AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **LAPO , BOGANI**
Referencia: RYC-2013-14823
Área Científica: Ciencia y Tecnología de Materiales
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Título:

Quantum effects in molecular materials: from single-spin sensing to coherent control

Resumen de la Memoria:

I want to establish an independent research line in Spain, providing strong integration at the national and EU level, also with support from previous high-profile proposals, such as my ERC and Sofja Kovalevskaja actions. My research will aim at: a) the development of ultra-sensitive sensors, capable of detecting single spins; b) the creation and study of molecular spintronic devices; c) the study of the fundamental interactions between spins and electrons, with an unprecedented level of detail and resolution; d) the control, both classical and quantum, of spin nanosystems and the related devices. My research will include all necessary steps, from synthesis and fabrication of the nanoscale systems, to the development of ultra-sensitive measurement techniques, and eventually the theoretical modelling of the systems. It thus follows the full development and investigation of novel materials, and has the possibility of providing direct, active feedback from the characterization and modeling parts to the synthesis of the systems, which can thus be tailored to provide optimized properties. The main common point is the presence of magnetic nanomaterials, which will be synthesized, measured and integrated into spintronic devices. The electronic detection methods (currently developed in the Sofja Kovalevskaja action) will lead to an ultra-sensitive, non-destructive readout of the spin-state of single molecules, and will make molecular spintronic devices possible, where the magnetic element will possess quantum behaviour. Ultra-clean, time-resolved investigation of spin-electron interactions will be pursued with novel approaches combining electron paramagnetic resonance and pulsed lasers (accepted ERC Starting grant). In addition to reading the magnetization of a single molecule I also want to control it with external stimuli, like light or an applied electric potential. This will allow the control and detection of single spins, possibly leading to the implementation of quantum logic operations with molecular magnetic materials. All these research lines thoroughly mix chemistry and physics, in the spirit of materials science, and, besides the fundamental interest, are already leading to potential applications in room-temperature memory units based on molecule memristors and novel ultra-sensitive scientific instrumentation.

Resumen del Currículum Vitae:

Lapo Bogani's work is strongly multidisciplinary and covers the whole spectrum of investigation of molecular nanomaterials, dealing with their electronic, magnetic and optical properties; it includes key synthetic advances, the development of ultra-sensitive technique, the fabrication of devices, and the theoretical modelling of the systems.

Bogani has already influenced the advancement of several research areas, including molecular magnetic chains, molecular spintronics and photomagnetic materials. He has provided major breakthroughs in the study of slow-relaxing magnetic chains, both in their chemistry (devising their first rational synthesis and creating full families of these compounds) and in their physics (showing the importance of finite size effects and switching the dynamics with light). In molecular spintronics, he has established several key concepts and methodologies (e.g. molecular spintronic double quantum dot devices) and developed the first hybrids of carbon nanotubes and single molecule magnets. Eventually, his interest in magneto optics and photomagnetism has led to the creation of highly-sensitive magneto-optical instrumentation and the switching of magnetic nanoparticles and chains.

This truly multidisciplinary approach has led to the publication of over 40 papers in chemistry, physics and material science. Several of these contributions have been groundbreaking, and have established our present understanding of the chemistry and physics of single chain magnets, and have opened new concepts in the field of molecular spintronics, establishing it as a key area of research in molecular magnetism. The quality of these contributions is evidenced by the fact that the papers have received more than 2000 citations in 8 years, for a corrected h-index of 20, averaging 230 citations per year, and about 49 citations per paper. The research activity has also been awarded several prizes and distinctions, including 5 covers of international journals, an individually-driven EIF Marie-Curie fellowship, the Giovanni Semerano italian national prize for the best PhD thesis, the 2009 Burgen award of the European academy of sciences and the Sofja Kovalevskaja award, awarded every two years in a competition among all disciplines. At 33 years he received the 2012 Raffaello Nasini Prize of the Italian Chemical Society (awarded to the best Inorganic Chemist under 40) and he is this year's recipient of an ERC Starting Grant, which will be developed from 2014, and of the 2013 Nicholas Kurti European Science Prize. He is the first Chemist to receive this latter honor, which counts very prominent Physicists and a Nobel Prize winner among its receivers. Lapo Bogani has received more than 40 invitations to international congresses and schools. He is referee for several high impact journals (Nature Journals, Angewandte Chemie, Advanced Materials, Physical Review Letters, etc...) and funding agencies, including the French Agence Nationale de la Recherche, the US Department of Energy and the British Royal Society.

Lapo Bogani has always backed his research lines by writing projects, obtaining individual grants for more than 4.5 M€. He has strong ties to many European laboratories and the European Institute of Molecular Magnetism. The applicative possibilities of L.B.'s research are

under evaluation for collaborations with SONY EU division (Dr. Florian von Wrochem) for sensors and molecular devices.

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

Nombre: **CRIVILLERS CLUSELLA, NURIA**
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Título:

Materiales orgánicos funcionales para aplicaciones en Electronica Molecular

Resumen de la Memoria:

Durante la carrera científica de NURIA CRIVILLERS, su principal línea de investigación se ha centrado en la preparación de materiales moleculares funcionales para aplicaciones en Electrónica Molecular. Su principal esfuerzo se ha dirigido a explotar las propiedades de interruptores moleculares como componentes activos en dispositivos electrónicos y en concreto para la preparación de memorias moleculares. La estrategia que ha seguido es la de usar las distintas propiedades que presentan los diferentes estados de sistemas bi- y tri-estables como elementos para almacenar información o para otorgar multifuncionalidad a los dispositivos.

Núria realizó la Tesis Doctoral en el Instituto de Ciencia de Materiales de Barcelona en el grupo de Nanociencia Molecular y Materiales Orgánicos bajo la supervisión de Prof.Concepció Rovira y Dr. Marta Mas. Núria disfrutó de una beca de Formación del Profesorado Universitario (FPU) para llevar a cabo su Tesis. Con los resultados de su Tesis se demostró el gran potencial que tiene el uso de monocapas auto-ensambladas formadas por radicales orgánicos libres para la preparación de memorias moleculares. Además, estudios de transporte de carga a través de estas capas abrieron la posibilidad de usar estos sistemas en electrónica uni-molecular, y en concreto en el campo de la Espintrónica. Con el fin de estudiar y entender el tipo de interacciones que intervienen en el auto-ensamblaje, se llevó a cabo la investigación de la formación de organizaciones supramoleculars de especies electroactivas en superficie. Además, y en paralelo con este trabajo, Núria, realizó la síntesis y caracterización de moléculas que fueron después empleadas como semiconductores en transistores orgánicos de efecto de campo.

En la Tesis llevó a cabo un trabajo muy multidisciplinario, trabajando en distintas disciplinas como la síntesis orgánica, la química física y la ciencia de los materiales. Estos conocimientos constituyeron una base muy fuerte para poder desarrollar el proyecto de su post-doc. Núria realizó una estada doctoral de dos años y medio en el Institut de Science et d'Ingénierie Supramoléculaires (ISIS) en Estrasburgo, Francia. Núria disfrutó de una beca Marie-Curie IEF para desarrollar su proyecto. Este consistía en la fabricación de transistores orgánicos de efecto de campo que sus características eléctricas pudieran ser moduladas usando la luz. Para eso se usaron también interruptores moleculares pero en este caso moléculas fotocrómicas.

Actualmente Núria trabaja como investigadora Juan de la Cierva en el Instituto de Ciencia de Materiales de Barcelona, en el grupo NANOMOL siguiendo en el desarrollo de dispositivos más avanzados en el campo de la electronica molecular y en el campo de la espintrónica molecular. Núria es actualmente coordinadora de un proyecto europeo colaborativo enfocado al estudio de la aplicación de moléculas electroactivas las propiedades magnéticas de las cuales propiedades puedan ser moduladas eléctricamente.

Resumen del Currículum Vitae:

NURIA CRIVILLERS tiene un total de 29 publicaciones científicas con un índice de impacto medio (I,índice actual) de 9.15 y un índice-h de 13, con un 66 % de publicaciones con un índice de impacto alto (igual o superior a 5). Entre estas revistas cabe destacar: Chemical Reviews (1); Nature Chemistry (2); PNAS (1); Advanced Materials (3); Angewandte Chemie Int. Ed. (1); Journal of the American Chemical Society (2); Small (1) and Chemical Communications (4).

Posee una patente Española (ES20062663)"Procedimiento para la obtención de derivados del dicalcógenofeno-tetracalcógenofulvaleno (DC-TCF)" y es co-autora de un capítulo de libro: "PTM radicals for Molecular-Based Electronic Devices" en el libro: "Architecture and Design of Molecule Logic Gates and Atom Circuits", publicado por Springer. Realizó la Tesis Doctoral en el Instituto de Ciencia de Materiales de Barcelona en el grupo NANOMOL liderado por el Prof. Jaume Veciana, obteniendo el título en mayo de 2008. El título de su Tesis Doctoral es: "Organizaciones bi y tridimensionales de moléculas electroactivas para aplicaciones en dispositivos".

Durante su doctorado realizó varias estancias cortas en otros centros de investigación de alto prestigio internacional como el MESA+ Institute for Nanotechnology de la Universidad de Twente en Holanda (estancia de 4 meses), en el Instituto de Ciencia de Materiales de Madrid (estancia de 2 semanas), en el Katholieke Universiteit Leuven en Bélgica (estancia de 1 mes) y en la Jagiellonian University de Krakow en Polonia (estancia de 2 semanas).

La estancia postdoctoral (enero 2009-junio 2011) la realizó en el Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Université de Strasbourg, Francia, en el grupo del Prof. Paolo Samorì. La investigación que desarrolló fue: Diseño, preparación y caracterización de transistores orgánicos de efecto de campo modulados con luz y estudio de la interfase electrodo/SAM/semiconductor. Para la estancia doctoral disfrutó de la prestigiosa beca Marie Curie Intra-European Fellowship (IEF) (IEF-OPTSUFET PIEF-GA-2009-5967).

Actualmente Nuria Crivillers disfruta de un contrato Juan de la Cierva en el Instituto de Ciencia de Materiales en el grupo NANOMOL. En la actualidad es investigadora principal (IP) de dos proyectos europeos: 1) Marie Curie Career Integration Grant-CIG (PCIG10-GA-2011-

303989) y 2) es coordinadora de un proyecto colaborativo FET-Open (FET Young Explorers) que empezó en enero de 2014. El título del proyecto es Electrical Spin manipulation in electroactive molecules acrónimo ACMOL. Además, ha participado en 3 proyectos nacionales y en 6 proyectos europeos.

Nuria ha participado en 16 congresos, escuelas y workshops internacionales (EU y non-EU) con 7 contribuciones orales, 1 charla invitada en uno de los centros donde realizó una estancia y 9 contribuciones con póster. También, ha participado en 4 congresos nacionales, con 4 contribuciones orales, una de ellas invitada.

Ha dirigido el trabajo de dos master de Erasmus, colabora en la supervisión de dos estudiantes de doctorado y es oficialmente co-directora de un PhD contratado bajo el proyecto ACMOL.

El pasado año 2013 recibió el premio de la Real Sociedad Española de Química RSEQ-Sigma Aldrich a Jóvenes Noveles en el área de Química. En 2013 fue seleccionada para participar en el prestigioso encuentro "63rd Lindau Nobel Laureate Meeting".

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **MUÑOZ ESPI, RAFAEL**
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Título:

Colloidal Systems for the Design of Polymer/Inorganic Hybrid Nanostructures

Resumen de la Memoria:

The research line proposed here focuses on the application of colloidal systems for the design of polymer/inorganic hybrid nanostructured materials. On one hand, colloidal particles (both polymeric and inorganic) can act as a support for crystallization processes on their surface. On the other hand, the colloidal structures generated by micelles and surfactant-stabilized droplets serve as soft templates or nanoreactors for the controlled precipitation of inorganic materials, yielding nanoparticles and nanocapsules of with defined morphology. In addition, the application of heterophase-based colloidal techniques is also useful for the synthesis of multifunctional hybrid particles, for instance by miniemulsion polymerization in the presence of functionalized inorganic nanoparticles. In this context, three related research topics are presented: (1) the application of polymers and polymer colloids as controlling agents in crystallization processes; (2) colloidal systems as templates for crystallization and confined synthesis for complex inorganic compositions; and (3) design and engineering of polymer/inorganic multifunctional hybrid nanoparticles.

The effect of the confinement provided by colloidal systems in the control of crystallization processes is the main driving scientific problem to be addressed. We aim to investigate how precipitation and crystallization processes are confined at the surface of particles, to the interior of droplets, and to liquid–liquid interfaces. In all cases, the templating effect of particles and droplets can be understood in terms of "confinement", because the precipitation/crystallization is forced to happen in defined spaces. The investigations for the understanding of the interfaces and the structure–property relationships of the resulting materials are far from being a trivial question and offer an exciting research scenario.

Resumen del Currículum Vitae:

Rafael Muñoz-Espí studied chemistry at the University of València, completing his degree in 2001. From 2002 to 2006 he worked in the group of Professor Gerhard Wegner at the Max Planck Institute for Polymer Research (MPI-P) in Mainz. He received his doctoral degree in 2006 from the Johannes Gutenberg University of Mainz for a thesis analyzing the effects of functional latex nanoparticles on the growth and physical properties of zinc oxide. In 2007, he moved to the USA as a postdoctoral associate in the group of Prof. Benjamin Chu at the State University of New York at Stony Brook, where he stayed for two years. During this time, he was mainly involved on the polymer-assisted formation and structural characterization of polyoxometalates and transition metal oxides. Since 2009, he has been group leader for "Colloid-Assisted Crystallization" at the Max Planck Institute for Polymer Research in the department headed by Prof. Katharina Landfester. He has coauthored more than 30 publications in international scientific journals. His research interests include mineralization processes, crystallization in colloidal systems, and the study of the interaction of polymers with inorganic matter.

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **CORDOBA GALLEGO, JOSE MANUEL**
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Área Científica: Ciencia y Tecnología de Materiales
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Título:

Materials for extremely hostile environments (Aerospace, Aeronautical, Military and Energy Industries)

Resumen de la Memoria:

The candidate has got two Master Degree, in Materials Science (Solid State Chemistry) and in Engineering Chemistry (Genetic and Biomolecular Chemistry), and he got his PhD degree with the cum laude mark. During his stay as Assistant Professor in the Nanostructured Materials Group (Linköping University (Sweden), he had experience as the main responsible of the set-up and maintenance of the laboratory. Also, he has experience as teacher in the Physical Metallurgy and Materials for Energy courses. He has supervised three PhD student, one master degree student and one licentiate degree student. He has carried out successful collaboration with industrial partners (Impact Coating AD (Sweden), IMA Engineering Services Limited (Malta), etc.) as well as universities (Drexel University (USA), Fraunhofer FEP (Germany), etc.) and research centers (CNRS (Italy), etc.). The scientific production of the candidate can be summarised in 54 papers (48, published; 2 accepted and 4 in progress) in high quality international journals. In the most of them the candidate is the first author showing the high involvement level in the research carried out. Several of the manuscripts, in which the candidate is the second or the last author, have been developed by the students (PhD and/or Licenciate Thesis) supervised by him. Also, the candidate's research has been disseminated in 46 congress communications (14, oral presentations) (39, international and 7, national). Also, the candidate is co-author of the industrial patent P201131835 and a chapter in a book. Finally the candidate has developed labors of main researcher and leader in different national and international projects.
The need for materials operative at temperatures above 2000ºC with no or limited oxidation and ablation arises from future leading applications in several sectors such as military, aerospace, energy, or chemical industry (Ultra-high-temperature ceramics (UHTCs). Potential applications as thermally stable and protective systems in extreme environments like hypersonic flight, atmospheric re-entry, and rocket propulsion; in heaters and igniters; in refinery and refractory process vessels and internals; etc, depend on the development of new materials with higher temperature capabilities than the current state-of-the-art materials can provide. For these high and ultra-high temperature applications, ceramic matrix composites have to be used principally. These materials, which are now in development, are based on refractory carbides, nitrides, and borides of the early transition metals, as exemplified by ZrB2, ZrC, ZrN, TiB2, HfB2, HfC, HfN, TaB2, and TaC, because of their high melting points, high hardness, good chemical inertness and oxidation resistance, good thermal conductivity, low electrical resistivity, wear resistance, and high-thermal stability.
The main research of the candidate has been focused on the use of MSR process as an affordable and reproducible manufacturing process for unexplored solid solutions in the MT-C-N and MT-B systems. The candidate has employed these pre-made solid solution-based compositions instead of unalloyed mixtures as the raw materials for the fabrication of high and ultra-high temperature materials, cermets and ceramic matrix composites, which should allow the achievement of a higher level of quality and reliability in their final properties. The work carried out by the candidate has leaded to the formation of an international network on this field.

Resumen del Currículum Vitae:

The candidate got his degree in Chemistry in 2000, after that, he obtained a master degree in Chemical Engineering (2002). He got his PhD in Chemistry (2007) from the University of Sevilla-ICMS (CSIC), Spain, under the supervision of Dr. Fco. José Gotor (CSIC). During this period, the candidate got a master degree in Materials Science (2005) in the field of Solid State Chemistry.
After the PhD period, he got postdoctoral experience [(01-05-2007 to 30-04-2008) postdoctoral student and (01-05-2008 to 31-12-2010) Assist. Professor)] in the Nanostructured Materials Group (Linköpings University) leaded by Prof. M. Odén. He was one of the founders of the Nanostructured Materials Divison. During the first months of the stay he was working in the planning, organization and purchase of all of the necessary facilities of a new division of materials science. During the stay, he was the main responsible of the laboratory and equipment. During the stay he was the co-supervisor of the PhD students, Emma M. Johansson (Mark: A) and Mohamed A. Ballem (Mark: A), as well as, the licenciate thesis student, Hao T. Tsei, and supervisor of the licenciate thesis student Jennifer Ullbrand. Also, he acquired teaching experience in the Materials for Energy and Physical Metallurgy courses. During the abroad stay, he has taken care of the start-up and development of the group main research research line.
The candidate was back on the ICMS (Seville) by the JAE-Doc Program (2010-2013). During this period, the candidate worked on the research line, materials for extremely hostile environments and he started a new research line based on the use of new deposition techniques of transition metal diborides for aeronautical and aerospace applications. The work carried out by him leaded to the formation of an international networking (Spain, Italy, Austria, Slovakia, etc). During this period, the candidate has been the co-supervisor of the Dr. Mr. Ernesto Chicardi

He has done several stays in prestigious research centers (Universite Paris Sud and Stockholm University) and companies (IMA Engineering Services Limited, Invited Researcher). During these stays, high quality experience in XRD, electron microscopy and wet-chemical were achieved. Also, the candidate has given a talk in the Leibniz Institute for Solid State and Materials Research, Dresden.

The scientific production of the candidate can be summarised in 54 papers (48, published; 2 accepted and 4 in progress) in high quality international journals (e.g. Journal of Materials Chemistry, Nano Letters). In the most of them the candidate is the first author showing the high involvement level in the research carried out. In several, in which the candidate is the second author, have been developed by the students (PhD and/or Licenciate Thesis) supervised by him. Also, the candidate's research has been disseminated in 46 congress communications (14, oral presentations) (39, international and 7, national). Also, the candidate is co-author of the industrial patent P201131835 and a chapter in a book.

The candidate has participated in several research projects (European FP6, Convenio CSIC/Slovakia Science Academy, EC in Erasmus Mundus Programme). Also, ha has carried out collaborations in the field of structural materials with the Swedish companies Norstel AB and Impact Coating AB. Finally, the candidate is referee in prestigious journals edited by the RSC, the ACS, Elsevier, The American Ceramic Society and SpringerLink.

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

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Título:

Development of a computational framework for designing optimal atom- and energy-efficient forms of matter with tailored properties

Resumen de la Memoria:

My research interests focus on integration of recent advances in computational chemistry and materials science with new developments in chemical and material informatics to provide a novel framework and algorithms for efficient materials discovery. At its core, I aim to create and apply tools for materials design, in which chemical systems with desired properties or performance are easily identified. Over the last five years, my efforts have been mainly focused on discovery of porous materials for energy applications such as carbon dioxide capture and methane storage. However, through collaborations and releasing open-source software, my developments are now reaching other applications such as ionic liquids, catalysts and battery materials design.

In my work, I am merging many different ideas and methodologies. For example, I have used computational geometry and partial differential equations-based techniques to analyze studied chemical structures and the associated data such as electron densities or pores structure of each system. I have used optimization algorithms to select systems to undergo characterization, as well as machine learning tools to control data collection, build property-predicting models and perform analysis of sets of molecules or materials. Parallel and large scale computing have been employed to perform simultaneous classical and/or electronic structure characterization of many carefully selected (statistically relevant) chemical systems. My goal has been to build computational machinery that can perform almost unsupervised discoveries of new chemical systems.

Enabling efficient design of materials is my greatest research ambition. My career goal is, however, more broad. I'd like to build a strong and recognized research program in the area of material informatics. I have been realizing this goal since 2008 when I joined the Lawrence Berkeley National Laboratory (Berkeley, CA, USA). My five most significant achievements so far are: (1) I have conducted high quality research, both independently as well as in collaboration with other groups, summarized as publications in top-notch scientific journals (ca. 45 publications in the last 5 years, 83 total); (2) I have been able to secure research funds via competitive grant calls (10 grants in the last 5 years) to create and support a group of 6 (myself, 3 postdocs, 2 students); (3) I have created unique software tools (e.g. Zeo++ code for analysis of porous materials) as well as web-based material databases (e.g. www.carboncapturematerials.org) used by hundreds registered users worldwide from both academia and industry; (4) my research has gained international visibility reflected in numerous invited presentations, journal covers and newsletter articles. (5) relying on my internationally gained experience, I have become independent investigator supervising junior researchers, reviewing peers' work (publications, US and EU grant proposals) and serving the scientific community (e.g. organization of symposia).

Resumen del Currículum Vitae:

Maciej Haranczyk is a Staff Scientist in the Scientific Computing Group at Lawrence Berkeley National Laboratory (Berkeley Lab) in Berkeley, CA, USA. Dr. Haranczyk received a PhD (2008) and MSc (2003) degrees in Chemistry from University of Gdansk, Poland. He spent his post-doctoral appointment as a 2008 Glenn T. Seaborg Fellow at the Berkeley Lab, and was promoted to a Research Scientist position in 2010, and then a Staff Scientist position in 2014.

Dr. Haranczyk has extensive research experience gained through international mobility. He stayed at different institutions in The Netherlands, Germany, UK and USA for periods lasting from two months to 1.5 years. In particular, he stayed as a research student at the Utrecht University (Summer 2001), at the Pacific Northwest National Laboratory, Richland, WA, USA (3 months in 2002, and 16 months in 2003-2004), at the Technical University of Muenchen (2 months in 2002). During his graduate education, he performed part of his research project at the University of Sheffield (7 months in 2007) and at the University of Southern California in Los Angeles (6 months in 2007-2008).

Dr. Haranczyk has co-authored 1 book chapter and 83 publications, which have been cited over 1100 times (h-index of 21). He has also received numerous awards for his research including American Chemical Society CINF-FIZ Chemie Award for Scientific Excellence (2006), Jacques-Emile Dubois Award from the Chemical Structure Association Trust (2008), Charles Kittel Award for Best Theoretical Research (2008) as well as awards for his thesis and doctoral dissertations (Janina Janikowa Award for the most outstanding Master Thesis of 2003 in the field of chemistry by the Polish Chemical Society; The 2008 Most Outstanding Doctoral Dissertation in Chemistry. Award from a three-

party committee of the Polish Chemical Society, University Gdansk, and Technical University of Gdansk).

As a researcher at the Berkeley Lab, Dr. Haranczyk is leading a research team working in the area of material informatics. His research activities are funded through competitive research grants. Over the last five years, he has been awarded single Principal Investigator (PI) awards from the US Department of Energy (US DOE) Office of Basic Energy Sciences and US DOE Office of Advanced Scientific Computing Research (ASCR) (4 projects, ca. 1M USD for 4 years), and the Berkeley Lab's Laboratory Driven Research and Development program (ca. 0.6M USD for 3 years). He has also participated as a co-PI on large projects such as the US DOE BES Energy Frontier Research Center for Gas Separations (10M USD for 5 years), the US DOE BES Center for Functional Electronics (11M USD for 5 years), a US DOE Advanced Research Project Agency Energy-funded project on carbon capture (3.6M USD for 3 years) and a US DOE National Energy Technology Laboratory-funded project on gas separations (1.1M USD for 3 years).

Dr. Haranczyk is a member of the American Chemical Society(ACS), the Molecular Graphics and Modelling Society and the Materials Research Society. He serves in the Programming Committee of the COMP and CINF divisions of the ACS.

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **COLL BAU, MARIONA**
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Título:

Preparation of functional oxide thin films with atomic-scale control by low-cost chemical approaches and soft-lithography

Resumen de la Memoria:

Over 11 years of experience as materials scientist,my know-how ranges across the synthesis and characterization of nanoscale engineered functional oxide thin films (including insulator, magnetic, superconductor and ferroelectric materials) prepared by chemical methods combined with soft-lithography patterning(SL) and chemical surface engineering skills.During my PhD at ICMAB-CSIC I made significant contributions to the superconductivity community helping establishing the basics to develop a new approach to prepare chemical solution deposited (CSD) YBa2Cu3O7 (YBCO) superconducting films resulting in world leading YBCO performances. It was essential to understand the relationship between the chemistry of the metalorganic precursors, the kinetics and the thermodynamics involved in the thermal treatment of CSD oxides and their structural, chemical and physical properties acquiring a solid experience in all these areas, thanks also to the stays I performed in internationally recognized labs in USA and Europe.This work was transferred to the spin-off Oxolutia. My skills placed me in an excellent position to currently lead a research line at ICMAB, within the framework of an EU project, aiming to develop radically new chemical approaches to prepare superconducting YBCO films incorporating oxide nanoparticles to widely explore the huge capabilites associated with these new type of nanocomposite (NC) materials. I am recognized in the superconductivity field to have developed a new YBCO NC composition that has been crucial to underline the universal and distinct behavior of CSD-NC. These results will be transferred to EU companies to be scaled-up fabricating several hundred meters of superconducting cables constituting an important breakthrough.I uniquely combine this expertise with chemical surface engineering and SL strategies acquired during my postdoc in U.Maryland-NIST, USA.There, I led a US project and I demonstrated for the first time the fabrication of reliable molecular electronic devices placing the top metal electrodes by SL and preserving the integrity of the self-assembled molecules which could one day miniaturize the electronic industry with single molecules acting as electronic switches.I broadened my skills performing a thorough study of the chemical interaction between molecule and metal contact.This multidisciplinary knowledge has driven me to launch and lead a new research line at ICMAB to prepare ultrathin films and nanostructures by atomic layer deposition (ALD) combined with SL strategies.I opened the field to develop ultrathin epitaxial oxides at low temperatures (300ºC) with different functionalities (insulating, magnetic, ferroelectric) and also the stabilization of new phases which are very challenging goals from a processing point of view and have a huge impact in film properties, applications and fabrication cost. I work in close collaboration with worldwide recognized experts in the field (Prof. K.Nielsch and Prof. S.Mathur) and private companies. I will continue this research line devising ALD epitaxial ferroelectric perovskites oxides with gradient composition to build a new emerging concept of solar cells. I recently submitted a national project as PI in this topic reinforcing my research independence and leadership.

Resumen del Currículum Vitae:

I received my degree in chemistry from UBarcelona in 2002. In 2007, I earned my PhD degree in Materials Science from UAB performing the research at ICMAB-CSIC with a FPU grant.I was a postdoctoral researcher at U.Maryland,USA holding a joint appointment at NIST, USA for 3 years. In 2010 I joined back ICMAB, awarded with 2 postdoctoral grants (BP and JdC). At present, I am a contracted postdoc within the framework of an EU project.My research focuses on the development of radically new processes to generate and stabilize nanoscale engineered functional oxide thin films and nanostructures combining chemical solution deposition (CSD), atomic layer deposition (ALD) and soft-lithography (SL).I have made relevant contributions to the field of superconductivity helping establishing the basics to develop a new chemical approach to prepare high quality (nanostructured)-YBa2Cu3O7 thin films to obtain world leading performances when CSD were just emerging as an alternative to the well established vacuum techniques.Also, I put forward feasible CSD oxide buffer layer candidates to integrate on metallic substrates. I performed stays in international labs in EU and USA. Now, as a postdoc, I lead a research line on this topic within the framework of an EU Project. I published in high impact journals (Nature Mater., Phys.Rev.B, Chem. Mater).I presented my work as oral contributions in EU, USA and Japan (MRS, EMA, ASC) including 2 invited talks.I supervised 5 students (2 MSc,1 PhD internship,2 PhD thesis ongoing). In the field of chemical surface engineering and SL I successfully devised a robust approach to fabricate molecular junctions keeping the integrity of the molecules that one day could miniaturize the electronics industry with single molecules acting as electronic switches. I published my work in JACS, APL, JPCC, some of them highlighted by the press.I also attended prestigious conferences: ACS,APS,E-MRS,ECS,GRC. I established intl. collaborations (U-Maryland USA, WFU USA, EMPA,Switzerland).I participated in 3 US projects (leading one of them) and I supervised an undergrad student. I was a referee of the Washington Editorial Review Board.This multidisciplinary background strengthened my research career and leadership in the preparation and characterization of functional nanomaterials and in 2011 I have launched a new research line at ICMAB based on innovative chemical routes to obtain epitaxial oxides combining ALD and SL being the first in the ALD community to obtain low-temperature epitaxial oxide thin films and stabilize new phases

having a deep impact in materials properties and fabrication cost. I already have 1 publication (Chem.Mater), and 1 under evaluation (Nano Letters). I have a submitted national proposal as PI. I presented this work in MRS, E-MRS and BALD-ALD.I supervised 3 students(2 undergrad,1 PhD internship).I collaborate with worldwide recognized researchers:Prof.Mathur,Prof.Nielsch-Germany, Prof.Corma, Spain.I am very active in technology transfer and outreach activities.I am on the editorial board of Scientific Reports (Nature group). In summary, I have 32 publications (1st author in 12) including 1 invited review and 1 invited paper.Cites>480 and H=12, 75% first quartile,1 patent granted and 1 book chapter.2 invited talks, 35 orals in intl. conferences and invited colloquiums.I participated in 19 research projects (including 5 EU,3 USA,1 Japan), 1 national project as a PI under evaluation. I supervised 9 students.

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **CANAL BARNILS, CRISTINA**
Referencia: RYC-2013-14676
Área Científica: Ciencia y Tecnología de Materiales
Correo Electrónico: criscanal@yahoo.com

Título:

Low temperature plasma tuning of drug release & biological interactions from biomaterials for restorative and regenerative medicine

Resumen de la Memoria:

Dr. Cristina Canal started her research in the textile field, working on surface modification of textiles with low temperature plasmas for the substitution of conventional processes, gaining expertise in different surface characterization techniques for materials, as well in textile finishing techniques.

Since then, during her post-doctoral research period, she has progressively reoriented her research towards biomedical materials. She has made significant scientific contributions to her scientific field. In particular, in 2007, she found the main species of plasmas responsible for the surface modification of materials by the use of plasma diagnostics on post-discharge plasmas[1,2], which constitutes a step forward in the field of surface treatments by low temperature plasmas. Later, in 2009, her work allowed grafting F on the surface of textiles through the use of fluorine containing plasmas to confer them with antibacterial properties with views on medical dressings[3].

Taking advantage of her experience in nanoscale surface modification of polymers and textiles for improved wettability (among other properties) by cold plasmas[4,5], she developed a series of works on nonwoven membranes for use as conditioning material in plasma sterilization processes[6,7,8], allowing the transmission of atomic species from plasmas through the membranes to sterilize materials wrapped in them and developing specific indicator materials for such processes, essential to allow transfer of plasma sterilization technologies to the market.

This experience was also applied on the development of nanostructured solid foams from highly concentrated emulsions which could be successfully modified by remote plasmas[9] and used as models for the development of pharmaceutical dosage forms for delivery of low molecular weight drugs[10].

More recently, within a series of novel and innovative works in one of the current research lines of the candidate on biomaterials for soft tissue therapy, focusing on the regulation of drug release from textile materials by means of low temperature plasma, it has been possible to show that through fiber surface modification with plasmas it is possible to alter the interactions with drugs and modify their release behavior[11,12]. Lately (2011 and 2012) Dr. Canal has published two review works focused on biomaterials for hard tissue regeneration and repair (with Calcium Phosphate Cements); one for drug delivery[13] and another for formation of composites with fibers (her original field), being the first review work in this topic[14], both of which have had significant impact within the scientific community, and have set the basis for publications in both directions[15,16,17] dealing with biomaterials for bone regeneration have been recently published or are ongoing where Dr. Canal is either first or corresponding author.

[1]Plasma Process Polym.4(2007)445 [2]Plasma Chem. Plasma Process.27(2007)404 [3]Int.J.Pharm.367(2009)155 [4]TextileRes.J.77(2007)559 [5]J.Adhesion Sci.Tech.13(2004)1077 [6]Plasma ProcessPolym.5(2008)867 [7]Appl.Surf.Sci.254(2008)5959 [8]Patent WO2008078053(2006) [9] Plasma Processes Polym.6(2009)686 [10]J.Pharm.Pharmac.Sci.15(2012)197 [11]Plasma Chem.Plasma Process.30(2010)885 [12]Plasma ProcessPolym.9(2011)165 [13]Adv.DrugDeliver.Rev. 64(2012)1090 [14]J.Mech.Behav.Biomed.Mater.4(2011)1658 [15]ActaBiomater. 9(2013)8403 [16]J.Amer.CeramicSoc. Accepted(2014) [17]Plasma ProcessPolym. Submitted(2014).

Resumen del Currículum Vitae:

Dr. Cristina Canal graduated in 2001 in Chemistry at the UAB (Bellaterra, Spain), and joined the Surfaces Products and Textile Processes group (UPC - Terrassa, Spain). In 2002 she joined the Surface Chemistry Group in the IIQAB – CSIC, to perform the PhD Thesis on plasma modification of textiles under Prof. P. Erra, being awarded 1st prize of AEQCT in 2003. In 2005 she was awarded her PhD Cum Laude, with European Mention, at UPC. In 2006 the PhD thesis received the 1st prize by Institut d'Estudis Catalans.

Since then, she has been awarded successive relevant competitive post-doctoral grants which have allowed her working in different international research centres; In particular, in 2006 she joined the team of Prof. André Ricard to work on plasma diagnostics and their application on textile materials with views on medical applications, at the group Plasmas Réactifs Hors Équilibre - LAPLACE (CNRS – Toulouse, France) with a grant of the French Ministry. In 2007 she moved to the team on Development of Medicines in Nanostructured Systems of Prof. M.J. Garcia-Celma at the Faculty of Pharmacy (UB - Barcelona, Spain) with a "Beatriu de Pinós" competitive fellowship, to work on drug delivery from nanostructured systems and where she started developing her own research line on modification of materials with plasmas for biomedical applications. In 2010 she joined the Biomaterials, Biomechanics & Tissue Engineering group (UPC – Barcelona, Spain), with Prof. M.P. Ginebra with a "Juan de la Cierva" fellowship where she is currently working on biomaterials for bone substitution or for soft tissue repair, plasma modification and drug delivery.

As a researcher, Dr. Canal has also made different research stages in France, Portugal and Slovenia.

- 38 SCI papers, most in 1st Quarter: 1st author in 20; 2nd author in 7; last/corresponding author in 4 (+3 sent).
- 3 patents (2 licensed). 1 book & 4 international book chapters with ISBN. 12 non-indexed publications.
- 4 Scientific awards (highlight: L'Oreal-Unesco for Women in Science Spain 2012)
- Supervisor of 6 PhD Thesis (UPC): 1 presented in 2011, 3 Foreseen in 2014 (March, June, July). Supervisor of 2 Master thesis (Master Nanoscience & Nanotechnology - UB) and 3 Engineering Final Projects (CMEM- UPC).
- Member of International Scientific Commitees in: 9th EU-Japan JSPP2014; 69th IUVSTA (2012) Workshop; 62nd IUVSTA (2010); 21st IFATCC (2007) Congress, Session Chair & Co-editor of the Proceedings ISBN-13: 978-84-612-2641-2
- Member of Organising & Scientific Committee in BIOCERAMICS26 (November 2014).
- Organiser of 2nd Cost Action TD1208 Annual Meeting (March 2015).
- Acredited as Lecturer Professor (6 recognitions AQU, ANECA)
- Universitary Teaching since 2005: Bachelor (Pharmacy UB), Engineering (Materials UPC), and Master (Nanoscience and Nanotechnology; Research & Development of Drugs UB, Biomedical Engineering; Materials Science; Textile Technology and Management UPC).
- Expert member in the elaboration of the European Comission BREF Document on BAT for the Textile Industry and many other International Textile Committees and WGs.
- Elected member of: Cloister of the UPC (2013), Board of the Faculty of Pharmacy, UB (2009).
- Member of: SGR Consolidated group; Associated unit to IBEC; CIBER-BBN.
- Industrial experience: Farmaban S.A. (2001).

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **WALL , SIMON**
Referencia: RYC-2013-14838
Área Científica: Ciencia y Tecnología de Materiales
Correo Electrónico: projects@icfo.es

Título:

Ultrafast dynamic control of correlated materials

Resumen de la Memoria:

Simon Wall has been a NEST fellow and junior group leader at ICFO since 2012. He received his undergraduate, masters and doctoral degrees from the University of Oxford. From 2009 to 2012 he worked at the Fritz Haber Institute of the Max Planck society where he was awarded a fellowship from the Alexander von Humboldt foundation. His research has focused on using multiple ultrafast techniques to study the femtosecond, non-equilibrium processes in materials, in particular, examining the dynamics of electrons, the lattice, spin and orbital degrees of freedom in correlated materials. His research combines both lab-based experiments and the use of cutting edge large scale facilities around the world.

His 3 most significant research achievements are:

1. Measuring the role of lattice vibrations and the structural pathway of the photoinduced insulator metal phase transition in VO2. These experiments led to new interpretation of the photoinduced transition which were published in Nature Communications (2012) and Physical Review B (2013). This work also led to a new method to generate, characterize and compress low power, broad-band pulses which was published in Applied Physics Letters (2011). This work resulted were enabled by a grant from the Alexander von Humbolt foundation, which enabled an independent project. The work received wide recognition and resulted in invited talks at several international conferences on material science, including ICPEPA USA 2012, Photonics West USA 2013, and MRS Japan 2013.

2. Demonstrating the role of quantum electronic coherence on the ultrafast charge-transfer processes in Mott insulators. This work showed dynamics on an unprecedented timescale and was published in Nature Physics (2011). This work was realized through LaserLab Europe and was highlighted in the group's annual publication and resulted in invited talks at international conferences on organic solids (ISCOM Poland 2011) and ultrafast surface science (USD7 Croatia 2010).

3. He has made significant contributions to the physics of manganite materials, with publications in Nature Materials (2007), Physical Review Letters (2009, 2011) and Physical Review B (2009, 2011, 2012) and an invited review in IEEE selected topics in quantum electronics (2011). These works were started during the PhD and the collaboration was maintained during post-doctoral studies and examined a broad range of phenomena in manganites. They made use of a combination of optical and X-ray techniques and made use of several international user facilities, including the ALS – Berkeley – USA, LCLS – Standford – USA and Diamond – Oxford – UK.

His work at multiple research centers around the world, together with his experience with range of experimental techniques has led to him being requested to write several letters of support for experimental installation at large scale user facilities. He has strong collaborations with groups at the IR FEL at HZDR-Dresden, FHI-Berlin, Diamond and the University of Oxford and Hamburg and has coordinated several projects between these groups.
His scientific credentials and innovative ideas are recognised though a Marie Curie CIG grant for young researchers, excellent publication record, and success in obtaining experimental time at multiple user facilities.

Resumen del Currículum Vitae:

Simon Wall's research career has taken place at some of Europe's premier research institutes. He was awarded a first class master's degree in physics from the University of Oxford. His results in examinations resulted in an undergraduate scholarship and book prizes and his master's project was on quantum computation under the supervision of Prof. Dieter Jaksch.

He remained at the University of Oxford for his post graduate, obtaining a DPhil in atomic and laser physics under the supervision of Prof. Andrea Cavalleri on "photo-induced dynamic in complex materials probed with femtosecond X-rays and few cycle optical pulses" in 2009. His research quality was recognised by St. Johns College Oxford, which awarded him a North Senior Scholarship. His research focused on generating ultra-short optical and X-ray pulses to study correlated materials, primarily focusing on research into dynamics in manganites.

During his DPhil, he taught statistical mechanics and quantum physics at undergraduate level and was also an academic mentor for

undergraduate students with disabilities.

After his DPhil, Simon was awarded a fellowship from the Alexander von Humboldt foundation and took a post-doctoral research position in the 2007 Nobel-prize-winning Department of Physical Chemistry at the Fritz Haber Institute of the Max Planck Society in Berlin, from 2009-2012. His research focused on developing ultra-broad-band probing techniques for use in time resolved non-linear optics of surfaces, interfaces and magnetic systems, photoemission and the use of coherent phonons to study changes in the interatomic potential. The latter was applied to study the photo-induced phase in VO2 and showed that a prompt change in the lattice potential drives the phase transition process.

In 2012 Dr. Wall was awarded a NEST fellowship at ICFO in Barcelona and started his own research group. His current research focus is on the femtosecond dynamics of crystalline-to-amorphous phase transitions in phase change materials, THz control of domain structures and light control of magnetic ordering. In 2013 he was awarded a Marie Curie Career Integration Grant (CIG) for promising researchers from the European Union.

As well as research based in laboratories, he has also worked at a large range of user facilities around the world. These include the synchrotrons: Diamond Light Source - UK, BESSY – Germany and ALS – USA. As well as the free electron lasers: LCLS – USA, FLASH - Germany and FELBE – Germany. This has enabled him to build up a world-wide reputation and has written letters of scientific support for several beamline instruments.

The quality of his research is highlighted through continued publications in high impact journals, including Nature, Nature Physics, Nature Materials, Nature Communications and Physical Review Letters, as well as multiple invitations to present at international conferences around the world, in addition to smaller departmental invitations.

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **GARCIA CAÑADAS, JORGE**
Referencia: RYC-2013-13970
Área Científica: Ciencia y Tecnología de Materiales
Correo Electrónico: jorge.garcia.canadas@gmail.com

Título:

Characterisation and fabrication of semiconductor devices for optoelectronics and energy related applications

Resumen de la Memoria:

I obtained my degree in Chemistry in 2000 at the Universidad Autónoma de Madrid (UAM). I started my MSc/MPhil in the area of electrochemistry at the Department of Chemistry in the UAM based on the electrosynthesis and chemical characterisation of conducting polymers. In 2002 I spent 6 months as a visitor researcher in the Group of Prof. Laurie Peter at the University of Bath (United Kingdom) working in the preparation and photo-electrochemical characterisation of nanostructured electrodes and electrochromic materials.

After completing my MSc/Mphil, I joined in 2003 the Photovoltaic and Optoelectronic Devices Group of Prof. Juan Bisquert at the Universitat Jaume I of Castellón as a PhD student. During my PhD I was involved in the preparation, characterisation and the development of physical models for electrochromic materials (a-WO3, conducting polymers and viologen functionalised electrodes). In addition, I also worked in the preparation and characterisation of solar cells; especially dye-sensitized solar cells by means of impedance spectroscopy, voltage decays and other photo-physical techniques.

After finishing my PhD in October 2006 I was offered a position as a R&D Manager in the recently created spin-off company Xop Física S. L. in the Science Park of the Universitat Jaume I, where I led the development of soil moisture, conductivity and temperature sensors based on transparent conductive oxides. In 2011 I was contracted by Cardiff University (United Kingdom) to work in the Thermoelectric group of Dr. Gao Min in the School of Engineering. In Cardiff, I have been working in the fabrication of thermoelectric devices and the design and construction of thermoelectrical characterisation techniques. Moreover, I have established new research lines for the development and characterisation of flexible dye-sensitised solar cells and the use of impedance spectroscopy in thermoelectricity.

In conclusion, I have developed the characterisation and preparation of semiconductor devices as my main research line along my career. Most of the semiconductors with applications in the optoelectronics and energy harvesting areas. I have co-authored more than 25 papers in international journals, I am the inventor of two patents and I have participated in more than 10 regional, national and European research projects.

Resumen del Currículum Vitae:

This are the most relevant merits from my currículum:

1. Most relevant publications:

-T.A.N. Peiris, K.G. U. Wijayantha and J. García-Cañadas.
Insights into mechanical compression and the enhancement in performance by Mg(OH)2 coating in flexible dye sensitized solar cells.
Physical Chemistry Chemical Physics 16, 2912-2919 (2014).

-J. García-Cañadas, A.V. Powell A. Kaltzoglou, P. Vaqueiro and G. Min.
Fabrication and evaluation of a skutterudite-based thermoelectric module for high temperature applications.
Journal of Electronic Materials 42, 1369-1374 (2013).

-G. Garcia-Belmonte, J. García-Cañadas and J. Bisquert.
Correlation between volume change and cell voltage variation with composition for lithium intercalated amorphous films.
Journal of Physical Chemistry B 110 (10) 4514-4518 (2006).

-F. Fabregat-Santiago, J. García Cañadas, E. Palomares, J. N. Clifford, S. A. Haque, J. R. Durrant, G. Garcia-Belmonte and J. Bisquert.
The origin of slow electron recombination processes in dye-sensitized solar cells with alumina barrier coatings.
Journal of Applied Physics 96 (11) 6903-6907 (2004).

-J.García-Cañadas, A. P. Meacham, L. M. Peter and M. D. Ward.
A near infrared electrochromic window based on a Sb-doped SnO2 electrode modified with a Ru dioxolen complex.

Angewandte Chemie-International Edition 42, (26) 3011-3014 (2003).

2. Patents

-J. García-Cañadas, P. Guillamón Castillo and J. Mayor Alabau.
Sistema de medida de la conductividad (system for the measurement of the conductivity).
Patent No: ES2400653 (2013).

-J. García-Cañadas, J. M. Pérez, A. G. Quiroga, M. A. Fuertes, C. Alonso and C. Navarro-Ranninger.
Determination of catalase activity in samples treated with [ZnCl2(isopropylamine)2]: a novel zinc complex that slows down the decay in activity of catalase extracts.
Journal of the Chemical Society. Dalton Transactions 11, 2283-2288 (2002).

3. Most relevant funded projects I have participated:

-Thermoelectric Heat Recovery from Low Temperature Exhausts of Steel Processes.
European project (1.506.651 €), started 01/07/2013, 3 years duration.

-Accelerated Metallurgy - the accelerated discovery of alloy formulations using combinatorial principles.
European FP7 project (23.800.986 €), started 15/06/2011, end date: 14/06/2016.

-Global solar spectrum harvesting through highly efficient photovoltaic and thermoelectric integrated cells.
European FP7 project (3.972.560 €), started 01/03/2013, 3 years duration.

4. Most relevant grants obtained

-Torres Quevedo, started 01/04/2008, 3 years duration.

5. Other merits:

-Co-director of PhD thesis:
1. Full-spectrum solar energy harvesting using nanotechnology-enabled photovoltaic/thermoelectric hybrid system. Hasan Talib Hasim. Date of reading: 09/2014.
2. Solar Powered Thermoelectric Cooling System. Hayder Sami Saleh Al-Madhhachi. date of reading: 12/2016

-Overseas stays:
1. University of Bath (United Kingdom) from 04/2002 to 09/2002.
2. Cardiff University (United Kingdom) from 01/2011 up to now.

-Invited talks:
1. Characterisation of energy related devices: from photovoltaics to thermoelectrics.
Device Integration Workshop. Swansea University (United Kingdom), 29/04/2013.
2. Characterisation methods for nanostructured materials € a thermoelectric approach.
Seminar of the Instituto de Microelectrónica CSIC, Madrid (Spain), 05/09/2012.

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

Nombre: **GARCIA FERNANDEZ, PABLO**
Referencia: RYC-2013-12515
Área Científica: Ciencia y Tecnología de Materiales
Correo Electrónico: garciapa@unican.es

Título:

Engineering of novel materials using electron-vibration interactions

Resumen de la Memoria:

Electronic and structural degrees of freedom strongly interact in many materials and are a source of novel phenomena that can be exploited to obtain new functionalities. My main research line consists in understanding these interactions in a wide variety of systems and proposing new materials that display enhanced magnetic, optical, dielectric or transport capabilities. This kind of research is strongly multidisciplinary as it requires a deep knowledge of the underlying physics of the problem and a good formation in chemistry to obtain new systems with the desired properties. My discoveries involve the proposal of an oxide superlattice that has a half metallic state which is fully confined in 2 dimensions, a whole new family of spin-crossover systems presenting very long lifetimes or the finding of a Ni2+ complex with the highest magnetic anisotropy in a transition metal system.

I have worked on how magnetic and optical properties of transition-metal impurities in insulator are influenced by the local distortions of the complex (publishing an invited review on the problem in J. Phys. Condens. Matter in 2006) and the problems of dynamics and complex magnetic behavior of systems that display a half-filled degenerate shell that defines a new kind of spin-crossover material far from the usual FeX6 complexes (1 Phys. Rev. Lett.).

My focus in recent years has been the field of complex oxides in different forms: bulk both pure and doped and heterostructrures. My contributions for these systems range from understanding the origin of hybrid improper ferroelectricity (published in Phys. Rev. Lett.), design and understanding of the magnetic and transport properties of strongly confined bidimensional metals (1 Phys. Rev. Lett., 1 Phys. Rev. B) or the chemical control of the octahedral rotations in perovskites (1 J. Phys. Chem. Lett, 1 Phys. Rev. B) or the dynamics of impurity centers (1 Phys. Rev. Lett.). A second area of application is the magnetic bistability of single-ion molecular magnets and the quest to achieve higher blocking temperatures, a problem which is directly connected to magnetic tunneling and spin-phonon coupling. As indicated above my contributions in this field involve the discovery of Ni2+ complexes with colossal magnetic anisotropy that provides the spin in these complexes an stability which is very close to that of molecular magnets (Chem. Science).

Currently I am working on a new second-principles method that I will present in the March Meeting of the American Physical Society that is able to perform simulation with tens of thousands of atoms at an accuracy level close to that of ab initio simulations and fully taking into account electronic and lattices degrees of freedom. I plan to use this method to research transport properties (thermoelectricity), systems displaying metal-insulator transitions and polarons in various oxides in order to find new interesting materials for future electronic devices as described in detail in the main text of the proposal.

Resumen del Currículum Vitae:

EDUCATION AND FORMER APPOINTMENTS: Dr. García-Fernández graduated in Physics at Universidad de Cantabria in 2000 and got his PhD. funded by a FPU fellowship in the same University in November 2004 supervised by Prof. M. Moreno. He has also a wide view of different research schemes thanks to two long stays in foreign Universities: first in the United Kingdom (six months in DeMontfort University, Leicester, in Prof. Bayliss group), and then in the USA (2.6 years supported by the Welch foundation in the University of Texas, Austin, in the group of Prof. Boggs and Bersuker, the world leader in Jahn-Teller effects in solids). In 2008, Dr. García Fernández returns to Spain, initially with a Juan de la Cierva fellowship (2008-2011) in Prof. Moreno's group, and currently with a postdoctoral research contract founded by an European Project in Prof. Junquera's group.

METHODOLOGICAL CONTRIBUTIONS: He is an expert in various first and second-principles methods with emphasis in strong-electronic correlation (CASSCF, CASPT2, hybrid DFT) and non-Born-Oppenheimmer dynamics that play an important role in high-Tc superconductivity or photochemistry.

APPLIED CONTRIBUTIONS: Thanks to his stays in three different Universities and the contacts made on them, Dr. García-Fernández has broad research interest, that go from the study of systems with exotic electronic properties (high-magnetic anisotropy, degeneracies,...) and modelling of structural, optical and magnetic properties of impurity centers, to the new phenomena emerging at complex oxide interfaces. My current international collaborations include I.B. Bersuker (USA), P. Ghosez (Belgium), D.I. Bilc (Romania), M. Gruden-Pavlovic

(Serbia), N. English (Ireland), C. Daul (Switzerland).

INTERNATIONAL RECOGNITION: Dr. García-Fernández has published 59 publications in peer-reviewed-journals. Among them 5 in Phys. Rev. Lett. (Impact Factor, IF=7.37), 1 in J. Phys. Chem. Lett. (IF=6.58), 1 in Chemical Science (IF=8.38), 1 cover article in Phys. Chem. Chem. Phys. (IF=4.01), and an invited review in J. Phys: Cond. Matter. Other publications include 37 papers in journals with an IF>3.0. I am main author of most of my publications (40 as first, last and/or corresponding author). My publications have been cited at least 572 times, my h-index is 14 and the number of citations per year is rising steadily (112 in 2013). I have presented 53 communications in international symposia, including 14 oral, 7 invited and 2 plenary talks (2 invited and 1 plenary in 2014).

I am an active referee in several journals including Phys. Rev. Lett., Phys. Rev. B or Inorg. Chem., and has participated in two project evaluation comittees (from the Research Council of Katholische Universitat Leuven and the Romanian National Research Council). I have already supervised a PhD Student (Dr. A. Trueba), who obtained maximum marks and the award for best science thesis at the University that year.

FUNDING: Dr. García-Fernández has participated actively in the writing and execution of an European Project within the 7th Framework Programme (OxIDes). Right now, another two FP7 projects are under peer-review-evaluation-process. He has obtained a bilateral Spanish-Serbia collaboration project on the development of room-temperature single-ion magnets. Finally, he acts as the local coordinator of the Santander node of the CODECS COST action.

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

SECRETARÍA DE ESTADO
DE INVESTIGACIÓN
DESARROLLO E INNOVACIÓN

SECRETARÍA GENERAL
DE CIENCIA, TECNOLOGÍA
E INNOVACIÓN

DIRECCIÓN GENERAL
DE INVESTIGACIÓN
CIENTÍFICA Y TÉCNICA

SUBDIRECCIÓN GENERAL
DE RECURSOS HUMANOS
PARA LA INVESTIGACIÓN

AYUDAS RAMÓN Y CAJAL
CONVOCATORIA 2013

Nombre: **GRAZU BONAVIA, MARIA VALERIA**
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Área Científica: Ciencia y Tecnología de Materiales
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Título:

Biofunctionalization of micro and nanostructured materials for biotechnological and biomedical applications

Resumen de la Memoria:

During 20 years of research activity the main research line that I carried out was "Biofunctionalization of micro and nanostructured materials for biotechnological and biomedical applications". In this sense, the development of an appropriate biofunctionalization strategy is no mean feat, as the biomolecules to be joined to the surface of the material could vary significantly in terms of size, chemical composition, 3D complexity, location of its biological active site. Thus, no universal methodologies exist to cover the wide variety of materials and biomolecules available for this purpose and each particular case (material+biomolecule) requires optimization of the most adequate functionalization protocol. All these years of research have showed me that if properly designed, a functionalization strategy could be a powerful tool to improve the stability, activity, specificity and selectivity of the attached biomolecule which results in more bioactive materials and in substantial improvements of its subsequent biotechnological or biomedical application. During my pre-doctoral work (1994-2006) in the group of Dr. Francisco Batista-Viera (Faculty of Chemistry, Uruguay) and as PhD student in the group of Dr. José Manuel Guisán Seijas (ICP-CSIC, Madrid), I focused my work within this line of research in the development of tailor-made novel functionalization strategies of different microstructured materials with enzymes in order to improve their subsequent biotechnological applicable purpose: synthesis of drug intermediates, synthesis of probiotics, and reutilization of industrial by-products. Since my incorporation as postdoctoral researcher at the Institute of Nanoscience of Aragón (INA) (2006-2013), I have translated this experience in the development of novel oriented functionalization protocols of different nanoparticles (gold, magnetic, quantum dots, silica), carbon nanotubes and cantilevers with antibodies (Ab) and other biologically relevant biomolecules (cell adhesion proteins, fluorescent dyes, carbohydrates, cell internalization peptides, nucleic acids). The obtained functionalized nanomaterials have been used to develop two different new sub-lines of research based on innovative applications of these materials: i) the development of novel biosensing strategies, and ii) the development of a novel controlled drug release methodology based on hyperthermia and magnetic NPs. The main objective of my work in Nanodiagnosis was to combine a good Ab functionalization with the interesting physical properties of nanomaterials in order to improve selectivity and sensibility of different novel biosensing schemes. With all of them we were able to improve in several orders of magnitude the limit of detection of several analytes in comparison with the gold standard biosensing technology used in clinical diagnosis. In the field of Nanotherapy, one of my achievements was to develop a novel strategy to obtain mutlfunctionalization of NPs based on the use of complementary nucleic acid (DNAs) chains. This work resulted in a patent that was the cornerstone in the foundation of Nanoimmunotech SL (NIT). Finally, all the acquired experience in the field of biofunctionalization of materials allowed me to be actually in charge of the Research&Development Department of NIT where I am in charge of: all the research of the company and the transference to the market of the multifunctionalization strategy of materials that I previously helped to develop at INA.

Resumen del Currículum Vitae:

As a native of Montevideo (Uruguay), I attended in the Faculty of Sciences of the University of the Republic of Uruguay, and was graduated in 1999 in Biochemistry. Since 1994 I started to work in the group of Dr. Francisco Batista-Viera at the Faculty of Chemistry. I received a grant to carry out a Junior Research Project by "Fondo de Investigación Clemente Estable" (1997-1999). Following my graduation in 1999, I won a competitive teaching position as Assistant Professor at the Institute of Biological Chemistry in the Faculty of Sciences (1999-2003). Besides, I have awarded a highly competitive MsC Fellowship-PEDECIBA-QUIMICA (2000-2002). This fellowship allowed me to carry out a joint master thesis between Dr. Batista-Viera¿s laboratory and Dr. José Manuel Guisán¿s laboratory (Institute of Catalysis and Petrochemistry, ICP-CSIC, Madrid, Spain). In 2003, I went to Dr. JM Guisán laboratory to carry out my Ph.D. After graduating with a Ph.D. at the Autonomous University of Madrid in June of 2006, I had a proposal offer to work as postdoctoral research fellow at the Institute of Nanoscience of Aragon (INA). Having already made several long-term stays in international renowned I+D centers and even my PhD abroad, I decided to accept this challenge instead of doing a postdoc outside Spain. This way I had the opportunity of co-founding the Biofunctionalization of Nanoparticles and Surfaces Group (BioNanoSurf), later renamed as Group of Nanobiosensors and Nanotherapy (GN2) together with Jesús Martinez de la Fuente. This was an excellent opportunity to acquire skills in settling up laboratory facilities, opening new areas of research, establishing interdisciplinary national and international collaborations, management of funding and human resources, writing of National and European financial proposals, etc. During 7 years at INA, I have worked in the development of novel mono and/or multifunctionalization protocols of different nanomaterials for their use in diagnosis and therapy. As I believed that undertaking periodical stays in research centers is essential for a varied and rich scientific career, once the GN2 group was settled up, I visited the laboratory of Dr. Helene Feracci at the Centre de Recherche Paul Pascal (CRPP)-CNRS (Bordeaux) on two occasions (1 month in 2010 and 6 months in 2011). In 2012, thanks to a competitive grant that I awarded from the Aragon Regional Government, I was able to

carry out a 6-month secondment in the Nano-Imaging facility of the Andalusian Centre for Nanomedicine and Biotechnology (BIONAND, Malaga). Finally since January of 2014, as Research and Development Director of Nanoimmunotech SL, I am responsible of all the research of the company and a technical department formed by 8 PhDs. Fruit of 20 years of scientific work, I have 5 patents (3 of them licensed), 55 papers (36 in the last 5 years), 37 posters and 12 oral communications in National and International congresses, 7 book chapters, 1 book editorial, 1063 citations and a H-index of 20. I have given 10 invited talks. I supervised 3 Master and 3 PhD students. I have been a member of 6 PhD tribunal thesis. I have participated in 18 National and 3 European projects. I am IP of a Large-Scale FP7-NMP project (1.200.000 €). I cofounded NanoImmunotech SL and I am a member of its Board of Directors. Finally, I have participated in 3 science divulgation projects in order to improve the public's understanding of science.

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Título:

Functional ceramics and electroceramics for industrial applications: Research and Development of products for market

Resumen de la Memoria:

Since 1998 and until October 2005, I worked at the Ferroelectric Department in the Materials Science Institute of Madrid, CSIC, where I obtained my PhD grade in April 2003 in lead free piezoceramics. My formation during the PhD student stage was completed with stays at the Universite du Maine-Le Mans (France) and at the Josef Stefan Institute (Eslovenia). From November 2005 to July 2007, I completed my postdoctoral training working at the R&D department of the multinational company EPCOS. My task was the study of materials for their use in high power capacitors, with direct application into the market. I was responsible of several research projects, as the study of the effect of oil on some type of polypropylene to reduce the costs and increase the performance of the capacitors; the application of resins as a component to protect and reduce the number of components of the capacitors, increasing its performance in certain applications with a lower cost; and new and lower-cost polypropylene materials in high power capacitors. From January 2008 I work at the Electroceramic Department in the Ceramic and Glass Institute, CSIC, in the processing and characterization of ceramic materials for SOFC applications, multiferroic materials and manganite oxides in a first stage. From April 2012 I work at the Ceramic for Smart System Group (CSSG), under the supervision of the Professor José Francisco Fernández Lozano. My activity is mainly focused in three research lines. One is related to thermoelectric materials for energy recovering. A novel method of combined high energy milling process (mechanosynthesis) and Spark Plasma Sintering gives place to a nanostructured that combines the appropriate electrical and thermal conductivity. The second deals with piezoelectric materials as energy harvesters, in which the task was the fabrication and characterization of the so-called piezoelectric cymbals; and the third one is the study of materials materials as security document markers in industrial applications. The experience acquired during the stage in Epcos relates with these lines that I am working in the CSS Group in the last years. In my projects, the interaction with private industry will be a strong line to be developed, as a way to increase the funding and also to keep incorporating the Development activity (the D of the R&D concept), in a similar way as the works I carried out in EPCOS and in some of the parts of the Industrial projects I am developing at the ICV.

Resumen del Currículum Vitae:

As a result of my work during these years, I have published 51 papers, 46 of them in international journals within the Science Citation Index. One of them, A. Moure, et al, Progress in solid state chemistry 37, 15-39, 2009 is a review of high temperature piezoelectric materials. I have published in 21 different journals within different fields of Materials Science, Physics, Chemistry and Energy. In 26 of the published papers (59% of the total), I figure as first author, and in 6 of them as second author (more than 70% of the works as first or second author). These works have received 377 cites until February 2014. My h index is 12. The 69% of the papers were published in journals of the Q1 quartile and 13% in journals of the Q2 quartile (more than 80% in Q1 and Q2 quartiles). My publication with the highest impact factor as a first signing author was published in the journal Chemistry of Materials (i. f. =6.400 in the publication year) in 2010. I have published papers in other journals with high impact factor, as Acta Materialia, Journal of Power Sources or Fuel Cells or Progress in solid state chemistry.

I have participated in 11 National, European and Industrial research projects for the study of polycrystalline materials. My job was the processing and characterization of bulk materials, mainly electroceramics with different applications (as piezeoelectric, dielectric, materials for SOFC, magnetorresistive, etc). During my stay at the Epcos Company, I was also responsible of several R&D projects to study adequate materials and developments that allow minimize costs and increase the performance of high power capacitors. They were the study of the effect of oil on some types of polypropylene, with the aim of reduce costs and improving the lifetime of high power capacitors. Other project studied the application of resins on capacitors working at relatively low voltages, with the purpose of reduce the number of pieces of the capacitors, reducing thus their cost while maintaining a good performance. The resin also acts as a protector of the dielectric capacitor again humidity. I also studied the applications of new polypropylene materials in high power capacitors.

I have presented a total of 45 works in 30 conferences. 6 of them were national conferences and the other 24 were international conferences. One of the works was an invited talk, as second author. For the rest of the works, 10 of them were presented as an oral communication as first signing author and 2 were oral communications as second signing author. The rest of the works were presented as poster, being the first author in 8 of them.

I am the management Committee Substitute Member of the COST Action "Single- and multiphase ferroics and multiferroics with restricted geometries (SIMUFER), 2010-2014". I was Member of the Steering Comitee of the 3rd Iberian Symposium on Hydrogen, Fuel Cells and Advanced Batteries (HYCELTEC-2011) and Chairman of the same congress. I was vocal of the Sub-Comitee of Local Affairs of the Orginizer Comitee of the International Meeting of Ferroelectricity-10. I am referee of 14 international journals. I have also teached in

several courses and seminars, as in the "Master en energías renovables, pilas de combustible e hidrógeno", of the Universidad Internacional Menéndez Pelayo. I have directed different end of course projects and I am co-directing nowadays a Doctoral Thesis at the Instituto de Cerámica y Vidrio.