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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: RAMOS DIAZ, JAVIER

Referencia: RYC-2011-09585

Area: Ciencia y Tecnología de Materiales

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Título:

Design and application of structure-property relationship methods to the functionality study of macromolecular model materials.

Resumen de la Memoria:

The ultimate goal of research in macromolecular science is to understand and predict the behaviour of macromolecular materials at different length and time scales from the knowledge of the atomic structure and the forces interacting among the components. Unfortunately, a single strategy cannot be used to address the massive disparity in the time-length scales on which the important events occur. It is clearly necessary to carefully design hierarchical or multiscale approaches consisting of several stages of modelling and experimental work, with each stage tackling phenomena over a specific window of length and time scales. The central idea is that each stage receives input information from a more elemental level (more detailed) and provides information for more coarse-grained (less detailed) models. The input information for each stage can be obtained from detailed computer simulations, statistical theories and/or experiments. Although, a set of well-established and efficient computational and experimental approaches to handle the relevant phenomena have been developed at each level over the years, the links between multiple scales needs to be addressed yet in a proper and consistent way. My experience in this field can be applied to understand some selected problems which are of academic and technological relevance in material science: i) Crystallization of semi crystalline polymers, ii) Molecular compatibility of polyolefin blends and iii) Study of the membrane-protein interactions (in particular cannabinoid membrane receptors) to understand biology functionality and to help in drug design.

Resumen del Curriculum Vitae:

I am co-author of 39 articles (6 of them in revision status and 1 divulgation article) in prestigious international journals which accumulate 218 cites and h-index = 8 (source Scopus). I am the first or second author in 28 of these publications, which gives an idea of the high level of authorship, furthermore I am the corresponding author in two of them (Macromolecules 2008 and J. Polym Chem Part A 2011). The 69% of the articles are published in journals within the first quartile (Q1) and the 90% in the Q1 and Q2 categories. The 70% of the articles are published in journals with an impact factor greater than 3.0 and a quarter of the articles in journals with IF >4. In addition, I have contributed to 28 national and international meetings. I have acquired experience in student training; having co-supervised two Ph.D theses and one more started in 2008. I would like to remark that during the progress of my research career, I have attained substantial experience interacting with industrial staff in Repsol-YPF and Mitsui Chem Co as well as colleagues in both CSIC and NTUA institutions. Remarkably, I did a postdoctoral stay (24 months) in the Prof. Theodorou's team in Athens which is a group of excellence in the field of Monte Carlo, molecular dynamics and multi-scale simulations of macromolecular systems. Recently, I came back to this group for 4 months thanks to a *Jose Castillejo* fellowship to develop Monte Carlo methodology to study polymer blends. Furthermore, I have acquired experience in the organization of meetings forming part of the organizing committee in five meetings. One of them is being celebrated each year in the IEM-CSIC. As a result of this experience and interactions, I have a deep understanding of academic and industrial problems in the field of polymer materials from the synthesis to the final properties.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: SAUCEDO SILVA, EDGARDO

Referencia: RYC-2011-09212

Area: Ciencia y Tecnología de Materiales

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Título:

New materials, processes and device concepts for sustainable next generation solar energy technologies

Resumen de la Memoria:

This Project proposes the synthesis and development of thin layers of kesterite compounds ($\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$) and new related materials and alloys, with the aim to replace most important II-VI and I-III-VI photovoltaic materials in thin film solar cells technologies ($\text{CuInGa}(\text{Se},\text{S})_2$ and CdTe). This is because the storage problems of In and Ga, and the high toxicity of Cd and Te compounds which claims for their immediate replacement by materials and processes based on earth abundant and non toxic elements. The demonstration of the strong potential of these new materials for the development of sustainable photovoltaic technologies compatible with mass production requirements needs for a strong research effort in the next years. Furthermore, the exploration of low cost chemical based routes (spray pyrolysis, printing) compatible with the future massive industrial deployment of these technologies has to be investigated, including techniques compatible with roll-to-roll processes and equipments of automatic processing of complete devices production. The research strategy will be based in the development of procedures for the synthesis of kesterite absorbers, including a modification of the spray pyrolysis technique with a possible high technological impact, consisting in the utilization of a controlled atmosphere by the design of a closed chamber. Different strategies will be essayed for the synthesis of the kesterites (different precursors from solutions to nanoparticles, different atmospheres, inclusion of novel concepts like ultrasonically assisted spray pyrolysis, etc.). Furthermore the Project proposes to explore printing processes based on the synthesis of nanocrystalline precursors using new nanoparticle based inks and their sintering to produce photovoltaic grade material. The optimization of the complete photovoltaic device (back contact, buffer and windows layer) will be performed, searching for the light conversion efficiency maximization. Adaptation of the proposed processes and layers for the development of new photoelectrochemical CZTS based devices will be investigated. The evaluation of the potential of these materials to function as efficient electrodes, for the direct conversion of solar energy into chemical energy via photoelectrochemical water splitting will be performed, developing new energy storage concepts for a more efficient exploitation of solar energy for production of electricity. This will imply the need for a detailed analysis and processing at nanoscopic level of the device surface.

Resumen del Curriculum Vitae:

Edgardo Saucedo studied Chemical Engineering at the University of the Republic, Montevideo, Uruguay, followed by a Master in Material Science at the same University. After finishing his Master Thesis, he moved to the Materials Physic Department at the Universidad Autónoma de Madrid, Madrid, Spain, where he made his PhD Thesis (obtained in March 26, 2007), with a FPU Fellowship of the Science and Innovation Ministry of Spain (AP2003-1388). His thesis work was focused on the preparation of high quality single crystals of CdTe and on the analysis and control of their doping with heavy elements, with several stays in very recognized research centers around Europe: Università degli Studi de Parma, Italy; Institute for Material Research of the Freiburg University, Germany; and Charles University, Prague, Czech Republic. After the PhD Thesis, the applicant joined the Institut de Recherche et Développement sur l'Énergie Photovoltaïque IRDEP (Paris, France) in 2007, with a CNRS associated Researcher fellowship, where he was involved in the research of new electrochemical/chemical based routes for low cost and high efficiency photovoltaic devices, with special emphasis in the synthesis of the $\text{CuInGa}(\text{Se},\text{S})_2$ absorber and ZnO conductive window layers. Then, in 2009, he joined NEXCIS, a spin-off created at Rousset, Bouches du Rhône, France. At NEXCIS, he had contributing in the installation and organization of a new Characterization Laboratory for the spin-off. Finally, in 2009 he obtains a Juan de la Cierva Fellowship (JCI-2009-04606), and in March 2010 he joined the Catalonia Institute for Energy Research (IREC), with the aim to develop new low cost materials and processes for high efficiency thin film photovoltaic devices. At IREC, the applicant is in charge of the investigation line devoted to the development of new routes and materials for low cost and high efficiency photovoltaic devices. In all these periods, he has participated in 13 Projects (at national and European level), published 54 articles in reviewed international Journals of high prestige (29 as the first or second author), including: Chemistry of Materials (IF=5.368), Journal of Physical Chemistry C (IF=4.224), Applied Physics Letters (IF=3.554), Progress in Photovoltaics (IF=4.702), Solar Energy Materials and Solar Cells (IF=3.858), New Journal of Chemistry (IF=3.006), Journal of Applied Physics (IF=2.072), etc. He has also 67 presentations at International recognized conferences mostly in Europe and USA (with several invited Conferences), and has been co-chairman of two important Congresses, with an h index of 10 and a high number of citations (more than 300). He has three patents (one in exploitation and one under exploitation/negotiations) and is the supervisor of two PhD Thesis and is also regular referee of two journals. The applicant exhibits a high experience in industrial transfer of technology with particular emphasis in the photovoltaic field.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: MOYA RAPOSO, XAVIER

Referencia: RYC-2011-09500

Area: Ciencia y Tecnología de Materiales

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Título:

Magnetolectric and multicaloric effects in nanostructured multiferroic materials

Resumen de la Memoria:

Los materiales funcionales son un pilar esencial de nuestra sociedad. En ellos descansan buena parte de nuestras tecnologías y tienen un impacto directo en nuestra manera de obtener y usar energía, en nuestra salud y en las tecnologías informáticas y de comunicación. Por todo ello, el desarrollo y aplicación de nuevos materiales funcionales es un aspecto clave para afrontar los retos del siglo XXI, tanto desde un punto de vista tecnológico y ambiental como socio-económico. La línea de investigación que propongo pretende estudiar propiedades funcionales de materiales ferroicos y multiferroicos, tanto voluminosos como nanoestructurados, con especial atención en las propiedades magnetoeléctricas y calóricas. El efecto magnetoeléctrico ofrece un amplio rango de aplicaciones prácticas. Entre ellas, la más prometedora es el almacenamiento de datos mediante escritura eléctrica y lectura magnética, combinando así lo mejor de las memorias ferroeléctricas y magnéticas. Los sistemas formados por la unión de materiales ferromagnéticos y ferroeléctricos, tanto en compuestos como heteroestructuras, basados en el acoplamiento mediante deformaciones de los grados de libertad magnéticos y eléctricos son los más prometedores ya que solventan el rango limitado de temperaturas y campos externos de operación de los materiales multiferroicos de una sola fase. Mi investigación se centrará en estos materiales bifásicos, tanto compuestos como nanoheteroestructuras. Por otro lado, el estudio de efectos calóricos (magneto-/electro-/elasto-) promete tecnologías de refrigeración respetuosas con el medio ambiente y energéticamente más eficientes que los sistemas actuales basados en compresión de gases. De entre los tres tipos de efectos mencionados, el efecto electrocalórico es de particular interés ya que se opera con una fuente de voltaje y por tanto es mucho más factible de implementar comercialmente que los otros dos efectos. No obstante, su estudio se encuentra mucho menos desarrollado que su equivalente magnético y por ello le dedicaré especial atención. Los amplios conocimientos que adquirí sobre efectos magnetocalóricos durante mi tesis doctoral, junto con la experiencia acumulada en la Universidad de Cambridge en el estudio de ferroeléctricos, serán de vital importancia para llevar a cabo dicha investigación. También estudiaré el efecto de la variación simultánea de varios grados de libertad del material sobre las propiedades calóricas. Por ejemplo, los materiales ferroeléctricos también son piezoeléctricos y por tanto es posible modificar sus propiedades electrocalóricas mediante deformaciones. Asimismo, es posible a priori modificar las propiedades magnetocalóricas mediante la aplicación de campos eléctricos en multiferroicos ferromagnéticos y ferroeléctricos. De nuevo, la investigación que realizo actualmente será de gran utilidad para abordar el estudio de propiedades cruzadas. En ambos estudios aquí propuestos, mi experiencia en el estudio de materiales multiferroicos tanto voluminosos como nanoestructurados, así como mis conocimientos sobre acoplamientos magnetoestructurales y magnetoeléctricos, permitirá la elección de un amplio abanico de materiales, y el gran número de técnicas experimentales con las que trabajo permitirá su estudio en profundidad.

Resumen del Curriculum Vitae:

Obtuve mi licenciatura en Física en 2003 y me doctoré en Física en marzo de 2008 en la Universidad de Barcelona (UB), con calificación de excelente cum laude y mención europea. Mis estudios de doctorado fueron posibles gracias a una beca de Formación de Profesorado Universitario otorgada por el Ministerio de Educación y Cultura. Tras finalizar mi tesis doctoral me trasladé a Cambridge en junio de 2008, donde estoy realizando una estancia postdoctoral en el Departamento de Ciencia de Materiales de la Universidad de Cambridge, gracias primero a una beca de formación de personal investigador Beatriu de Pinós otorgada por la Generalitat de Catalunya y actualmente a una Herchel Smith Fellowship. Mi investigación se centra en el estudio de transiciones de fase exhibidas por materiales ferroicos y multiferroicos y en las propiedades funcionales que de ellas se derivan. Estoy especialmente interesado en fenómenos físicos exóticos que suceden fruto de la fuerte interrelación entre propiedades básicas de los materiales. Durante mi tesis doctoral estudié transiciones de fase magnetoestructurales en aleaciones metálicas de tipo Heusler y descubrí dos nuevos efectos consecuencia del fuerte acoplamiento entre sus grados de libertad magnéticos y estructurales: el efecto magnetocalórico inverso (Nature Mater. 2005, PRB 2007 y Adv. Mater. 2009) y la superelasticidad magnética (PRB 2007). En Cambridge estudio un tipo completamente distinto de materiales. En este caso se trata de heteroestructuras multiferroicas de óxidos magnéticos y óxidos ferroeléctricos con el objetivo de estudiar materiales con fuerte acoplamiento entre los grados de libertad estructurales y eléctricos. Mi trabajo en Cambridge ha sido publicado en revistas de alto impacto como Phys. Rev. Lett., Nature Mater. y Science. En total, mi trabajo ha dado lugar a 36 publicaciones en revistas internacionales, las cuáles han recibido más de 870 citas (factor $h=13$). He presentado mi trabajo en 9 conferencias internacionales (3 charlas invitadas) y cuatro seminarios realizados en universidades extranjeras de prestigio. Dicho trabajo ha sido financiado mediante la participación en 6 proyectos de investigación, nacionales e internacionales. He sido investigador principal de un proyecto anglofrancés realizado entre la Universidad de Cambridge y la Unité Mixte de Physique CNRS, de una Royal Society Internacional Travel Grant y de tres proyectos de investigación en el sincrotrón Diamond Light Source. Soy evaluador de artículos para diversas revistas de prestigio de física de materia condensada y de proyectos para el laboratorio nacional de Oak Ridge. He recibido premios y distinciones de prestigio tanto en Barcelona como en Cambridge, como el Premio Ramon Margalef 2009 al mejor artículo en el ámbito de Ciencias Experimentales y de la Salud publicado en una revista internacional surgido de una tesis doctoral realizada en la UB por mi artículo publicado en Nature Materials en 2005 o el nombramiento como Junior Research Fellow por Wolfson College en Cambridge. Desde que inicié mi carrera científica he combinado mi investigación con tareas docentes y de divulgación científica. Durante el doctorado di clases en la Facultad de Física de la UB, y durante mi etapa postdoctoral complementé mi trabajo de investigación con clases de laboratorio de Ciencia de Materiales en la Universidad de Cambridge.



Nombre: SEVILLA SOLIS, MARTA

Referencia: RYC-2011-07647

Area: Ciencia y Tecnología de Materiales

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Título:

Production of sustainable carbons from renewable organic substances and their use for gas adsorption, energy storage and as catalysts

Resumen de la Memoria:

Energy and environment protection are two of the most important topics in the 21st century. The depletion of energy sources due to the ever-increasing energy demand of the current society and the increasing environmental concerns caused by excessive relying on fossil fuels and industrial polluting processes, call for the development of energy storage and conversion devices that are highly efficient and low pollutant, as well as seek for more environmental-friendly production processes. In this context, supercapacitors and fuel cells are under serious consideration as alternative energy/power sources due to the fact that they play an important role in the development of zero-emission vehicles and the substitution of fossil fuels for renewable energy. However, we need to improve their performance substantially to meet the higher requirements of future systems by developing new materials capable of storing large amounts of energy (supercapacitors) or hydrogen (for fuel cells) in a safe and efficient way. In parallel, improved technologies for CO₂ capture with lower energy consumption are necessary to fight against the global warming caused by the current fossil fuel-dependent society. In this same environmental-concerned context, there is a high demand of more environmental-friendly production processes, such as the use of solid-acid catalysts for the production of biodiesel and other valuable chemicals. The overall aim of the proposed research project is to design novel nanoporous carbon materials with different structural and chemical characteristics based on the hydrothermal carbonization process (HTC) and to explore their use for energy storage (supercapacitors), hydrogen storage, CO₂ capture and as solid-acid catalysts. The structural and chemical characteristics of the materials will be tuned via modification of the synthesis conditions (carbon precursor, time or temperature of reaction, use of additives) or application of a post-synthesis treatment (activation, ammoxidation,...). The strength of the proposal lies in the use of green and economic processes, such as HTC, as well as renewable, cheap and widely available precursors, such as biomass (i. e. wood sawdust) or saccharides (i.e. glucose, starch, cellulose, etc) for the synthesis of carbon materials with outstanding and tailored properties. What is more, these materials will be used for environmental-friendly applications, such as storage of electrical energy and H₂, capture of CO₂ and solid-acid-based catalytic processes.

Resumen del Curriculum Vitae:

I have a multidisciplinary CV, with knowledge of Science and Technology of Materials, Nanotechnology and Electrochemistry. My first approach to the research world was through a fellowship for the introduction to research of university students in their penultimate year of the degree, funded by C.S.I.C. in 2002. I finished my BSc in Chemical Engineering in 2003 and obtained my PhD between 2005 and 2008 under the supervision of Prof. Dr. A. B. Fuertes in the National Institute of Coal (C.S.I.C.), funded by the Science and Education Ministry (MEC) via a FPU fellowship. The title of my PhD Thesis is: Novel Carbon Materials for Energy Storage and Production, and was centered in the development and characterization of carbon materials with a variety of structural properties through different techniques, and the study of their behavior as electrodes in electrochemical capacitors or as electrocatalyst supports for fuel cells. I have been awarded the San Alberto Magno 2008 Prize to the best research project by the Official Association of Chemists of Asturias and León, and the Extraordinary Doctorate Award from the Department of Chemical Engineering and Environmental Technology of the University of Oviedo. After the PhD, I worked on the development of magnetic nanocomposites (mesoporous superparamagnetic polymers, superparamagnetic colloidal nanocomposites of an inorganic and hybrid nature, and inorganic nanoparticles confined within a hollow mesoporous carbon shell) and their application to the adsorption of organic molecules. Since 2009 I am working at the University of Nottingham with a postdoctoral fellowship funded by MICINN. My research topic is porous carbon materials for hydrogen storage. Overall, I have published 39 articles (and another 5 are under revision) in journals of high impact factor (up to 8.5), as well as a highlight in Journal of Materials Chemistry that has been identified as Hot Article for the journal. I have presented as well 19 contributions in conferences. My h-index is 12, with 220 citations in total (excluding self-citation) and an average citation per article of 9.20. My work in the preparation of porous carbon materials, graphitic carbon nanostructures and in the hydrothermal carbonization topic has made me being selected as referee for articles related to those topics by many journals, what probes acknowledgement of the quality of my work in those fields by other scientists.



Nombre: BALAS NIETO, FRANCISCO

Referencia: RYC-2011-07641

Area: Ciencia y Tecnología de Materiales

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Título:

Nanosafety: Monitorization Techniques for Risk Assessment of Nanoparticles

Resumen de la Memoria:

The great expectations laid by the Scientific Community and Industry in the use of Nanotechnology are now a reality in the form of new materials with innovative and, in many cases, unique characteristics. Moreover, novel analysis and diagnosis systems with extremely sensitive and specific properties are currently under development, as well as highly selective and efficient chemical and biological catalysts, drug carriers able to recognize their targets, interference pigments, clean energy nano-vectors of high capacity, chemically inert and mechanically tough coatings, carbon nanotubes and nanowires with unprecedented properties, nanoporous interfaces for molecular recognition and sieving or even high-performance composite nanomaterials. These are just some examples of the industrial applications of Nanotechnology. Due to the originality of this subject and to the speed in which it is developing, the market of nanotechnological products and processes is shortly regulated and therefore the information and operation guidelines are limited in this area. This should not be a reason for being outside of such dynamic sector but quite the contrary. The needed knowledge basis must be created for the expansion of new technologies and scientific techniques that allow a sustainable development of Nanotechnology and for ensuring the production processes, workplaces and harmless products to the human health and environment safety. This represents an essential requirement for assuring that the great effort in R+D under development would not be thwarted by unknown emerging risks or poorly evaluated up to date. The objective of this research topic is, therefore, the development of scientific and technical basis for assessing the potential risks associated to both processes and products of Nanotechnology. Indeed, the techniques and technologies derived from the results of this research will set up the necessary means to help in the early decision of the viability of certain "nano" products in the research and development stage, to design environmentally friendly and health harmless industrial processes and to ensure the safety in the final products. Consequently, my proposal is focused in a. Assessing, in a general way and in some precise cases, the risks to which are exposed the researchers in the laboratories specialized in nanomaterials, as it is specifically found for the Institute of Nanoscience of Aragón (INA). b. Analyzing the efficiency of several protection systems (laminar flow hoses, personal masks, etc.) for facing the work with nanoparticles, together with the study of the efficiency of several methods for the capture of nanoparticles loaded in gas flows. c. Developing novel treatment methods for risk reduction by the appropriate agglomeration of nanoparticles up to reach conventional sizes for waste management. Finally, the rising nature of this research topic is proved by noticing that it is also the matter for two research projects recently funded by the Spanish Ministry of Science and Innovation. This is the case of projects MAT2008-01319/NAN "Development of Monitorization and Capture Techniques for Nanoparticles", in which I participate as Main Researcher, and the project PSE-420000-2008-3 "Nanosost: Towards a Responsible, Safe and Sustainable Nanotechnology", where I am the leader of one of its subprojects (PSS-420000-2008-14) in which is divided.

Resumen del Curriculum Vitae:

Francisco Balas Nieto (July 7th, 1973) Academic- BSc in Chemistry, UCM, 1996.- PhD in Chemistry, UCM, 2002. Scientific and professional activities -FPI Scholarship. UCM Jan 1997 - Dec 2000-Post-doctoral scholarship. Grad. Sch. Eng - Kyoto Univ (Japan) 2002 - 2003-Post-doctoral scholarship. Grad. Sch. Mater Sci - Nara Adv Inst of Sci and Technol (Japan) 2003 - 2003-Researcher. Japan Science and Technology Agency (JST) 2003 - 2005-Assistant professor. Fac Farmacia (UCM) 2005 - 2007-Researcher. CIBER-BBN, 2007-Scientific productivity-Participation in 18 research projects. Principal investigator in 3. -32 publications in peer-reviewed scientific journals (852 citations). H-index = 15.-35 congress communications Selected publications -F Balas, M Kawashita, T Nakamura, T Kokubo. Biomaterials 2006, 27, 1704-1707.-F Balas, M Manzano, P Horcajada, M Vallet-Regí. J Am Chem Soc 2006, 128, 8116-8117.-F Balas, T Kokubo, M Kawashita, T Nakamura. J Mater Sci Mater Med 2007, 18, 1167-1174.-F Balas, M Rodríguez-Delgado, CO Areán, F Conde, E Matesanz, L Esquivias, J Ramírez-Castellanos, JM Gonzalez-Calbet, M Vallet-Regí. Solid State Sci 2007, 9, 351-356.-M Colilla, F Balas, M Manzano, M Vallet-Regí. Chem Mater 2007, 19, 3099-3101.-M Vallet-Regí, F Balas, M Colilla, M Manzano. Solid State Sci 2007, 9, 768-776.-M Vallet-Regí, F Balas, D Arcos. Angew Chem Int Ed 2007, 46, 7548-7558.-IB Leonor, HM Kim, F Balas, M Kawashita, RL Reis, T Kokubo, T Nakamura. J Mater Chem 2007, 17, 4057-4063.-M Manzano, V Aina, CO Areán, F Balas, V Cauda, M Colilla, MR Delgado, M Vallet-Regí. Chem Eng J 2008, 137, 30-37.-F Balas, M Manzano, M Colilla, M Vallet-Regí. Acta Biomater 2008, 4, 514-522.-P Horcajada, C Serre, G Maurin, NA Ramsahye, F Balas, M Vallet-Regí, M Sebban, F Taulelle, G Férey. J Am Chem Soc 2008, 130, 6774-6780.-M Vallet-Regí, M Manzano, F Balas, M Colilla. Prog Solid State Chem 2008, 36, 163-191.-A Nieto, F Balas, M Manzano, M Colilla, M Vallet-Regí. Micropor Mesopor Mater 2008, 116, 4-13.-S Sanchez-Salcedo, I Izquierdo-Barba, F Balas, M Vallet-Regí. Acta Biomater 2009, 5, 2738-2751.-F Balas, M Arruebo, J Urrutia, J Santamaría. Nat Nanotech 2010, 5, 93-96.-A Nieto, M Colilla, F Balas, M Vallet-Regí. Langmuir 2010, 26, 5038-5049. Selected projects in the last 5 years-Materiales para la sustitución ósea. Japan Science and Technology Agency (JST). Kyoto University, Chubu University and JST, from 2003 to 2005, IP: T Kokubo.-Desarrollo de estrategias de imagen molecular y de fenotipo, in vivo de modelos murinos de tumores gliales y de enfermedad de Alzheimer. Preparación de la extensión translacional a pacientes. CIBER-BBN. From 2008 to 2009, IP: C Arús.-Desarrollo de Técnicas de Monitorización y Captura de Nanopartículas. MAT2008-01319/NAN. CIBER-BBN, from 2009 to 2011, IP: F Balas.-NANOSOST. Hacia una nanotecnología responsable, segura y sostenible. Subproyecto 1. Caracterización, Metrología y Generación de Referencias, PSS-420000-2008-11, from 2008 to 2010, IP: J Santamaría.-NANOSOST. Hacia una nanotecnología responsable, segura y sostenible. Subproyecto 4. Bases científicas para la medición del riesgo. PSS-420000-2008-14, from 2008 to 2010, IP: F Balas.-Nanopartículas poliméricas para aplicaciones biomédicas. Control del tamaño mediante síntesis confinada PI148/08. CIBER-BBN from 2008 to 2010, IP: F Balas.



Nombre: MUÑOZ ROJAS, DAVID

Referencia: RYC-2011-09498

Area: Ciencia y Tecnología de Materiales

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Título:

Synthesis of novel functional materials for energy applications

Resumen de la Memoria:

The limited availability of fossil resources and their inhomogeneous distribution in the Earth crust requires a change in the energy mix of modern societies. However, the renewable energy technologies already available are not yet capable of competing with fossil fuels due mainly to a poor ratio cost/efficiency. A clear example is photovoltaic energy, for which high costs and moderate performances yield too long payback times, despite the huge amount of solar energy constantly reaching the Earth. The key to more efficient and cheap renewable sources of energy lays in the materials at the heart of the different technologies. Therefore, the synthesis of novel materials with superior tailored properties for each particular energy application, and the development of cheap and scalable fabrication protocols is crucial if renewable energy technologies are to take a main share of modern society energy mix. Within materials, oxides and related compounds are particularly important due to their multiple functionality and properties (e.g. electrical, ferroelectric, magnetic, optical, ionic conducting, thermoelectric, semi-conducting). Indeed, oxides encompass almost all solid state functions ranging from high k dielectrics to superconductors. In addition to oxides, hybrid functional materials are an exciting field of research where synergies between the hybrid components bring superior and often surprising properties. Moreover, the presence of different functionalities (organic and inorganic) allows a finer control and tailoring of the material's properties. Thus, the research line proposed focuses on the synthesis and study of novel materials, especially oxides and organic/inorganic hybrid materials, with tailored properties for energy applications using and developing facile, low-cost and scalable approaches. The hydrothermal method has proven to be a very effective synthetic approach yielding known and new phases. Moreover, it is a low cost method and easily scalable. The candidate has also shown the efficiency of hydrothermal reactions for the fabrication of hybrid nanostructures. Additionally, other low-cost, solution based methods will be explored (electrochemistry, chemical oxidation, etc.).

Resumen del Curriculum Vitae:

I graduated in Organic Chemistry by the Instituto Químico de Sarrià (IQS-URL) and obtained the title of ingeniero IQS after performing a research project in the Polymer Institute (University of Detroit Mercy) for 7 months. This research project was awarded the P. Salvador Gil, S.I. 2000 prize, given by the IQS's alumni association (AIQS) to the best project and academic expedient. I obtained my Ph.D. in materials science (Universitat Autònoma de Barcelona), having performed the research in the Solid State Chemistry Group at the Materials Science Institute of Barcelona (ICMAB), under the supervision of Prof. N. Casañ-Pastor. During the Ph.D. I performed 3 stays in foreign laboratories (University of Pennsylvania (USA), University of Exeter (UK) and Laboratoire de Réactivité et Chimie des Solides (LRCS, Amiens, Fr)). After the Ph.D., I spent 11 months working in the prestigious LRCS, directed by Prof. J-M Tarascon. I then returned to the ICMAB to work in a project with Air Products Inc. After 4 months I was also awarded an I3P contract to join Prof. P. Gómez-Romero's group in the CIN2 (Research centre in Nanoscience and Nanotechnology, Barcelona), and worked in the two projects until October 2008. Since then I work with Prof. J. Driscoll in the Device Materials Group (Univ. of Cambridge), initially as a Marie Curie IEF fellow and since October 2010 as a Beatriu de Pinós fellow. I am specialized in the synthesis and characterization of novel compounds and materials (I have synthesized two new silver-copper mixed oxides and novel Ag@PPy and Cu₂O@PPy hybrid nanostructures), and in energy applications, namely, batteries, supercapacitors and solar cells. I have as well developed novel low cost synthetic procedures such as the synthesis of oxides by electrochemical oxidation of aqueous suspensions and heterogeneous hydrothermal redox reactions. I have published 25 papers in peer-reviewed journals in topics related to organic, inorganic and solid state chemistry, electrochemistry, crystallography, polymer chemistry and nanoscience. Of those, I am first author in 15 (60%, with an average impact factor of 3.34), corresponding author in 9 (36%, IF: 4.44) and both first and corresponding author in 6 (24%). My work has been featured in the cover of Materials Today (index: 11.45), accompanied by an invited article, and a back cover of Journal of Materials Chemistry (4.80). I am co-inventor of 2 patents and co-author of a book chapter. I have also presented 26 communications (10 oral & 16 posters) in meetings, including one invited oral presentation, being co-author of another 22 communications. I referee papers for the ACS, IUPAC, Elsevier, Springerlink and ASP. I am co-supervisor of one Ph.D. thesis and have supervised postdocs and undergraduate, Mphil and Ph.D. students. Finally, I participate in and coordinate science vulgarization and outreach activities.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: PARDO CASTRO, VICTOR

Referencia: RYC-2011-09024

Area: Ciencia y Tecnología de Materiales

Correo electrónico: victor.pardo@gmail.com

Título:

Ab initio calculations in spatially confined magnetic materials

Resumen de la Memoria:

My area of expertise is condensed matter physics, and particularly the design of materials with new electronic properties from ab initio (starting only from first principles of physics, using no models or approximations) calculations. In the last few years, my activity has comprised studies on several classes of compounds (mainly oxides and similar magnetic systems in which strong correlations, magnetism and/or spin-orbit coupling are important), in particular those where spatially confined electrons determine the electronic, magnetic and conduction properties. These will be either nanostructures like oxide thin films and interfaces, but also bulk materials where spatial confinement caused by the structure of the compound, or surface effects play a key role. The study of this kind of oxides has been rekindled due to its profound implications in the physics of topological insulators and oxide interfaces. The computational techniques, mainly based on density functional theory and tight-binding-based model Hamiltonians, that I am experienced with are state-of-the-art and have been proven successful in the study of not only oxide interfaces and topological insulators, but also the recently discovered pnictide superconductors, to name the most prominent examples in my field. The main goal of this type of research is to design and predict new functionalities for new (or already known) materials, especially in the cases where computational experiments are easier to be carried out because of the peculiarities of the compound or the nature of the problem itself. In many situations, in a computational experiment, the crucial variables can be tuned and the consequences of those modifications can be predicted with a better control than in real experiments, serving as a complement to the experimental works available with synthesized materials. Due to the complexity of this type of studies, a multidisciplinary study involving experimentalists and theorists is mandatory for being able to discern the relevant phenomenology from the accidental one. During my career, I have had experience interacting in such environments. Situations where a perfect nanostructuring, high applied pressures, studies of strain and distortions, etc are required to understand the materials properties are perfectly suited for the type of calculations in my area of expertise, where a certain degree of precision in the calculations is required, beyond the phenomenological treatment given by less accurate techniques.

Resumen del Curriculum Vitae:

I did my PhD studies in the Applied Physics Department in the University of Santiago de Compostela (USC), Spain, from October 2001 to March 2006 under the supervision of Daniel Baldomir. In 2004 I spent 3 months in the Vienna University of Technology working in the group led by K. Schwarz and P. Blaha, the developers of the software WIEN2k, licensed by more than 1500 groups in the world. During 2005-2006, I was a frequent visitor to Vienna in the context of a Joint Project Spain-Austria focused on ab initio calculations on magnetic cobalt oxides. I obtained a European PhD in March 2006 and I got the Outstanding PhD thesis Award 2006 given by the USC. From August 2006 to July 2007 I was a post-doctoral researcher at the USC. I participated in a project on a mixed theoretical and experimental work on transition metal oxides funded by the Ministry of Science and Education (MEC) from 2006 to 2009. In June 2007, I visited the University of Cologne to collaborate with Daniil Khomskii, in the context of a Joint-Project Spain-Germany that ran through 2007-2008, focusing on compounds close to a metal-insulator transition. In February 2008 I was appointed as substitute professor in the Applied Physics Department of the USC. The teaching duties were concentrated in one semester per academic year, so I could use the other semester for postdoctoral research stays at the University of California Davis. Since October 2007 I have been a frequent visitor at UC-Davis, under the supervision of Warren Pickett. Since October 2010 I ceased my contract in Santiago and became a permanent postdoctoral researcher at Davis, where I have a contract until June 2011. I participated in a project funded by MEC starting in 2009 to study ab initio properties of materials close to metal-insulator transitions and its connection with their transport properties. Since the beginning of my PhD, I have published 37 papers (23 articles and 14 proceedings papers) in international journals. I am first author of 18 of those (13 articles and 5 conference proceedings). Seven of those articles have only two authors, and another two have just three authors. My publications include one article in Nature Materials, 7 in Physical Review Letters (4 of them as first author), 12 in Physical Review B, or one in Applied Physics Letters. By February 2011, my publications accumulate close to 200 citations (85 of them in 2010), and my h-index is currently 9. I have given 5 talks (two invited) in international conferences, one in a national conference and co-authored about 20 posters presented in both international and national conferences. To publish those results, I have integrated in groups with diverse areas of expertise (including frequent collaboration with experimentalists), in different countries, showing my initiative to propose new projects and ideas. This year I will chair a session on Electronic Structure at the APS March Meeting to be held in Dallas. Also, I am a co-organizer of the conference "The New Generation in Strongly Correlated Electron Systems 2011", to be held in Santiago de Compostela in July 2011. I have taught over 600 hours of classes (theory, laboratory, and computational) in the Applied Physics Department in the USC, where I have also co-supervised the PhD thesis of Alberto Piñero, that will be submitted in 2011. I am a frequent reviewer of Phys. Rev. Lett. and Phys. Rev. B, and occasional reviewer of J. Chem. Phys., Inorg. Chem., Appl. Phys. Lett., and others



Nombre: **SABIROV , ILCHAT**

Referencia: RYC-2011-08881

Area: Ciencia y Tecnología de Materiales

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Título:

PROCESSING-STRUCTURE-PROPERTIES RELATIONSHIP IN ADVANCED ULTRA-FINE GRAINED AND NANOSTRUCTURED METALLIC MATERIALS

Resumen de la Memoria:

The present project focuses on the theoretical and experimental research in the area of ultra-fine grained (UFG) and nanostructured materials processed by severe plastic deformation (SPD) methods using advanced techniques. It will provide a further development of SPD processing methods and a better understanding of the nature of plastic deformation in SPD processed UFG and nanostructured materials. The work combining both applied and fundamental research consists of two parts: 1. Severe plastic deformation of advanced metallic materials and physical simulation. The first part of the project aims to optimize the processing parameters in advanced SPD methods through their physical simulation using state of the art GLEEBLE 3800 system. The main problem of accumulative roll bonding (ARB) is a low degree of bonding between different layers in the ARB-processed samples. Physical simulation of the accumulative roll bonding process will be performed to predict the optimum set of processing parameters that would lead to the highest degree of bonding during accumulative roll bonding of commercially pure Zr. The results of the physical simulation of the cryorolling process of pure Al and Al alloys will link the processing parameters and chemical composition of materials to their microstructure and mechanical properties. This model is important for research in the area of cryorolling as the final microstructure and mechanical properties of materials are very sensitive to the processing parameters due to the extremely low processing temperatures. Optimization of the processing parameters and design of die will be done for the newly invented SPD method, equal channel angular pressing with parallel channels (ECAP-PC) to improve the SPD technique. Series of experiments will be also performed in order to verify the developed models. 2. Mechanical and physical properties and deformation behavior of advanced ultra-fine grained and nanostructured metals and alloys. The second part of the present project focuses on the experimental study of the mechanical and physical properties of the UFG/nanostructured materials as well as their deformation behavior. Temperature jump tests and stress relaxation tests are proposed to study thermal activation mechanisms in UFG/nanostructured materials. Evolution of deformation mechanisms and microstructure in the UFG/nanomaterials during plastic deformation will be also investigated in detail. Thermal expansion behavior and phase transformation of the UFG/nanomaterials will be studied using dilatometry technique.

Resumen del Curriculum Vitae:

Education PhD (Mining and Metallurgy), July 2004, University of Leoben, Austria Engineer (Materials Science and Engineering), June 1999, Ufa State Aviation Technical University, Russia Professional Experience 2009-present Researcher at IMDEA Materials Institute, Madrid, Spain 2005-2009 Academic Researcher at Centre for Material and Fibre Innovation, Deakin University, Australia 2004-2005 Postdoctoral Fellow at Erich Schmid Institute for Materials Science, Austria 2000-2004 Research Assistant (PhD student) at University of Leoben, Austria Publication/Scientific Merit Snapshot; To-date, I have published 30 papers in several peer-reviewed journals and gave 18 oral talks at European and International Conferences. In about 75 % of my papers, I am the first or the corresponding author and I have made the main contribution to these works. Regular reviewer for some international journals in the area of materials science and engineering, including Acta Materialia, Philosophical Magazine. My work is state-of-the-art for the area of severe plastic deformation and structure-properties relationship in metallic materials. Participation in Research Projects To date, I have participated at 9 research projects, in 4 projects I was a principal investigator. Among these projects there are 2 European projects funded by European Union, 3 projects funded by the Spanish Government, 2 projects funded by the Deakin University via CRGS scheme, and 2 projects funded by the Austrian Fund for Fundamental Research. Expertise My research activities have been mainly focused on development and optimization of novel methods of severe plastic deformation of metallic materials, effect of severe plastic deformation on the microstructure and mechanical properties of metallic materials. I have a significant expertise in the evolution of microstructure during severe plastic deformation of metallic materials and composites. I made a significant contribution in the area of structure-properties relationship in UFG and nanostructured metallic materials produced via severe plastic deformation. Five most relevant publications [1] I. Sabirov, M.T. Perez-Prado, J.M. Molina-Aldareguia, I.P. Semenova, R.Z. Valiev. Anisotropy of mechanical properties in ultra-fine grained pure Ti processed via a complex severe plastic deformation route. Scripta Materialia. 64 (2011) 69-72. [2] I. Sabirov, R.Z. Valiev, I.P. Semenova, R. Pippan. The effect of equal channel angular pressing on the fracture behavior of commercially pure Ti. Metallurgical and Materials Transactions A. 41 (2010) 727-733. [3] B.P. Kashyap, P.D. Hodgson, Y. Estrin, I. Timokhina, M.R. Barnett, I. Sabirov. Plastic flow properties and microstructural evolution in an ultra-fine grained Al alloy at elevated temperatures. Metallurgical and Materials Transactions A. 40 (2009) 3294-3303. [4] I. Sabirov, M.R. Barnett, Y. Estrin, P.D. Hodgson. The effect of strain rate on the deformation mechanisms and strain rate sensitivity of an ultra-fine grained Al alloy. Scripta Materialia. 61 (2009) 181-184. [5] I. Sabirov, O. Kolednik, R. Z. Valiev, R. Pippan. Equal channel angular pressing of metal matrix composites: Effect on particle distribution and fracture toughness. Acta Materialia. 53 (2005) 4919-4930.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: HERNANDEZ VELASCO, REBECA

Referencia: RYC-2011-08737

Area: Ciencia y Tecnología de Materiales

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Título:

Hybrid colloidal materials for applications in nanobiotechnology

Resumen de la Memoria:

My main research line is focused on the development of hybrid colloidal materials derived from biopolymers for specific applications in nanobiotechnology. The final goal is to obtain drug delivery systems controlled through magnetic fields that exhibit high quality thermal response for applications in magnetic hyperthermia and, to achieve that aim, on the one hand in vitro experiments of cell internalization of the hybrid nanogels will be carried out and on the other hand their ability to achieve temperatures above 42 C (cell necrosis) and release model drugs controlled by alternating magnetic fields will be monitored. It is anticipated the development of novel preparation methods of polymeric hybrid nanogels (

Resumen del Curriculum Vitae:

After I graduated in Chemistry from the University Autónoma of Madrid (2000), I was awarded with a FPU fellowship from the Spanish Ministry of Education to carry out my PhD: `Structure and Viscoelastic Properties of novel hydrogels based on polyvinyl alcohol; in the Institute of Polymer Science and Technology (ICTP-CSIC). During my PhD, I spent research stays in internationally recognized centers (6 months, Institute Charles Sadron, CNRS, France and 3 months, North Caroline State University (USA)). The PhD qualification was `Sobresaliente Cum Laude; and received the European Mention and the 2nd award for outstanding Doctoral Research in Polymer Science given by the Spanish Polymer group (2005). In 2005, I started a two-year postdoctoral stay funded by the Heart, Lung, and Blood Institute of the National Institutes of Health (NIH) and Aortech Biomaterials (a multinational company) at the Penn State University (PSU) in the United States. Since 2008, I am a JAE researcher at the ICTP-CSIC where I am responsible for a new research line for the development of hybrid colloidal materials for applications in nanobiotechnology. I have participated in 6 national projects (1 as a IP that is currently under evaluation) and 4 international projects (1 as IP). I have published 30 papers (1 submitted, 23 in Sci Journals (70% in Q1 journals), 3 as conference proceedings and 2 non Sci publications). I am first author in 23 papers and corresponding author of 6. My h-index is 7 (Scopus). In addition I am reviewer for ACS and Elsevier journals. I have actively participated in 25 national and international meetings (12 oral communications, 2 invited conferences) and I have been member of the organizing committee in 2 International conferences. I organize monthly group seminars and I am actively involved in science divulgation activities. Regarding the formation of scientific personnel, I currently supervise 2 PhD students and I have supervised MSc and BSc students. I have been lecturer in MSc programmes in Polymer Science (Materiales Poliméricos coordinated by the Universidad de Valencia and Materials Science and Engineering at PSU). My scientific interests are also focused in technology transfer activities to the industry. My postdoctoral research at PSU was partly funded by Aortech Biomaterials to which I transferred technological results aimed to introduce products improvements regarding the biostability of commercialized polyurethanes. In this same area of biomedical polyurethanes, I also studied the structure-properties relationship in commercial materials and the results were reported in technical documents delivered to Bayer and Medical Hershey Center. In addition, I have actively collaborated with several industries (Qualicups, Nanoquimia and Schering-Plough) and I have participated in 1 contract with Nanoquimia.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: CABALLERO MESA, ANA RAQUEL

Referencia: RYC-2011-08521

Area: Ciencia y Tecnología de Materiales

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Título:

New materials and new designs of solar cells for sustainable low cost photovoltaic technologies: kesterite thin films and plasmonic photovoltaics

Resumen de la Memoria:

One of the great challenges facing society today is the supply of low-cost, environmentally friendly energy sources that can meet the growing demands of an expanding population. Photovoltaic (PV) power has the potential to meet these needs, because the amount of radiation striking the earth's surface is three orders of magnitude higher than the current world usage. However, it is necessary to reduce the costs and improve the PV-cells efficiency to be competitive with the traditional sources. The objective of this multidisciplinary project is to explore new materials and new solar cell design concepts for sustainable low cost PV. Some alternatives are presented. Thin film solar cells have the potential to significantly decrease the cost of PV. A highest efficiency of 20.3 % has been achieved for CIGSe thin film solar cells technology. However, large mass production is compromised by the scarcity of In and Ga. An attractive solution to this can be found in the kesterites $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$, which are composed of abundant elements and with a similar crystal structure to that of the chalcopyrites. They have a strong potential for low cost thin film PV technologies due to their high optical absorption and direct optical band gap. Recently, kesterite-based cells with an efficiency of 9.6 % have been produced by a hydrazine-based routine. However, not a lot of information about kesterites fundamental properties is known yet. Therefore, it is proposed to perform i) conventional and synchrotron X-ray diffraction, spectroscopy and neutrons diffraction measurements, as well as Raman spectroscopy and spectroscopic ellipsometry on the material in the bulk form or on quality epitaxial layers to investigate its structural and crystalline properties, electronic structure and optical constants; ii) deposition of thin films by evaporation techniques with the composition defined according to the results from i) and their characterization (XRD,XPS,XRF,Raman,SEM,Hall effect,PL); iii) demonstration of the potential films from ii) by thin film solar cells fabrication. An enhanced device performance is expected by depositing the absorber layer by evaporation techniques because these lead to high crystalline and electronic quality material. On the another hand, light trapping is particularly critical in thin film devices in order to increase the optical absorption and hence cell efficiency. The use of metallic nanostructures that support surface plasmons, such as Ag, Au, Al or Cu nanoparticles, is proposed for achieving light trapping in thin film solar cells. It will be necessary to optimise the size and shape of these nanoparticles as well as the best position within the cell structure to achieve the optimum photocurrent. Optical transmission/reflection, SEM and EQE measurements will be applied. Enhanced absorption will make it possible to reduce the absorber layer thickness (μm ultrathin film solar cells, in a near future), which not only reduces costs but also improves the electrical characterization of the solar cell. Finally, plasmonic tandem geometries can be considered to improve the device performance. The successful development of this project will be based on the experience acquired by the candidate in the field of materials for PV applications for the last 10 years. It will be also very interesting to extend the range of applications of these materials.

Resumen del Curriculum Vitae:

June 1998: graduated in Physics at the University of Granada. 1999: fellowship from the Ministry of Industry and Energy to do a Master in Nuclear Energy at University Autonoma of Madrid (UAM). In 2000: FPI fellowship from the Ministry of Science and Technology to do a PhD in chalcopyrite materials for photovoltaic applications at CIEMAT. In 2004: PhD for UAM with the maximum mark. Nov.2004-Nov.2006: postdoc fellowship from MEC to work at the Hahn-Meitner Institut (HMI) in Berlin. There, I developed transparent CuGaSe_2 thin films as top cell for tandem devices obtaining the highest Voc reported, in the group of Prof. Siebentritt. Nov.2006-Jan.2007: postdoc fellowship from HMI. Since then I joined the Institute for Technology working with Prof. Schock (Becquerel prize 2010). Since February 2007 I am scientific staff in Helmholtz Zentrum Berlin für Materialien und Energie (HZB, former HMI) at the same institute. I have worked on the technology transference from CIGSe thin films preparation on rigid substrate to different flexible ones. Since April 2008 some of those cells on Ti foil are working in the nanosatellite Delfi-C3. I actively work in a project funded by DLR to develop CIGSe solar cells on polyimide for space applications. I have made important contributions on the low temperature growth of CIGSe thin films. An example is the world-record certified efficiency CIGSe-based device on a polyimide flexible substrate by using a NaF precursor layer. The continuous alliance with the industry (PVFlex Solar, Solarion, HTS, Global Solar Energy Deutschland) reflects the relevance of my work. 2009-2010: researching at large scale synchrotron and neutron facilities at BESSY, Berlin and at ILL, Grenoble. In particular, I have been working on real-time XRD measurements at BESSY to investigate the growth kinetics of chalcopyrite compounds. In 2009 I stayed in the group of Prof. Serna at the Institute of Optic, CSIC, to analyse CIGSe thin films by spectroscopic ellipsometry. Thanks to this collaboration, I started a new research line with the insertion of Ag nanoparticles to enhance the photocurrent of cells. In 2009 I also started working with ZnO nanorods for superstrate and tandem devices. I have a great experience in thin films fabrication via evaporation methods as well as in many characterization techniques of materials and electronic devices: (GI)XRD, Raman, XPS, XRF, transmission/reflection, IV-T, admittance spectroscopy, EQE. I present 42 peer-reviewed publications (18 as first author) in journals such as Phys.Rev.Lett., Appl.Phys.Lett., Acta Materialia, Progr.in Photovoltaics, Sol. En. Mat. and Sol. Cells, J. Appl. Phys. 2 papers more in revision and 4 in preparation (2 as first author). I am co-author of a chapter of a book. I have contributed to 57 congresses (27 oral and 1 invited talk). I have participated in 10 European projects of high interest. Invited to lecture in the Doctoral Program of Uni. Barcelona in 2009, seminars at Instit. Ener. Solar in Madrid and at TSB in Berlin. Intensive collaborator with research groups of Spain, Germany, Luxemb. and USA. I am also regularly referee for prestigious journals. In 2005: co-supervisor of a Diploma student. 2007-2010: supervisor of students in the summer program from HZB. Assistant supervisor of PhD and Master students. Positive assesment by ANECA as "Profesor contratado doctor" in 2010.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: GARCIA LASTRA, JUAN MARIA

Referencia: RYC-2011-07782

Area: Ciencia y Tecnología de Materiales

Correo electrónico: jumagala@fysik.dtu.dk

Título:

Towards high-efficient solar cells: ab initio theoretical studies of organic photovoltaic and dye-sensitized devices.

Resumen de la Memoria:

Uno de los retos más importantes de la ciencia de materiales es el desarrollo de dispositivos capaces de generar energía limpia y renovable, en particular usando células solares eficientes y de bajo coste. Las células solares orgánicas y las sensibilizadas por colorantes (o células Gratzel) son candidatas prometedoras para lograr este objetivo. Actualmente alcanzan eficiencias en torno al 6 %, valor cercano al umbral del 10 % a partir del cual serían competitivas comercialmente. Para alcanzar este límite sin utilizar la estrategia habitual de prueba/error, que suele ser cara y no ofrece resultados a corto/medio plazo, es necesario comprender mejor los mecanismos básicos (absorción de luz y transferencia de carga) que tienen lugar en este tipo de sistemas. El objetivo general de esta línea de investigación es precisamente éste, contribuir, mediante estudios teóricos con cálculos ab initio, a entender dichos mecanismos. Se utilizarán los métodos de cálculo más avanzados en cada uno de los niveles de estudio: i) Teoría del Funcional de la Densidad (DFT), incluyendo funcionales van der Waals, para determinar la estructura de los distintos componentes del sistema (colorantes, dadores, aceptores y electrodos), así como su disposición relativa. ii) Cálculos Many-Body Perturbation Theory para estudiar la absorción de la luz en colorantes y dadores y el alineamiento de sus niveles energéticos con los de los aceptores. Como resultado de i) y ii) se obtendrá una biblioteca de niveles de energía de moléculas relevantes para células solares y de los cambios de dichos niveles en contacto con electrodos nanoestructurados (nanohilos y nanopartículas) y electrodos metálicos. iii) En un último paso se utilizará DFT dependiente del tiempo para estudiar los procesos de transferencia de carga. Finalmente, con todos estos datos se pretende postular nuevas estructuras moleculares a sintetizar para mejorar la eficiencia de las células fotovoltaicas. La investigación se llevará a cabo en colaboración con grupos experimentales de Estados Unidos, España y Japón, lo que permitirá un continuo *feedback* entre teoría y experimentos.

Resumen del Curriculum Vitae:

Licenciado en Física por la Universidad de Cantabria en 2001 con el mejor expediente de la promoción. Doctor por la Universidad de Cantabria en 2006 en el grupo del Prof. Miguel Moreno con una tesis titulada: *Estudio computacional de centros complejos en materiales impurificados: Efecto del campo eléctrico del resto de la red*, por la cual recibí el Premio Extraordinario de Doctorado. La línea de investigación principal durante el doctorado se centraba en el estudio mediante cálculos ab initio de las propiedades ópticas y elásticas de los complejos de transición que se forman al dopar sólidos aislantes con metales de transición. Mis trabajos sobre óxidos dopados con cromo recibieron reseñas en prensa general en España (El País) y Francia (Science et Vie). Realicé 4 estancias predoctorales, durante un total de 11 meses en las universidades de Ámsterdam, Ginebra, Friburgo y Austin. En 2006 me incorporé, a través de un contrato Juan de la Cierva (JdIC), al grupo del Prof. Ángel Rubio, en la Universidad del País Vasco (UPV). De los 36 meses de duración del contrato, 14 de ellos (10 financiados mediante el programa J. Castillejo del MEC) son realizados en el Center for Atomic-Scale Materials Design (CAMD) en la Universidad Técnica de Dinamarca (DTU), bajo la dirección del Prof. Jens Nørskov. En esta etapa abrí tres líneas de investigación, completamente distintas a la de la etapa predoctoral, que he venido desarrollando durante los últimos cinco años. Por un lado he trabajado en el estudio de las propiedades electrónicas de nanoestructuras de carbono (grafeno y nanotubos), haciendo hincapié en la influencia del dopado en el transporte electrónico. Asimismo, he llevado a cabo investigaciones teóricas, gran parte en colaboración con grupos experimentales (Prof. Himpsel en la Univ. de Wisconsin, Prof. Ortega en la UPV y Prof. Wakayama en la Univ. de Kyushu) sobre la interacción de capas de moléculas orgánicas depositadas sobre distintos sustratos. Finalmente, he realizado estudios de los gaps ópticos y de fotoemisión en distintos sistemas mediante cálculos Many-Body Perturbation Theory (GW y Ecuación Bethe-Salpeter). Después del contrato JdIC he continuado con estas líneas de investigación íntegramente en el CAMD (desde Diciembre de 2009), primero a través de un proyecto del programa FP7 de la UE (en cuya elaboración participé) y actualmente mediante una beca Ørsted (de gran prestigio en Dinamarca, solo se conceden 10 por año en régimen de competencia). Mi contribución científica incluye 50 artículos en revistas internacionales (con 271 citas en total), 5 de los cuales están publicados en revistas con índice de impacto >7 (Primer autor en 2 PRLs, primer autor teórico en un Adv. Func. Mat. y en un ACS Nano. Co-supervisor de la tesis que dio lugar a un Angew. Chem.), otros 26 en revistas en el primer cuartil de su área (PRB, JCP o JPC, siendo primer autor en 14 de ellos y segundo en otros 7), 3 capítulos de libro, 45 contribuciones en congresos (19 orales, 8 por invitación) y la participación en 13 proyectos de investigación. Mi índice h es 10. He sido referee en más de 10 ocasiones (p.ej. en PRB o JCP). En el aspecto docente he impartido clases en el Master in Nanoscience de la UPV (4,5 créditos) y en el Master in Physics and Nanotechnology de la DTU (4,5 créditos). Me ha sido reconocida la figura de Profesor Ayudante Doctor por la ANECA.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: GIMENEZ ROMERO, DAVID

Referencia: RYC-2011-07632

Area: Ciencia y Tecnología de Materiales

Correo electrónico: David.Gimenez-Romero@uv.es

Título:

BIOSENSORES ELECTROQUÍMICOS DE NUEVA GENERACIÓN BASADOS EN ELECTRODOS NANOESTRUCTURADOS

Resumen de la Memoria:

Actualmente hay una gran necesidad de atender demandas de información tanto en calidad como en cantidad, en tiempos cortos y con proximidad a quien toma decisiones o se ve afectado por ellas. Por ello, el desarrollo de modernos biosensayos electroquímicos con gran capacidad de trabajo y respuesta rápida tiene un gran potencial y puede dar respuestas muy interesantes a los retos planteados en campos tan dispares como en biotecnología, clínica, proteómica, agroalimentaria, medioambiente, etc. Teniendo en cuenta estas premisas, la línea principal de investigación propuesta está centrada en el desarrollo de nanomateriales híbridos para el diseño de metodologías de diagnóstico in-situ en campo. Los objetivos concretos son: a. Síntesis de nanomateriales híbridos a partir de sílice y polímeros conductores, ya que combinan las propiedades especiales de una matriz inorgánica (estabilidad química, morfología y porosidad moldeable, transparencia óptica y fuerza física) con las propiedades eléctricas y ópticas de los polímeros, lo que cuenta con una amplia gama de aplicaciones, tales como dispositivos sensoriales, microelectrónica o fotónica. La línea propone la modificación de las matrices de sílice con polímeros conductores, de modo que su funcionalización selectiva permita inmovilizar bioreceptores utilizables en el desarrollo de sistemas y metodologías para la detección masiva de dianas sin marcaje. Con ello se debe dotar a estos materiales de la capacidad de anclar en su superficie receptores específicos sin modificar irreversiblemente sus propiedades químico-físicas. Desarrollo de biosensores electroquímicos. A partir de los nanomateriales híbridos anteriores, se persigue el desarrollo de sistemas electroquímicos de detección. Se pretende poner a punto novedosos dispositivos electroquímicos que den lugar a una plataforma simple y barata para la detección precisa y sensible de determinados compuestos de interés biológico. La alta sensibilidad, especificidad, sencillez, y miniaturización inherentes a los modernos biosensayos eléctricos les permitirá competir con los más avanzados protocolos ópticos de diagnóstico. El objetivo fundamental es aplicar los desarrollos más prometedores a problemáticas concretas, aspirando a poner a punto sistemas competitivos para diagnóstico clínico o mejora de la seguridad alimentaria. Esta línea aspira a demostrar su utilidad en la aplicación de terapias personalizadas (home health monitoring), o in-situ en campo, adaptables a diferentes escenarios como p.e., la detección de enfermedades, la monitorización de organismos modificados genéticamente y la detección de residuos de fármacos en el medio natural. Por todo ello, los resultados de esta línea serán fácilmente transferidos a aplicaciones reales de gran interés para diferentes empresas tecnológicas y biotecnológicas, tales como medioambiente, alimentos, bioquímica, clínica, etc., facilitando así su financiación económica.

Resumen del Curriculum Vitae:

Mi Tesis Doctoral fue distinguida con el Premio Extraordinario de Doctorado por la Universidad de Valencia. Dicha Tesis se basó en el estudio de la transferencia electrónica de los metales de transición, participando como investigador en el proyecto CICYT MAT-2000-0100-P4. Además, esa investigación proporcionó resultados transferibles al sector industrial, como por ejemplo la patente P20042930. Posteriormente, realicé una estancia post-doctoral de 18 meses en el UPR15-CNRS (Francia) bajo la supervisión del Dr. Claude Gabrielli, que fue financiada mediante una beca post-doctoral de la Generalitat Valenciana. Durante ese periodo, el trabajo se realizó en colaboración con la empresa ALTIS (filial de IBM-INFINEON) y se basó en el estudio de los depósitos de cobre preparados a través del proceso Damascene mediante técnicas electroquímicas, gravimétricas y acústicas; este proceso es muy utilizado en la industria de microelectrónica. A continuación, disfruté durante 18 meses de una beca post-doctoral de Excelencia financiada por la Generalitat Valenciana, permitiéndome continuar mi carrera investigadora en el UPR15-CNRS. La investigación durante ese periodo se fundamentó en el estudio de la interrelación entre los flujos electrónicos, magnéticos e iónicos de los compuestos de la familia del hexacianoferrato férrico (Azul de Prusia). Además, colaboré en la caracterización del Azul de Prusia soluble por medio de la técnica de difracción de rayos-X en polvo con radiación sincrotrón complementada mediante un refinamiento Rietveld y la síntesis de Fourier de diferencias. De 2007 a 2009, disfruté de un contrato post-doctoral de dos años como investigador doctor en el Departamento de Química Física de la Universidad de Valencia a través del programa de Estancias de Doctores en Centros de Investigación de Excelencia, financiado por la Generalitat Valenciana. Las investigaciones llevadas a cabo encontraron evidencias de efectos de magnetorresistencia negativos en las películas de Azul de Prusia durante su ciclado voltamperométrico. Además, participé como investigador en el proyecto CICYT CTQ2007-64005/BQU, desarrollando un novedoso sistema de medida que permite obtener simultáneamente las funciones de impedancia eléctrica, de masa y de color. Paralelamente, codirigí una Tesis Doctoral (2009). En estos momentos, disfruto de un contrato post-doctoral como investigador doctor en la Universidad de Valencia a través de las Becas Carmen y Severo Ochoa, financiadas por el Ayuntamiento de Valencia. Cabe destacar que colaboro con diversos grupos de investigación, así como, con diversas empresas con programas I+D. Dichas colaboraciones facilitarán la interdisciplinariedad del proyecto de investigación presentado. Soy coautor de 57 artículos -J. Phys. Chem. B (6), J. Phys. Chem. C (7), J. Am. Chem. Soc. (2), Electrochem. Commun. (6), Electrochim. Acta (4), J. Electrochem. Soc. (6), J. Electroanal. Chem. (3), Appl. Phys. Letters (1), J. Solid State Electrochem. (5), Rev. Metal. (2), Mater. Sci. Tech.-Lond. (1), Matériaux & Techniques (2), Appl. Surf. Sci. (1), ECS Trans. (9), Anal. Ing. Mec. (1), Anal. Chim. Acta (1)-, 60 aportaciones a congresos, 1 patente, 2 libros y 7 capítulos de libro.



Nombre: REBOLLAR GONZALEZ, ESTHER

Referencia: RYC-2011-08069

Area: Ciencia y Tecnología de Materiales

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Título:

Laser nano- and microprocessing of polymers and biopolymers

Resumen de la Memoria:

The candidate proposes a research line in the field of laser nanoprocesing and nanostructuring of polymers and biopolymers, involving fundamental studies on the mechanisms responsible of the formation of structures, and applications derived in the fields of Biomedicine and sensing. Laser nanoprocesing and nanofabrication of polymer and biopolymer materials have attracted a great interest in the recent years and constitutes a fast growing field. The use of ultrashort laser pulses allows the patterning of polymers with improved spatial resolution and reduced mechanical and thermal deformation effects as compared with longer pulses in the nanosecond regime. Also, the possibility to temporally shape femtosecond pulses, with the corresponding time scale of processes involved, offers new avenues for controlling and tailoring the features of the created structures. The proposed research deals with the investigation of laser irradiation conditions that lead to the formation of micro- and nanostructures on the surface and in the bulk of the irradiated polymers and biopolymers and the assessment of the mechanisms involved. The objectives are the control of the morphology and chemical composition of the modified surfaces by exploring different laser processing procedures, and the development of new strategies of control and design of materials by optimizing the laser parameters. The formation of nanostructures (Laser Induced Periodic Surface Structures, LIPSS, (1D) and foams(3D)) will be investigated both in the ns and in the fs regime, and the use of temporally shaped fs pulses, matching the corresponding time scale of processes involved, will also be examined aiming at controlling the polymer nanostructuring. The methodology adopted to characterize the modified material involves the use of different techniques such as Atomic Force Microscopy, Scanning Electron Microscopy, Raman and Fourier Transform Infrared spectroscopies, or contact angle measurements. The use of X-ray based non-conventional techniques such as Grazing Incidence Small Angle X-ray Scattering (GISAXS) and Grazing Incidence Wide Angle X-Ray Scattering (GIWAXS) is newly proposed for the characterization of these structures and the development of a new methodology to assess the modifications induced by laser irradiation at PETRA III, HASYLAB, Hamburg, Germany. Applications of these nanostructures will be explored mainly for: (a) biomedical applications, by studying the cell culture, alignment and migration of different kinds of cells on surfaces with LIPSS, and cell culture and drug release on ζ nanofoamed ζ surfaces; (b) development of sensors, by testing the potential of the structures coated by metal films or nanoparticles as substrates for Surface Enhanced Raman Spectroscopy (SERS), and (c) alignment of nanoparticles (ferromagnetic or metallic) also for applications in the fields of biomedicine and sensing.

Resumen del Curriculum Vitae:

The candidate finished her Bachelor in Chemistry in 2001 in Universidad Complutense, Madrid and started her PhD in 2002 at the Instituto de Química Física Rocasolano, CSIC, under the supervision of Dr. Marta Castillejo. During the 4 years that she spent working on her PhD Thesis, she visited several times the Institute of Electronic Structure and Laser (IESL), FoRTH, Greece, as a Marie Curie Fellow (6 months) or funded by the COST Action G7 or by the Ultraviolet Laser Facility (ULF) operating at IESL, FoRTH, in several occasions. During this period she participated in 3 research projects, her work resulted in 21 publications, and presented 52 contributions to conferences. She presented her PhD entitled ζ Mechanisms and application of laser ablation of doped polymers ζ in Universidad Complutense, Madrid in 2006 and she obtained the title of European Doctor with the highest qualification. In her first postdoctoral stay she worked for 15 months in the Institut für Angewandte Physik, at Johannes Kepler Universität and in this period she participated in one project, her work resulted in 4 publications and presented 4 contributions to conferences. In a second postdoc in the Department of Applied Physics, Universidad de Vigo, she held a contract funded by the Xunta de Galicia and after a period of 15 months she started a contract as a young Doctor Angeles Alvarioño fellow. She obtained this contract in the call of 2008 (first position, maximum qualification of all the applicants). In total, she spent 2 years in Vigo, where she participated in 2 projects and a bi-lateral integrated action (Spain-Portugal), and her work resulted in 4 publications (1 more submitted), 8 contributions to conferences, one research contract with the Xunta de Galicia to perform several works related to the laser cleaning of granite, and one patent published in the USA. In this period she spent 3 months in the 3B ζ s group (Biomaterials, Biodegradables and Biomimetics) at the University of Minho. After these two postdoctoral stays the candidate returned to the Instituto de Química Física Rocasolano, CSIC, where she was employed first as a JAE Doc fellow and since December 2009 as a Juan de la Cierva fellow (contract obtained in the 2009 call as the number one in the area of Materials Technology). In this period she has participated in 2 research projects, 2 publications have been submitted, and 2 contributions to conferences have been presented. Additionally she attended to the 2nd International School ζ Laser surface interactions for new materials production: Tailoring structure and properties ζ in Venice, Italy in 2010, where she was awarded the Roger Kelly Award to the best poster. She spent 3 weeks at IESL, FoRTH as user of the ULF, and she has visited twice as user the BW4 beamline at HASYLAB in Hamburg, Germany. Additionally, during 2011 she will spend 3 months in the Institut für Physik, Universität Kassel funded by the ζ Convocatoria de ayudas a investigadores del CSIC para la realización de estancias en centros de investigación extranjeros ζ . In all, during her scientific career since 2002, the applicant has participated in 8 research projects and 1 bi-lateral integrated action, and has published 29 articles (3 more submitted). Her h-index is 9, she has presented more than 60 contribution to conferences (17 works published in proceedings), and published a patent in USA.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: MARCILLA GARCIA, REBECA

Referencia: RYC-2011-08093

Area: Ciencia y Tecnología de Materiales

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Título:

APPLICATION OF IONIC LIQUID-BASED MATERIALS IN HIGH PERFORMANCE SUPERCAPACITORS

Resumen de la Memoria:

The demand for clean energy is rapidly expanding worldwide and one of the most promising solutions proposed is non-polluting energy production by solar and wind energy. Supercapacitors (SCs), due to their capability to deliver high specific power during a few seconds or more, are presently considered as the electrical energy storage devices of choice for smoothing the strong and short-time power solicitations required in transportation and domestic applications powered by fuel cells or batteries, as well as for energy storage substations for voltage compensation in distributed networks. SCs present on the market are electrical double-layer capacitors (EDLCs), which make use of electrolyte solutions containing either aqueous solutions or an organic solvent which permits relatively higher operating voltages (about 2.5 V vs. 1 V for aqueous). The main drawback with the latter SCs is that the organic electrolytes often do not fulfill the requirements of environmental compatibility and safety for vapor generation, flammability and toxicity. This is the case for EDLCs with acetonitrile-based electrolytes, which are the most common high-voltage EDLCs on the market. The high vapor pressure of acetonitrile-based electrolytes requires a careful and expensive thermal control of the EDLCs when used in combination with fuel cells or batteries. The interest in ionic liquid (ILs) based electrolytes for electrochemical energy storage and/or conversion systems is growing worldwide. The key features that trigger this interest are their low vapor pressure, non-flammability, and high chemical and thermal stability, which make them promising electrolytes for the development of safe electrochemical systems. Additionally, ILs properly selected may allow increasing the operating voltage to values over 3.5 volts, which would mean a six-fold increase on the energy stored by current SCs. This Ramón y Cajal will support a research line having the following four key objectives: (i) development of a green and safe electrolyte chemistry based on ionic liquids for SCs ii) Investigation of the peculiar properties and specific interaction of these electrolytes with advanced commercial and self-prepared electrodes (both carbonaceous and conducting polymer based electrodes) with the goal of understanding and improving the electrode and electrolyte properties and thus their interactions iii) construction of supercapacitors (SCs) with outstanding performance by using optimized high capacitance electrodes in combination with IL-based electrolytes and iv) development of novel ionic liquid based solid electrolytes by processing together ionic liquids with novel polyelectrolytes designed to have good affinity with the ILs. These solid electrolytes will allow us to design devices with new architectures such as flexible bilayer SCs or fiber-shape devices. If awarded, this Ramon y Cajal will allow Dr. Marcilla to launch these new research lines consolidating her scientific career. Her solid background in fields such as functional ionic liquids, polyelectrolytes, conducting polymers and electrochemistry will contribute to the success of this research lines.

Resumen del Curriculum Vitae:

Dr. Rebeca Marcilla García got her Bachelor's degree (Chemical Engineering) in 2002 obtaining the best qualifications. After that, she performed her PhD in the University of the Basque Country (UPV/EHU) in close collaboration with the Research Center CIDETEC and the company CEGASA (2003-2006). In this period her scientific interest was focused on the synthesis of new polymeric ionic liquids (PILs) and their applications in nanotechnology and electrochemistry. During her PhD, she was hired for 6 months at the Technical University of Eindhoven (under a Marie Curie Research Training Network) to investigate the enzymatic polymerization in ionic liquids in the group of Prof. Cor Koning. Dr. Marcilla's scientific contribution has been very fruitful in multidisciplinary subjects such as ionic liquids, polymer chemistry, nanotechnology and electrochemistry. As a result she was awarded with the Best PhD in polymer science in 2005-2006 two-year period by the Grupo Especializado de Polímeros de la RSEQ. After the PhD she joined the New Materials Department of CIDETEC (Research Center specialized in Electrochemistry) in San Sebastián (2006-2010) as Junior Researcher being promoted to Senior Researcher after 18 months. There, she contributed with her experience in ionic liquids and polymers to develop electrochemical devices such as electrochromic devices, photoelectrochemical solar cells and Li-ion batteries acquiring important skills in conducting polymers such as PEDOT, nanomaterials (carbon nanotubes, quantum dots, metallic nanoparticles) and applied electrochemistry. In between, she joined the Prof. Franco Cacialli's group (London Center of Nanotechnology at University College London) for 6 months in 2007 to develop Light Emitting Electrochemical Cells (LECs) by using polymeric ionic liquids and acquiring experience in the assembling and electro-optical characterization of these devices. In October 2010 she moved to Madrid to work as Senior Assistant Researcher in the Unit of Electrochemical Processes at IMDEA-Energy Institute. During these 8 years this young researcher has published 37 scientific papers in peer-review journals (average citation per item 15, sum of times cited 504) having an h-index of 13 in February 2011. The average impact factor of the journals is 4 highlighting 2 articles in Advanced Materials (2009-10), one of them cover highlight, 1 in Advanced Functional Materials (2010), 1 in Small (2006), 1 in Chemistry of Materials (2007), 2 in Macromolecules (2006-08), etc. Moreover, she has participated in more than 20 national and international Conferences and/or Congresses and she has 2 international patents. During her scientific career Dr. Rebeca Marcilla García has participated in 15 Research projects (Regional, National and European funded together with Private Sector Initiatives) being Principal Investigator (PI) in 6 of them, highlighting within the last ones the CONSOLIDER National Project Hybrid Optoelectronic and Photovoltaic Devices for Renewable Energy-HOPE and the European Project (FPVI-Strep) Ionic Liquid-Based Lithium Batteries-ILLIBATT.



Nombre: PUIGMARTI LUIS, JOSE

Referencia: RYC-2011-08071

Area: Ciencia y Tecnología de Materiales

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Título:

Tethering Functional Molecular Materials to Microfluidic Platforms; Automated Integrated Lab on a Chip

Resumen de la Memoria:

The proposed research project will approach novel problems and major challenges in material sciences, molecular machines and microfluidics, and will establish three principle aims: (1) Molecular motors and liquid pumping at the microscale. Microfluidic platforms made of polydimethylsiloxane (PDMS) bonded to a glass surface will be functionalized with retinal molecules. This unit can isomerise by light-induced activation leading to mechanical motion. This process is known to be extremely fast; for example, neuronal signal activation during visual perception is attributed to retinal chromophore entities. Therefore, the modification and functionalization with photoactive retinal impellers of the PDMS chips will allow a new and promising research line regarding self-flow pump efficiency promoted from light-induced translocations and the development of Automated Integrated Microfluidics. (2) Pneumatic actuated valves and Light-actuated membranes for on chip application to bottom-up materials growth. Two kind of Pneumatic actuated valves will be used. The Type A will consist of a thin membrane of PDMS bonded between two PDMS microchips, and Type B will involve two PDMS layers where the bottom layer is deflected towards a surface by actuation of the top layer, also called control layer. These micro-reactors will be employ as research platforms to study crystallizations, assembly, localization and integration of functional materials (donor-acceptor systems) bridging nanoscopic organizations to read out components for analysis and function. A major challenge of supramolecular chemistry and microfluidic nature is the development of stand alone devices or automated platforms. For this reason, novel materials such as cross-linked polymers based on retinal units and flexible PDMS membranes will be studied towards the creation of light-active materials (e.g. light-driven valves). We scope to convert light energy directly into mechanical work, and therefore, provide with a battery of new functional and light-controlled automated platforms. This will imply free energy consumption, quick operability, remote control and precise actuated systems. (3) Microfluidics and patterning of functional molecular materials composed of donor (D) and acceptor (A) systems. The way microfluidics operate allowing parallel liquid layers co-flow (laminar flow), parallelization during synthesis, and pneumatic guided assembly makes this technology an advanced and powerful tool for a wide range of applications including integration and localization of structures. A promise of the proposed project will be to study whether all these microfluidic properties are capable of instigate differences trough intramolecular distances between the planes of donor and acceptor materials. This is an important topic in chemistry and material sciences since these systems can be used as artificial photosynthetic systems to convert light into energy. Therefore, the results of these studies could represent a breakthrough approach towards photovoltaic studies, solar cell development, and application.

Resumen del Curriculum Vitae:

With his background of chemistry studies, the candidate developed his PhD thesis entitled "Supramolecular Organization in Crystals, Monolayers and Fibers of Organic Molecules", under the guidance of Dr. David Amabilino of the Institute of Materials Science Barcelona and the experimental work was undertaken in Prof. Veciana's group (Universitat Autònoma de Barcelona). The thesis was framed on a Material Science programme where new organic conductors based on an electronically functional unit, tetrathiafulvalene (TTF), were synthesised and studied. During his work, JPL showed how to organise TTFs units via non-covalent interactions, attempting formation of a supramolecular structure with properties suitable for organic molecular electronic devices. Finally, he could successfully describe new conductors that show unexpected and novel properties when heated or even when forming hybrid states with inorganic nanoparticles. During his PhD, JPL had collaborations with several international research groups well known worldwide and has worked as a visitor in the following three groups; Prof. Mathias Brust (Liverpool, UK), Prof. Richard Nichols (Liverpool, UK), and Dr. Steven De Feyter (Leuven, Belgium). JPL continued the work in Dr. De Feyter's group as a postdoctoral fellow for two months after his PhD to finish several pending experiments in the collaboration. So far, he has published more than 20 articles (including two Angewandte Chemie, one JACS, one Advanced Materials and one Advanced Functional Materials, two Lab on a Chip, two Soft Matter, one Nanoscale), and several others are in preparation. The outcome of his work has been presented at various international meetings in oral and poster presentations. Furthermore, he has been awarded with Premi Antoni de Martí i Franquès de Ciències Químiques from Institut d'Estudis Catalans in 2008 and during his PhD JPL received the St. Jordi Award from Institut d'Estudis Catalans and Societat Catalana de Química for his work on Supramolecular Organic Fibres. Presently, he is at ETH Zurich at the Bioanalytics group. For two years, JPL has been an ETH Fellow for Post-Doctoral researchers. The ETH Fellowships are awarded to individuals with a promising proposal every year. Given the limited number of Fellowships available in a given year, it is clear that being designated an ETH Fellow is an honour and the result of a highly competitive process. He is familiar with various analytical techniques (HPLC, GC-MS chromatography) due to his research at the industry, at Bodegas Torres (Vilafranca del Panadès) and at Inganieria Analítica S.A (Sant Cugat del Vallès). To date, he has been using different techniques including single crystal X-ray diffraction, small-angle X-ray scattering (SAXS), laser desorption ionization mass spectrometry (LDI-MS), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM and SEM-EDX), Atomic Force Microscopy (AFM and current sensing-AFM) and Scanning Tunnelling Microscopy (STM and STS). Currently, JPL interests are microfluidic-guided assembly of functional molecular materials and fabrication of integrated on chip devices. The outcome of JPL's work has recently been published in outstanding journals such as Advanced Materials 22, 2255-2259 (2010, cover of the journal), Nanoscale DOI: 10.1039/C0NR00681E (2011), Lab on a Chip DOI: 10.1039/C0LC00270D (2011) among others.



Nombre: NAFFAKH CHERRADI-HADI, MOHAMMED

Referencia: RYC-2011-09437

Area: Ciencia y Tecnología de Materiales

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Título:

Design of novel multiphase polymer blend nanocomposites based on inorganic nanotubes: Toward new green materials for packaging, defence and security, and biomedical applications.

Resumen de la Memoria:

In the rapidly advancing technology landscape polymer blending provides a very versatile strategy because it enables the creation of materials with new or improved properties by mixing multiple constituents and exploiting synergistic effects. Also the expanding use of polymer nanocomposite materials is in response to growing demands for lighter, stronger, and more affordable materials with low nanofiller content. The principal objective of the proposed research line consists essentially in the integration of these two areas of investigation in order to obtain multifunctional materials that challenge traditional polymer blends and emerging polymer nanocomposites in terms of performance and cost. Specifically, it is proposed to develop advanced polymer blend nanocomposites for packaging, defence and security (protection materials), and biomedical (trauma, orthopedic and dental implants) applications. New preparative strategies will be explored for polymer blend nanocomposites based on inorganic nanotubes (INTs), e.g. WS₂, MoS₂, Halloysite, as economically and environmentally-friendly "green" nanofillers, alternatives to carbon nanotubes. The short-term objective consists in two landmarks: (1) The development of new routes for the effective dispersion of INs in order to assure good interfacial interactions (e.g. cold plasma functionalization, coating/wrapping of low molecular weight surfactants, etc.). The polymer blend nanocomposites based on potential spherical particles (inorganic fullerenes, carbon nitrides) will be another type of developing materials, and will serve as model references for the comparison of the results obtained with INTs. (2) The development of "intelligent" advanced materials processing strategies with new molecular architectures and controlled morphologies from both conventional and renewable resources. In order to do so, a wide range of designs can be achieved using non-reactive thermoplastic/thermoplastic blends and reactive thermoset/thermoplastic blends. In this respect, the main research line will be expressly addressed to investigate the influence of nanofillers on the structure, dynamics (e.g. competition between reaction-induced phase separation and crystallization) and interphase phenomena in these multiphase systems. Also, it is important to analyse the synergistic effects of different components to generate improved structural (mechanical) and functional properties (electrical, optical, etc.). The final objective of the project consists of developing greener plastics, based predominantly on renewable resources, with improved properties in order to compete with increasingly expensive petroleum based materials. The industrial interest of this application is notable due to the following fundamental reasons: (1) INTs do not require exfoliation, making it possible to obtain advanced materials without the complexity and processing cost associated with the dispersion of for example nanoclays and graphenes. (2) Processing will be undertaken via advantageously traditional melt processing techniques as economical and scalable routes. The project proposed answers to the MICINN prioritised research areas 1, 3 and 4 of the National Materials Plan 2008-2011: "Nanoscience and Nanotechnology", "New materials and new industrial processes", "Sectorial Technological Development and Innovation", and "Sustainable Technologies".

Resumen del Curriculum Vitae:

The education of Dr. Naffakh as a scientist has been interdisciplinary in the field of Materials Science and Technology. The candidate received a Ph.D from the Complutense University of Madrid in 2001. The predoctoral experience of Dr. Naffakh in the Institute of Polymer Science and Technology of Madrid (ICTP-CSIC), under the supervision of the Prof. Dr. Marián Gómez and Dr. Gary Ellis, was focused on the development of technological blends of thermoplastic polymers with liquid crystal polymers and the study of the structure-property relationship in polymer blends. Afterwards, he joined the group of Prof. Dr. Jean-François Gérard at Laboratoire des Matériaux Macromoléculaires (INSA of Lyon, France) and worked during 2002-2004 as a postdoctoral researcher. His investigation was integrated into the Eur. project POLYNETSET. During this period, Dr. Naffakh has developed advanced thermoset/thermoplastic polymer blends via the Resin Moulding Transfer (RTM) process for the first time. In December of 2005, he returned to the ICTP of Madrid in order to initiate work in new scientific area of polymer nanocomposites. The investigation most relevant to the present is entitled "Next-generation hybrid polymer nanocomposites based on inorganic fullerenes (IF) and their application as coatings". This line of investigation started within the framework of the Eur. Integrated project ζ FOREMOST ζ and, later, it was consolidated by means of a postdoctoral contract in the I3P programme of the CSIC. Dr. Naffakh was also contracted to work on NAN2004-09183-C10-02 project (Strategic action on Atomic Force Microscopy for Nanosci. & Nanotechnol.). Nanocomposite polymers based on carbon nanotubes is one of current specialities of the candidate (nat. project MAT2006-13167-C02-01, inter. coordinated proj. NRC of Canada-CSIC). In addition, he also created a new nanocomposites research line based on carbon nitrides and polymers in collaboration of Prof. Félix Zamora (head of Nanomaterials Group, UAM). Since January 2010, he has initiated his participation in a fundamental MICINN research project of polymer nanocomposites based on graphene (MAT2009-09335). During the last five years, Dr. Naffakh has directed one European Integrated project at the ICTP and four European projects at Synchrotron HASYLAB-DESY. Also, he has participated in several projects of synchrotron infrared microspectroscopy at Synchrotron SOLEIL. Currently he is working in a CSIC-PIE project at ICTP. He is the author: 32 ISI papers (first author=21, corresponding author=16, high-impact articles-Q1= 16 (4 under review), J. Mater. Chem., J. Phys. Chem. B, Carbon, Nanotechnology, etc.), 13 non-ISI papers (first author=8, corresponding author=8), international patents=2 (first author=2) and book chapters=4. He has also participated in 18 scientific projects and in 38 national and international congresses (first author=23, oral communication=17, invited plenary lecture=1 at TMCN10 Meeting-Weizmann Inst. of Science of Israel). The candidate has experience in the organization of R&D activities (e.g. European YRM at Niza) and supervision of the work of various young researchers in Hasylyab-DESY. Dr Naffakh has been an active reviewer for scientific projects (e.g. U.S.-Israel Binational Science Foundation) and scientific journals since 2005 (e.g. Nanoscale Res. Lett., Mater. Chem. Phys., Polym. Eng. Sci., etc.).



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: TERAN GARCINUÑO, FRANCISCO JOSE

Referencia: RYC-2011-09617

Area: Ciencia y Tecnología de Materiales

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Título:

Towards tailoring dynamical magnetic properties of magnetic nanoparticles for cancer treatment

Resumen de la Memoria:

The objective of this proposal is to consolidate my professional position in an excellence research centre in order to develop recently funded research projects focused on nanotechnology for cancer diagnosis and treatment. In particular, I am coordinator of a Plan Nacional project (NANOvsCSC MAT2010-21822-C02-01) and I participate in an EU project (MULTIFUN n° 262943). This framework favours multidisciplinary collaborations with research groups of different knowledge areas and expertises required to accomplish the proposed research activity. My main research line concerns the study of dynamical magnetic properties of iron oxide nanoparticles (NP) to determine the suitable conditions for their therapeutic use based on magnetic heating to kill cancer cells. The heating capability of magnetic NP originates from a hysteretic non-reversible magnetic behaviour expected at dynamic regime (i.e. when an alternating AC external magnetic field is applied). Part of the magnetic energy accumulated by iron oxide NP -when subjected to AC magnetic fields- dissipates into heat. The NP magnetic heating is currently being clinically tested as a novel treatment modality for solid cancers with promising early results. However, systematic studies of the dynamical NP magnetic properties to identify the onset of hysteresis of MNP and to characterise their dynamically-induced heating capabilities are still lacking. Therefore, I propose to investigate the dynamic magnetic properties of iron oxide NP aiming to optimise their heating capabilities for medical applications. Thus, I will study the dynamical magnetic properties of ferrite NP, as well as to determine their heating power capabilities, as a function of NP size, material coating composition and AC magnetic fields, by exploring both magnetic field amplitude and frequency (magnetic field sweep rates). In addition, thermotherapy based on optimised NP will be evaluated in cancer cells of pancreatic and colon tumours.

Resumen del Curriculum Vitae:

Dr. Francisco J. Teran graduated in Physics at Universidad Autónoma de Madrid in September 1997. He immediately started a PhD at the Grenoble High Magnetic Field Laboratory under supervision of Dr. Marek Potemski. Dr. Teran studied spin dependent phenomena in n-type modulation doped quantum well nanostructures. Dr. Teran acquired diverse technical skills in low temperatures, magnetic fields, high vacuum, optics, EPR, and electrical transport. Dr. Teran designed and set-up different experimental systems to perform unprecedented magneto-luminescence, magneto-transport and EPR experiments leading to several collaborations with international groups. Dr. Teran got the PhD degree at the Université Joseph Fourier-Grenoble I in November 2001. Then, Dr. Teran performed different postdoctoral stays at the University of Nottingham, Universidad Autónoma de Madrid and Grenoble High Magnetic fields Laboratory working on magneto-optical experiments in semiconducting nanostructures. Dr. Teran has been working in interdisciplinary activities obtaining relevant results. In 2007, Dr. Teran moved temporary to GAIKER Technological Centre to reinforce the innovation service related to transfer technology to industry. In 2009, Dr. Teran joined the Nanomagnetism Group at IMDEA Nanoscience. Since then, Dr. Teran works on magnetic properties of iron oxide nanoparticles for cancer treatment. Dr. Teran has published more than 40 papers in international scientific journals, more than 35 communications (6 invited talks, 14 oral communications) at international conferences and workshops. Dr. Teran has participated in more than 11 research projects. Actually, Dr. Teran coordinates one Plan Nacional 2010 project focused on improving biomedical applications of magnetic nanoparticles.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

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Título:

Processing of ZnO-based semiconductor ceramics by soft eco-friendly methods

Resumen de la Memoria:

The renewed interest of the scientific community in ZnO-based ceramic semiconductors originates in the wide variety of properties that they exhibit, some of them unattainable by now for other type of materials. Ongoing research can be grouped into two main areas: In terms of materials new or improved functions are required, and in terms of processing, the manufacturing of ZnO-based semiconductor ceramics has to be adapted to the balance between environment, resources and energy concerns, predicted as the crucial subjects of technology in the 21st century. Current processing of advanced electroceramics generally consists of a multi-step strategy comprising the synthesis of substances on a first stage and the materials consolidation/fabrication on a second one. However the consolidation process of ceramic particles usually requires high temperatures and consumes a lot of energy. Hence, if we want to reduce our ecological impact new processing approaches are needed to redesign a technology that it is not so reliant on energy. In this context, the concept of bio-inspired soft solution processing has been proposed in the last years as the sustainable way of processing advanced ceramics. This concept has superlative benefits like energy saving, simplicity, cost effectiveness, nor or little waste and low temperature operation, so, in essence, with an eye on the environmentally benign conditions and without leading to the global warming. Inspired by the natural processes and the energy by them required, it basically covers all kind of processes to prepare materials which can be operated under, near or just above the ambient conditions. Leaning on this approach the research line here proposed pursues to develop an eco-friendly processing for the obtaining of modern ZnO-based semiconductor ceramics, which generally are produced by processing techniques that consume high energy in terms of temperature, pressure, vacuum, as well as expensive/sophisticated equipment and/or multi-step fabrication. To succeed with this objective, the key concept might be found in joining together the synthesis and the consolidation processes, something that can be achieved by activating the deposition and growth of ceramic films in/from solutions or nanoparticles suspensions by different means: substrate characteristics, catalysts, focused energy sources (UV or MW radiation, local electric fields, etc). Moreover the simultaneous combination of several energy sources (microwaves, electrical, magnetic, hydrothermal, mechanochemical, etc.) can open as well a new chapter in the processing of advanced electroceramics because of its speed, cost, and environmentally benign conditions. This last approach again finds its inspiration in the natural occurring processes and is much more energy efficient than conventional methods, being this key point for the sustained human development. Hence, within this background, the obtaining of stable solutions and/or nanoparticles dispersions, the analysis of the deposition conditions and the selection of a proper activating agent for the eco-friendly processing of ZnO-based ceramic semiconductors constitute the core of the scientific investigation to be developed in the present research line.

Resumen del Curriculum Vitae:

I have a long experience on the synthesis, processing and characterization of diverse electroceramics with special emphasis in advanced processing technologies that can lead to ceramic materials and/or devices with enhanced properties. The knowledge about chemical and physical phenomena associated to grain and grain boundary processes is also a key factor in my formation. The most relevant and innovative scientific developments along my scientific career can be summarized from two main points of view: innovative processes for the enhancement of the materials performance and better understanding of the physical and chemical phenomena involved during the fabrication of functional ceramics. The different projects (competitive and with private companies) and publications in the top journals in the category of Materials Science/Ceramics, support this fact. Also, in the frame of these projects I have acquired a deep knowledge about the interphase phenomena related to the nanostructure development and the functional response of different types of ceramic materials. Nanoparticle synthesis from chemical routes, particle functionalization and selected nanocoatings on different particles are among the skills that have led me to succeed in the achievement of nanostructured materials and functional nanophases with scientific and industrial interest. In the course of my scientific career I have published 36 SCI articles in high quality international journals (Acta Mater, J Eur Ceram Soc, Mater Chem Phys), being the first author in 20 of them. I have presented my job to 39 national and international conferences, and have participated in different research projects, being part of the 525 Action of the European COST network (integrated by research teams of more than 20 countries) and the European Project CLEANSKY: Active Pressure, Position and Temperature sensors for Turbohaft engines. My formation also includes several stays at research institutions of recognized international prestige in the area of Materials Science, like the E.T.S.I. of Telecommunications (Universidad Politécnica de Madrid), Laboratorio de Electroquímica of Sao Paulo (Brazil), Jozef Stefan Institute of Ljubljana (Slovenia) and the C station of HASYLAB synchrotron facility DESY (Hamburg, Germany). I have participated in several contracts of special interest with the industry, collaborating and supervising the introduction of improved products in the market. As a result of the technological innovations developed during my work, I have participated in the creation of the spin-off company IKVaristores S.A. (Toledo, Spain), the first Spanish company producing high voltage ceramic varistors. I am also co-author of an industrial patent in process. More recently I take part in research projects with companies as renowned as ROCA SA and IBERDROLA SA. At present I supervise the Ph.D. thesis of three students, planned to be finished between 2013 and 2014. Besides, I am Professor of Doctorate and Master Courses imparting several lectures on Materials Science, and since 2010 I am Associate Professor of the Degree Course on Civil Engineering at the Universidad Carlos III de Madrid, where I impart the lecture Technology of Materials to more than 250 students. Because of my work on ZnO semiconductors I was awarded with the Young Researcher price by the Spanish Society of Ceramic and Glass.



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**SUBPROGRAMA RAMON Y CAJAL
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Area: Ciencia y Tecnología de Materiales

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Título:

Design and Characterization of Multifunctional Nanostructured Hybrid Materials for Optoelectronic Devices

Resumen de la Memoria:

The main goal of the research line is the design and the study of different (bio) hybrid materials with interesting technological applications:- By incorporation of appropriate photoactive molecules, such as xanthenes, cyanines, pyromethenes and NLO dyes, into different nanostructured materials, i.e. with 1D-elongated pores such as aluminophosphates (AIPOs) and aluminosilicates (zeolites analogues) or 2D arrangements such as layered clays and LDHs, a preferential orientation of the photoactive entity will be induced at nano-scale range. Then, by diverse methods (application of electric field, directional deposition of inorganic structures or surface functionalization) a 1D- or 2D-macroscopic alignment can be reached, leading to new materials with very interesting non-linear optics properties or as light waveguides. The final goal is the manufacture of antenna systems, by a controlled and ordered doping of dyes with different absorption range in Visible spectra into the above cited inorganic nanocrystals, to activate the semiconductor by a Energy transfer process to improve the organic photovoltaic cells performance.- By incorporation of luminescent organic linkers as part of the Metal Organic Frameworks (MOFs), new molecular fluorescent sensors will be developed. A chemiresponse by a highly sensitive change in the luminescence properties of the MOF will be expected by specific interactions (charge transfer process, exciplex formation, antenna effects;) of the framework with the different guest molecules into the pores.- By immobilization of several enzymes on functionalized ordered mesoporous materials (OMM), an improvement in the thermal stability and catalytic activity is expected. A study of the (bio)catalytic activity and lixiviation process of enzymes immobilized will be performed to find an optimal host for each enzyme for potential applications as biocatalysts in the industry. In most of the systems, besides the conventional techniques for materials characterization (SEM, AFM, XRD, termogravimetry...), Fluorescence microscopy techniques (confocal and wide-field), with sensibility at single-molecule detection level and high temporal (picoseconds) and spatial (sub-micron) resolution, will be applied. It will allow the characterization of the fluorescent mechanisms, distribution and orientation of dopant dyes into the matrices at the single crystal level and real-time dynamic studies of catalysts under in situ condition by using the strategy of fluorogenic substrates.

Resumen del Curriculum Vitae:

The candidate Virginia Martínez Martínez, graduated in Chemistry at the Basque Country University (UPV-EHU) in July 2001, awarded the Extraordinary Prize. In January 2002, thanks to FPU fellowship from MEC she started her Doctoral Thesis at UPV/EHU under the supervision of Prof. Dr. Iñigo and Fernando López Arbeloa, on the elaboration and characterization of dye adsorbed in ordered clay films. She obtained the PhD Degree at the UPV/EHU in December 2005, with Doctoral Thesis entitle: Intercalation of Rhodamine in Ordered Clay Films, awarded Extraordinary Prize on Chemistry of 2005. In 2004 she did a predoctoral stay at National Institute for Material Science, in Tsukuba (Japan) to synthesize Organophilic clays. During her doctoral period she collaborated on a second research project developed in the Molecular Spectroscopy Laboratory (UPV/EHU), focussing on the photophysical study of pyromethenes as active media of lasers. After the doctorate (January-June 2006), she has been supervising a new research line about dye aggregation on organophilic clays. From July 2006 until August 2008, she moved to Department of Chemistry at the Katholieke Universiteit Leuven (KUL), under the supervision of Prof. Dr. Johan Hofkens for a postdoctoral stay, where acquired high knowledge on the Fluorescence Microscopy applied to the study of catalytic reaction in bio- and chemo-catalysts at single molecule level. Currently, V. Martínez is hired as postdoctoral researcher (September of 2008) being responsible for the Time-Resolved Confocal Fluorescence Microscope. She has been co-supervising a PhD (registered in 2009 at UPV/EHU) and she has supervised two Master thesis (2006 and 2010). She has been collaborating in teaching: Physical Chemistry Experiments at UPV/EHU (40 hours x 4 courses, in 2010-2011, 2005-2006, 2004-2005 and 2003-2004) and took part in Doctorate course Fluorescence Applications in Chemistry (1 credit 2010 and 1 credit 2008) part of the ECTS Master "New Materials". Her topics are focus on the development and characterization of ordered functional hybrid materials by encapsulation of photoactive molecules and enzymes into different nanostructured materials (AIPOs, zeolites, MOFs, OMM). All those lines are included in 9 national and international projects (GV/EA IT339-10, MAT2207-65778-C02-02, KUL 3E040750-ZKB4266-GOA/2006/02, etc). From her research career she has currently a h-index of 15 (ISI), 31 international publications are derived (429 times cited with an average index impact of 3.9). To highlight: 1 chapter of a book (Annual Reviews in Fluorescence), 4 reviews (J. Photochem. Photobiol. C, Inter. Rev. Phys. Chem., Trends in Physical Chemistry and Anales de Química), 1 Nature Communication, 1 J. Mater. Chem., 1 JACS, 2 Chem. Mater., 2 J. Chem. Phys. B and 5 Langmuir and attended to 18 conferences (12 internacional y 6 nacional), 3 of them as invited speaker (I Jornadas de Nanotecnología Aplicada in Alicante 2010, Workshops on Single Molecule Fluorescence Imaging in Bilbao 2009 and Hybrid Materials CNRS meeting in France 2008). She has opened new lines and collaboration with both national and international research groups: Prof. J. Pérez Pariente (CSIC, Madrid), Prof. S. Kitagawa and Dr. S. Furukawa (Kyoto University, Japan), Prof. J. Hofkens (University of Leuven, Belgium) and Prof. R. Brown (Université de Pau, Francia)