on the spectroscopic-based characterization of proton reduction catalysts for Artificial Photosynthesis.
- My profile is oriented towards X-ray spectroscopy and physical chemistry studies on solar fuel catalysts. The use of synchrotron-based X-ray facilities involves applications of peer-reviewed proposals due to the high cost of the runs, estimated to be around 25000 per day. The beamlines and run time for public service is limited, this increases the competition and the acceptance rate is normally less than 20%. I have been PI in 38 accepted proposals in USA (APS, Chess), and European synchrotrons: ALBA (Spain), Elettra (Italy), Petra(Germany), and Soleil (France).

Supervision:
- Supervising PhD, masters and undergraduate students at IMDEA
-Supervision of PhD student during postdoctoral appointment at ANL
-Supervised 2 undergraduate students during graduate appointment at Purdue University

Teaching:
- 640 hrs. of teaching experience for undergraduate students at Purdue University between 2008 and 2009. Subjects: Linear Circuit Analysis
- 120 hrs. of teaching experience for undergraduate students at Smith College in 2006. Subjects: Mathematical Methods of Physical Sciences & Engineering

Administration tasks and Outreach:
-Expert evaluator for the Horizon 2020 INEA Energy Research and Innovation Fund projects
- September 2013-2014: Committee Member of Postdoctoral Society of Argonne National Laboratory
- Summer Undergraduate Research Fellowship to mentor 141 students in Engineering and Physics, Purdue University (May-Augu

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AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2020

Turno de acceso general

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Título:

3D printed living robots with advanced functionalities

Resumen de la Memoria:

My research activity is devoted to the development of synthetic/hybrid robotic platforms, exploring robots at different scales for both biomedical and environmental applications. The experience on synthesis and characterization of nanomaterials to be further integrated in miniaturized sensors I acquired during my PhD, provide me with a broad know-how of different point-of-care devices, ranging from miniaturized sensors, to lab-on-a-chip devices, and nano/micrometric mobile entities, also known as nano and micromotors. This last have been my field of expertise for the last 10 years, being able to work in the groups pioneer in the field, first as a PhD exchange student at the University of California San Diego (UCSD, USA) under Prof. Wang, later on as a postdoctoral researcher at IFW Dresden (Germany) under the supervision of Prof. Schmidt, and nowadays as a postdoctoral researcher at the group of Prof. Sánchez at the Institute for Bioengineering of Catalonia (IBEC).

While in my first experience at the UCSD I mainly worked with catalytic micromotors, fabricated by electrodeposition techniques and elucidating the main design parameters in a field that was just at its infancy, at IFW I mainly focused my attention on the development of biocompatible micromotors fabricated by strain-engineering. Always working at the microscale, I decided to move forward and continue my research at Purdue University, where I joined Prof. David Cappelleri s group, a reference on the automation of magnetic micromotors. The experience in a Mechanical Engineering department broadened my knowledge on the real challenges of well-established robotics, allowing me to thrive them in the microrobotics field while taking advantage of the actuation and design know-how acquired in my previous experiences. Also, during that period, I learned about 3D printing and its main potential to include advanced functionalities in synthetic robots, that were later tracked by vision-based algorithm to automate them.

My current position as a postdoctoral researcher leading the 3D bioprinted robotics team at IBEC encompasses all the disciplines I explored during my scientific career, considering not only exploring diverse fabrication techniques (3D printing, microfabrication) and materials of different nature, adding one more challenge: working with living entities by 3D printing them in biocompatible scaffolds. Such living elements are key to explore the emergent field of hybrid robotics, that include cells with contractile behavior in the robotic platform. My ongoing and future projects are focused on (i) the development of 3D-printed living robots with complex shapes and advanced functionalities by (ii) sensing of the undergoing biological events and (iii) accordingly program its actuation, later reaching its full automation by using vision-based control methods. This will be achieved by the convenient integration of nanomaterials and flexible sensors, which will facilitate local stimulation towards asymmetric contractility resulting in an efficient motion. This unique topic perfectly fits my research career, being a synergy over biosensing, robotics and automation by integrating sensing elements in bioengineered robots. Also, the impact of the current biohybrid platforms is not only key from the biorobotics standpoint, but for their potential use as biomedical models.
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Resumen del Currículum Vitae:

My scientific research career started at the Autonomous University of Barcelona, where I went for a degree in Chemistry and I later did a M.S. degree in Nanotechnology. I obtained my PhD in 2013 (Extraordinary Doctorate award) in the Catalan Institute of Nanoscience and Nanotechnology (ICN2) under the supervision of Prof. Arben Merkoçi, joining a multidisciplinary group focused on the development of miniaturized point-of-a-care devices for both environmental and biomedical purposes. The broad spectrum of platforms, ranging from screen-printed electrodes to lab-on-a-chip devices, allowed me to not only acquire specific skills on different fabrication techniques, but also on different analytical tools in the framework of electrochemistry. That basics served me to develop from advanced nanomaterials-based sensors to micromotors. This last, opened me the door to a groundbreaking field still in its infancy in 2011, where micrometric autonomous devices were envisioned as potential platforms for biosensing and pollutants degradation due to the mixing effect related to their motion. I could expand my knowledge on the field in one of the pioneer groups in the field, in the University of California San Diego (USA), leaded by Prof. Joseph Wang, resulting in 3 publication in high-impact journals in a 9-months internship.

In my first postdoc I followed the micromotors research line, joining a well-stablished group pioneer in the fabrication of rolled-up micromotors lead by Prof. Oliver Schmidt s at IFW Dresden (2013-2016). My research focus was the development of biocompatible micromotors for biomedical and environmental applications, avoiding the use of the toxic fuel hydrogen peroxide, commonly used for its motion activation. During that period, I was selected for and participated in the German-American Frontiers of Engineering Symposium in

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2015 sponsored by the Alexander von Humboldt (AvH) Foundation and the National Academy of Engineering. I was also awarded by the Follow-up Program by AvH to collaborate with Prof. David Cappelleri, whose research group I joined in 2016. At Purdue University, I worked on the (i) design, fabrication and automation of micro-force sensing mobile microrobots (μFSMM) for mechanobiology studies and manipulation tasks, (ii) development of micro tumbling magnetic microrobots with advanced climbing capabilities, and (iii) the fabrication of 3D printed magnetic helical micromotors with distinct integrated structural color features for vision-based tracking.

From 2018, I joined as postdoctoral researcher the Smart nano-bio-devices group, led by Prof. Samuel Sánchez at the Institute for Bioengineering of Catalonia (IBEC) (2018-2020, Juan de la Cierva-incorporación; 2020-2023 Beatriu de Pinós) to develop 3D printed autonomous living robots with advanced functionalities. I am currently leading the 3D bioprinted robotics division in the group, focused on the development of highly functional robotic systems based on 3D bioprinted living robots. Our research not only encompasses the key design elements and fabrication skills to obtain mobile robots based on living cells (i.e. skeletal muscle cells), but related automation challenges and understanding the undergoing biological events in biobots. Also, due to its inherent biological nature, such devices are also posed as potential 3D drug testing platform for medical purposes.

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Turno de acceso general

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Título:

Engineered nanospaces for the synthesis of high added value compounds

Resumen de la Memoria:

My research activities on the engineering of novel materials as heterogeneous catalysts for the manufacture of fine chemicals and pharmaceuticals are mostly focused on the following lines: (i) the design of the steric and electronic environment of nanospaces in multifunctional hybrid organic-inorganic reticular catalysts with versatile compositions and porous architectures, leading to relations between molecular architecture and catalytic performance; (ii) the clean and efficient synthesis of high added value molecules, i.e. biomass-derived oxygenate molecules and aza-(heterocyclic) compounds, by controlling the chemical transformations inside the engineered pores of the solids.

After completing a BSc in Chemistry at the University of Alicante (2005-2010), I have gained >10 years of broad research experience at the interface of reticular and organometallic chemistry toward fundamental understanding and control of chemical reactivity in the pores of advanced solid catalysts. My research career was developed in 3 prestigious institutions in Spain and Belgium:

(i) Instituto Universitario Mixto (Universidad Politécnica de Valencia & CSIC) de Tecnología Química, ITQ (MSc & PhD student, Spain, 10/2010-05/2016), where I worked (supervised by Dr. F. X. Llabrés i Xamena and Prof. A. Corma) on metal-organic frameworks (MOFs) with acid-base and redox-active sites (metal-oxo clusters, nanoparticles and organometallic complexes) that promoted one-pot multistep reactions towards fine chemicals (terpenes or bioactive amines) and biofuels. This resulted in 2 book chapters and 10 articles with average IF~5.6 (7 as 1st and 1 as corresponding in J. Phys. Chem. Let.), 1 patent requested and 7 conference contributions.

(ii) Centre for Membrane separations, Adsorption, Catalysis and Spectroscopy for Sustainable Solutions (CMACS), KU Leuven (Postdoc & Marie Curie-Individual Fellow, Belgium, 06/2016-09/2019), where I managed H2020-MSCA, KU-Leuven Industrial Research and ESRF-NWO funded projects as PI (>400k) within the group of Prof. D. De Vos, independently drafting and executing networks with top researchers from >7 different research institutions across Europe and USA, being speaker in 12 high-level international conferences. The combined use of tailor-made MOF, ionic liquids, MOF-derived clusters and robust aluminosilicates (zeolites & mesoporous organosilica) enabled environmentally benign manufacture of bioactive steroids, N-heterocyclic scaffolds and biomass-derived molecules, resulting in 1 book chapter and 18 articles (average IF~7.0), with 10 as corresponding & 1st, only or last author at high-level journals such as Angew. Chem., Green Chem. or ACS Catal. I also supervised 1 MSc+1BSc student.

(iii) Instituto de Ciencia Molecular (ICMOL), Universidad de Valencia (Junior Leader, Spain, 09/2019-present), where I am supervising 1 PhD+1BSc student and have authored 1 book chapter and 4 articles, being 1st/last and corresponding author in 3 (1 of them in Chem. Mater.), leading researchers from 3 different institutions and 1 project at ALBA. As PI, I am opening new research lines with the support of La Caixa foundation (>300k), on the design and understanding of chemical reactivity at enzyme-like nanospaces in greener reticular materials with rich hierarchical architectures and multiple functionalities based on abundant, non-toxic building blocks.

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Resumen del Currículum Vitae:

I obtained a BSc in Chemistry (University of Alicante, July 2010), MSc (Technical University of Valencia, September 2011), and completed a PhD with Cum Laude grade (promotors: Dr. F. X. Llabrés i Xamena and Prof. A. Corma, funded with a FPI fellowship, at ITQ/CSIC-UPV, March 2016), working on multifunctional metal-organic frameworks as heterogeneous catalysts. In June 2016 I moved to KU Leuven (Belgium) in the group of Prof. D. De Vos, where I gained multidisciplinary experience on porous solids and ionic liquids for organic synthesis (40 months, 24 of them as a Marie Curie Individual Fellow evaluated 98.60 over 100.00). In September 2019 I came back to Spain (ICMOL, University of Valencia) as a Junior Leader La Caixa Incoming to continue my independent career on tailor-made greener reticular catalysts for the environmentally benign synthesis of value-added products (>15 months).

I have proven ability to obtain and manage funding from international public and private sources (ca. 10 research projects including access to large European scientific infrastructures and networks with international academic and industrial partners), being PI in 5 of them within the last 4 years, funded by Marie Sklodowska Curie Actions (2017, 167 k), Industrial Research funds of KU-Leuven (2018, 247 k), La Caixa Foundation (2019, 305 k), as well as ESRF (2018) and ALBA (2020) synchrotron facilities. Overall I have consolidated >700 k as PI.

At the age of 33, I am proving track record of scientific contributions as an independent researcher, being author of 32 articles (25 within the last 4 years) in peer-reviewed international journals of the 1st quartile in their respective fields, with ca. 1000 citations in total, 75% of them in the last 4 years (h index of 15, i10 index of 20). I am first, last or single author in 18 (~56%), corresponding author in 14 (~44%) and 23 (72%) articles correspond to my postdoctoral period (without my PhD supervisors), from which I am first/last and corresponding author in high impact factor (IF>9.5) journals such as Angew. Chem. (2017), Green Chem. (2018), ACS Catal. (2019) or Chem. Mater. (2020). I am also author of 4 invited book chapters (2 as first and corresponding) in Elsevier and RSC, 2 covers and 1 patent requested.

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I have participated in >20 international conferences of the highest quality in chemistry, with oral contributions in 12 of them within the last 4 years in Europe (EuropaCat, EuroMOF, EUCHEMS) Asia (TOCAT, ZMPC) or America (ACS meeting), creating international academic or industrially oriented networks that resulted in high impact publications as lead author. I was invited to 4 science divulgation events by the Falling Walls Foundation and the Spanish Scientists in Belgium organization.

In 2018 I was awarded with the XIII Premio Científico Técnico Ciudad de Algemesí, finalist of the X SusChem Innova award and best contribution award at the Dutch Zeolite Association meeting. I have been part of the organizing committee of the FEZA 2011 school, evaluation committee of the 17th ICC 2020, reviewer of international high impact journals (IF>11.5) and editor in peer-reviewed open access journals (Molecules, Materials, BMC Chemistry and Frontiers in Catalysis). I have officially promoted 2 BSc final year projects, 1 MSc, 1 PhD (ongoing) and have been member of the evaluation committee in 3 PhD defenses.

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Turno de acceso general

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Título:

Design and development of tailored covalent organic frameworks

Resumen de la Memoria:

During her PhD with Prof. François Diederich at ETH Zürich, Laura M. Salonen gained expertise in the study of intermolecular interactions in protein-ligand complexes (Angew. Chem. Int. Ed. 2009 and 2011, Chem. Eur. J. 2012). During her post-doctoral stay with Prof. Dirk Trauner and Prof. Thomas Bein at LMU Munich, where she worked on the synthesis of covalent organic frameworks (COFs) for photovoltaic applications (J. Am. Chem. Soc. 2014).

She became fascinated by how organic chemistry methods and intermolecular interactions can be harnessed for the preparation of COFs, and she joined the INL in 2013 as a MSCA cofund fellow to develop a supramolecular strategy based on dipole moments to gain access to high-quality COFs (Chem. Commun. 2016). In addition, she also applied COFs for the first time for the capture of marine toxins from water (J. Chromatogr. A 2017), which sparked an interest for the application of these materials in water monitoring and treatment. Meanwhile, she also explored the use organic chemistry methods and dynamic chemistry for the functionalization of inorganic nanoparticles (supervision of PhD student N. Guldris 2017; J. Colloid Interface Sci. 2016, Bioconjugate Chem. 2017, Chem. Eur. J. 2018).

In 2017, Laura was promoted to Staff Researcher at the INL. Since then, she has pioneered the use of COFs for the capture of pharmaceutical pollutants from water (hot paper in Chem. Eur. J. 2018, Cover feature, ChemistryViews article), recently demonstrating that these materials also work in real water samples (Molecules 2020) and for the screening of pharmaceutical pollutants from water (under review). She was also invited to write a perspective article on tailoring COFs for the capture of water pollutants (Chem. Eur. J. 2019, Frontispiece). Currently, she is supervising a PhD student working on High-Quality Covalent Organic Frameworks to Capture Hazardous Compounds from Water (S. Fernandes, foreseen 2022).

Laura then became interested in the opportunities of enhancing the properties of COFs by preparing composite materials, and she supervised a post-doctoral fellow (V. Romero) funded by Xunta de Galicia, who worked on the synthesis of magnetic COF composites. These composites were much easier to separate from the sample matrix than the bulk COF, resulting in enhanced adsorption efficiency of target toxin compounds from water (Nanoscale 2019, Microporous and Mesoporous Mater. 2020, review in Molecules 2020, 1 article in preparation). Currently, in the context of ERA-NET BlueBio cofund project DIGIRAS, she is supervising a research assistant on the growth of COFs on other support materials for the implementation of these materials in recirculating aquaculture systems for the adsorption of off-flavor compounds.

Recently, Laura has started to explore COFs for catalysis, especially focusing on H2-related topics. In addition to participating in a study on the use of RuO2/COF material for the dehydrogenation of formic acid (Catal. Sci. Technol. 2020), she is currently supervising a PhD student (O. Oliveira, foreseen 2023) on High-Quality Catalytic Covalent Organic Frameworks through Enhanced Interlayer Interactions by Hydrogen Bonding , a post-doctoral fellow (MSCA individual fellowship) on COFs for hydrogenation of CO2, and she is the PI of COFforH2 project to explore COFs as artificial metalloenzymes for H2 activation.
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Resumen del Currículum Vitae:

Laura M. Salonen was born in Turku, Finland, in 1980. She obtained a Master s degree in Chemistry from the University of Turku on 2006, specializing in Organic Chemistry. After a research internship at F. Hoffmann−La Roche, Ltd. in Basel, Switzerland, she started her PhD research at ETH Zürich with Prof. François Diederich on the study of intermolecular interactions in protein-ligand complexes. After completing her thesis in 2011, she carried out postdoctoral research at LMU Munich under the supervision of Prof. Dirk Trauner and Prof. Thomas Bein with an LMU Research Fellowship. In 2013, she joined the International Iberian Nanotechnology Laboratory (INL) as a Marie Skłodowska-Curie Action COFUND fellow, and she was promoted to Staff Researcher in 2017. Since 2020 she is a tenured staff researcher at the INL.

During her independent research career since 2017, Laura has established a research line on the preparation of covalent organic frameworks (COFs) for the capture of contaminants from water. She has pioneered the preparation and use of COFs for pharmaceutical pollutant capture, and has since then demonstrated these materials to function in natural water samples as well as for the screening of pharmaceuticals (manuscript under review, P1 below), thus bringing COFs from technology readiness level (TRL) of 0 to 5 for monitoring of

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pharmaceutical pollutants in water. The relevance of this achievement is reflected, in addition to scientific attention (hot paper in Chem. Eur. J., Cover feature, article in ChemistryViews, full paper in Molecules, invited Concept article in Chem. Eur. J.), by relevant national media presence, including an article in the Portuguese newspaper Publico, and appearance in Portuguese news on the channel RTP and TVi.

On the other hand, she has recently started to explore COFs for catalysis with a view on hydrogen chemistry, which, in addition to a publication, is demonstrated by the co-supervision of a MSCA individual fellow working on COFs for the hydrogenation of CO2 and Laura being the PI of COFforH2 project exploring the use of COFs as metalloenzyme mimics.

Laura has established an international network of collaborators with scientists from Europe (e.g. Germany, Spain, Portugal, Czech Republic) and worldwide (USA, Israel). She is/has supervised 2 post-doctoral fellows, 2 completed and 2 ongoing PhD theses, 4 Master s/Diploma theses, as well as 4 research assistants and several visiting PhD students, exchange students and summer students. Her scientific independence is also reflected in that she is corresponding author in 50% of her publications. She has integrated in her institution through several responsibilities, such as serving as the Deputy Coordinator of the Clean Energy Cluster of the INL in 2021, as member of the institutional Safety Committee since 2017, in the organization committee of the Annual INL Research Symposium since 2018, and as part of the INL Learning Organization team since 2019.

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Turno de acceso general

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Título:

Desarrollo de Catalizadores Multifuncionales Avanzados y su Aplicación en Procesos de Catálisis Heterogénea para Superar los Retos de Desarrollo Sostenible

Resumen de la Memoria:

Research focused on heterogeneous catalysis, with a multidisciplinary profile: background in applied catalysis, wide experience in surface science, complemented with synchrotron light source studies. The aim: combining the fields to overcome heterogeneous catalysis challenges, currently starting up since the recent beginning of my 2nd project as PI.

I started in 2004 at the ITQ (Valencia, Spain), interspersing (until 2011) projects with industry and Ph.D. research (FPI fellowship MEC/Spain), developing alkane-based technology as a sustainable/cheaper alternative to industrial olefins-based processes to produce partial oxidation products (raw materials for most of the consumer goods). My research on this topic meant a significant technology transfer to industry (Sumitomo, Shell, PEMEX), especially: i) cyclohexanol/cyclohexanone from cyclohexane, ii) acrylic acid from propane, and iii) ethylene from ethane (the most important building block in petrochemistry).

In 2012 I faced the surface science field as PI of my own project, awarded with a Fulbright/ME postdoc. grant ($145.000,00), in the CFN at Brookhaven Nat. Lab. of the US DOE (24 months), developing: i) novel alloy oxidation strategy for highly stable Au-based nanocatalysts (Nanoscale Horizons, 2016); ii) Epitaxial graphene (Appl. Phys. Lett.,2013); iii) multi-technique (XPS, LEISS, QMS, TDS) surface science instrument (single responsible) intended as users facility for in-situ catalysis studies (Part.&Part. Syst. Charact. 2014; J. of Catalysis, 2017 & 2019).

In 2014, I moved to the Fritz-Haber-Institut, Berlin (Germany), a world leader in surface science and catalysis, where have participated in: i) ERC Starting Grant ENREMOS/FP7, ii) 2 Center of Excellence UniCat projects CH4 activation and COx activation , and iii) CRC 1109/1 project Understanding Metal Oxides/H2O Systems at Molecular Scale . Upgraded to Research Scientist position in 2016, I spent 48 months in total, focused on CO2 and water interaction/activation on metal oxide surfaces (Angew. Chem. Int. Ed., 2015 & 2018, J. Phys. Chem. C, 2018), and hydrogenation of unsaturated hydrocarbons (JACS, 2015; ACS Catal. 2017; PCCP, 2016).

After a short stay as an invited researcher, in early 2018, with Prof. R. Luque s group (Córdoba university), implementing projects on biomass revalorization (ChemCatChem., 2018; Appl. Sci., 2018; Electroanalysis, 2018; ChemistrySelect, 2018), I joined the Dept. Química Inorgánica y Química Técnica at UNED (April 2018), as PI of my own project (385,336,67) awarded by "Atracción de Talento Investigador. Modality 1" program of C. de Madrid (Spain). Addressed to the revalorization of CH4 and CO2 (Nanomaterials, 2020), the goals achieved so far include: i) direct conversion of CH4 and CO2 into ethanol below 250 ºC (MS. Thesis, B. Martínez Navarro, 2020; journal papers in process), and ii) direct transformation of methane into formaldehyde at 250 ºC (Nanomaterials, 2020), far below the temperatures reported (600-800 ºC) up to now. In order to combine with fundamental surface science studies, I have upgrades, in parallel, a multi-technique surface science instrument including X-ray photoelectron spectroscopy (XPS), secondary ion mass spectrometry (SIMS), and ion scattering spectroscopy (ISS), a unique technique extremely sensitive to the composition of the outermost atomic layer of condensed matter.

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Resumen del Currículum Vitae:

h-index 18, with 36 articles (SCI journals; 34 Q1), and 4 book chapters on catalysis and chemical engineering. From the 40 publications, 11 as first author and 7 as corresponding (5 as both first and corresponding author). Inventor of 9 patents (3 U.S. patents and 6 extensions), 44 communications in sci. meetings (12 as speaker; 37 International, 7 National), and 9 invited lectures in postgraduate schools, universities, and international research institutions, including the II Escuela de Espectroscopía de Sólidos Inorgánicos by the "Real Sociedad Española de Química" (Nov. 2018).

Reviewer in Nature journals, Applied Catal. A-General, J. Nanotech., Top. Catal., PCCP and others. Since Sept. 2018, Coordinator of Inorganic Chemistry and Chemical Engineering Module from the Master Ciencia y Tecnología Química (UNED), and member of the CFN Proposal Review Panel , reviewing/evaluating proposals to access facilities from the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory of United States DOE. Since Sept. 2019, member of the Editorial Board 100cias@uned Journal.

Researcher in 3 industry contracts (Sumitomo, Shell, and PEMEX; patents derived), and 12 research projects (6 national, 6 international) from competitive public calls, 3 of them as Principal Investigator: i) Fulbright/ME, $145.000; ii) Atracción de Talento Investigador Modality 1: Experienced Researcher, of C. de Madrid, 385,336,67 ; and iii) ALBA CALL 2020-II Project, ref. VA-2020024346. Awarded with the European Commission Seal of Excellence for the Horizon 2020 s MSCA-IF project, ref. 751882 (call 2016), and the Best Presentation Award at the 5th Int. Conf. Vibrations at Surfaces (2015). Granted with a postdoc. Max-Planck-Gesellschaft fellowship (2014-2016; 56.640), a postdoc. fellowship from Consejo Educación C. Valenciana; Ref. FMECD-2011/6543325555. (28.470), and a postdoc. UNED

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fellowship (86.400), Resol. 18 de Enero de 2017 (BICI nº 11).
75 months of international mobility: 3 months as FPI in IRCELYON (Lyon, France); 24 months as Fulbright fellow in CFN-BNL (Upton, U.S.); 48 months in the Fritz-Haber-Institut, FHI (Berlin, Germany), as MPG fellow (24 months) and as public service research scientist (24 months).
Director of 1 Ph.D. thesis (2017, Cum-Laude), 5 Master Sci. thesis in 2011, 2019, and 2020 (2 M.H., 1 Sobresaliente), and 2 Final Degree Projects in 2019 (1 M.H., 1 Sobresaliente).
Member of the UNED teaching staff in subjects from both the Degree in Chemistry, and the Science and Chemical Technology Master, since 2018. Member of Evaluation Panels in 6 Final Degree Projects (Chemistry), 9 M.S. Thesis (Science and Chemical Technology), and 3 M.S. Thesis (Occupational Risk Prevention, Chemistry Module).
Laboratory Officer Group A1 (2009-2010; public service competitive call) at Chem. Dept. of UPV (Valencia, Spain): main responsible for 2 laboratories, their equipment, scientific instruments, and staff.
Experience in Synchrotron Light-Source experiments/projects: i) XANES at BM31 beamline from ESRF in Grenoble (France) (Catalysis Today, 2014), ii) NAP-XPS beamline at NSLS-I from Brookhaven Nat. Lab. in Upton (NY, US) (Nanoscale Horizons, 2016), iii) NEXAFS and XPS at the beamline UE52-PGM in BESSY-II (Berlin, Germany), and iv) EXAFS as Principal Investigator (granted project, 2020) at CLAESS (BL 22) beamline in ALBA (Barcelona, Spain).