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Referencia: RYC-2011-09706

Area: Tecnología Química

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Título:

Rationally designed nanostructured adsorbents and membranes for CO₂ capture and valorization from post-combustion emission sources

Resumen de la Memoria:

There is growing scientific consensus that the rising atmospheric levels of greenhouse gases, especially CO₂, as a result of man-made activities are responsible to a great extent for the warming effect on climate. A reduction of CO₂ emissions is therefore an urgent and strategic issue. One solution to reduce CO₂ emissions relies on its capture or separation in gas streams, transport and long-term storage (sequestration). CO₂ chemical adsorption using ethanolamines constitutes the reference technology for CO₂ capture. Adsorption is however limited due to the large surface layouts required and high-energy demands. In contrast, pressure-swing adsorption (PSA) and membranes are economically advantageous. The aim of this project is therefore to conceive and develop of PSA and membrane-based processes relying on novel and original materials coupling phys- and chemisorption properties or steric selectivity for CO₂ separation from gas streams with reduced energy demands. The research program involves 5 axes: a. Synthesis of functionalised micro- and mesoporous materials (zeolites, MOFs, functionalised MCM and SBA) and evaluation of their CO₂ adsorption/diffusion properties. b. Formulation of the best candidate materials in membrane and hollow-fibre form for the preparation of high-flux nanocomposite membranes by embedding the target material into the porous structure of a support. MOFs constitute the most challenging materials to put in membrane form due to their flexible frameworks. c. Testing the separation performance of adsorbents (2) Adsorption, to evaluate the affinity of each target material to CO₂; (3) Membranes, to synthesize the nanocomposite materials and perform gas permeation and separation tests; (4) Heterogeneous Catalysis for CO₂ valorization; (6) nanoscience, to understand CO₂ capture in adsorbents and (7) Chemical Engineering, for modelling purposes. My broad undergraduate & research background in the fields of Engineering and Chemistry will provide the necessary multidisciplinary skills to embark on such a challenging project for CO₂ capture. Moreover, the program fits the research policy of the hosting institution (Catalan Institute of Energy, IREC) for the next 5 years.

Resumen del Curriculum Vitae:

Marc Pera-Titus, 33 years old Born in 1977 in Barcelona, Catalonia, Spain 2000 Graduated in Chemical Engineering with honours (Univ. Barcelona) 2002 Graduated in Physical Chemistry (Univ. Barcelona) 2003 Advanced Studies Diploma in Product and Environmental Engineering (Univ. Barcelona) 2004 Master in Chemical Engineering (Univ. Barcelona) ζ Synthesis of zeolite membranes 2004-2006 PhD in Materials Science & Membrane Technology (Univ. Barcelona / Univ. Zaragoza) ζ Supervisors: Profs. Joan Llorens, Fidel Cunill & Jesus Santamaria ζ Preparation, characterization and modelling of zeolite NaA membranes for the pervaporation dehydration of alcohol mixtures. 2007 Master in Numerical Methods in Engineering (Applied Mathematics) (Polytechnic Univ. of Catalonia / CIMNE). 2006-2008 Post-Doc at IRCELYON/CNRS (Marie Curie Fellow EIF) ζ Supervisors: J.-A. Dalmon / S. Miachon, Study of gas solubility in nanoliquids. 2008 Permanent CNRS staff at IRCELYON in the group of C. Mirodatos (ranked 3rd over 200 candidates in CNRS national competition). Group leader since February 2009. 2008-2009 Visiting researcher at Hong Kong University of Science & Technology (HKUST, 6 weeks) ζ K.L. Yeung Selected publications related to the field: 1. V. Rakotovo, R. Ammar, S. Miachon, M. Pera-Titus. Influence of the mesoconfining solid on gas oversolubility in nanoliquids. Chem. Phys. Lett. 485 (2010) 299-303. 2. M. Pera-Titus, R. El-Chahal, V. Rakotovo, S. Miachon, J.-A. Dalmon. Direct measurement of gas oversolubility by microvolumetry: beyond Henry's Law. ChemPhysChem. 10 (2009) 2082-2089. 3. M. Pera-Titus, S. Miachon, J.-A. Dalmon. Increased gas solubility in nanoliquids: improved performance in interfacial catalytic membrane contactors. AIChE J. 55 (2009) 434-441. 4. S. Miachon, V.V. Syakaev, A. Rakhmatullin, M. Pera-Titus, S. Caldarelli, J.-A. Dalmon. Higher gas solubility in nano-liquids? ChemPhysChem. 9 (2008) 78-82. Scientific outcome: 45 publications in peer-reviewed journals, 3 patents, 7 book chapters & pre-prints, more than 80 conference proceedings, 2 keynotes (invited), 24 oral presentations in international conferences and about 600 citations (H=9). Awards & Honours 2009 Elsevier Award for highly cited author in Catalysis (rank 3 in 25th most cited papers). 2008 Finalist of the ζ Premi Claustre de Doctors ζ award given by the Univ. Barcelona and the Catalan Regional Government to the best PhD thesis defended in the year 2006. 2008 Best poster Award on the Plenary Conferences of the Club Français des Membranes (CFM), edition 2008. 2007 1st Prize of the 15th French Carrefours de la Recherche (section Engineering) given the Rhône-Alpes Futur Foundation (7000 euros). 2007 Post-doctoral Award given by the Association des Amis de l'Université de Lyon and the French Rhône-Alpes Region (1500 euros). 2007 Ph.D. Thesis Award (Premio Extraordinario de Doctorado) by the Univ. Barcelona. 2001 Top Student's Award of Chemical Engineering (Premio Extraordinario de Ingeniería) by the Univ. Barcelona.



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Título:

ELECTROCATALIZADORES AVANZADOS PARA TECNOLOGÍAS DE PILA DE COMBUSTIBLE DE ELECTROLITO ALCALINO

Resumen de la Memoria:

Los avances más recientes en la preparación de membranas sólidas de intercambio aniónico han despertado un renovado interés en la tecnología de pilas de combustible de electrolito alcalino (AMFCs), como alternativa a la generación eléctrica en pilas de membrana de intercambio protónico (PEMFCs). En medio alcalino, la influencia positiva del alto pH en la cinética de las reacciones involucradas hace posible la utilización de catalizadores basados en metales no nobles y menos costosos, como Ni o Ag. Una importante ventaja de estos sistemas es su mayor tolerancia a la presencia de CO. Tanto si se alimenta hidrógeno procedente de reformado, como metanol u otros alcoholes, la presencia de CO en el combustible o como intermedio en la electro-oxidación de metanol (alcoholes), resulta en una importante pérdida de actividad catalítica, por pasivación de los centros metálicos del catalizador. Aparte, en el caso de las pilas de metanol directo (DMFCs), o de alcohol (DAFCs), el impacto de la permeación de combustible a través de la membrana se ve sustancialmente reducido en medio alcalino, debido al sentido inverso del flujo, de ánodo a cátodo, junto con la mayor tolerancia del catalizador a la presencia de metanol. De este modo, en pilas de combustible de membrana de intercambio aniónico (AMFCs) existen, en principio, mayores posibilidades de conseguir un mejor rendimiento y durabilidad a menor coste. En los últimos años, la utilización de soportes carbonosos con propiedades avanzadas ha demostrado ser una vía más que interesante para la preparación de electrocatalizadores más activos, consiguiéndose un uso más eficiente del metal empleado. En este sentido, estudios recientes demuestran que la utilización de materiales como nanofibras de carbono (CNFs), xerogeles de carbono (CXs), nanoespirales de carbono (CNCs) y carbones mesoporosos ordenados (OMCs), ha permitido la preparación de catalizadores con mayor actividad en la electro-oxidación tanto de hidrógeno como de metanol, más tolerantes a la presencia de CO, eso sí, en medio ácido. La línea de investigación principal propuesta se basa en la utilización de estos materiales carbonosos para la preparación de electrocatalizadores que operen en medio alcalino, con vistas a su aplicación en AMFCs. La mayor actividad catalítica intrínseca del electrocatalizador en este medio, permitirá sustituir total o parcialmente los metales nobles empleados, normalmente Pt y/o Ru, por metales no nobles y menos costosos como Ag, Au, Cu, Fe, Ni o Co, en ánodo y cátodo. Además se estudiará la funcionalización de los diferentes materiales, introduciendo heteroátomos como O, N y/o S, bien como grupos superficiales o en la misma matriz carbonosa. Es ampliamente conocido el efecto positivo de la presencia de grupos oxigenados en la superficie de un soporte carbonoso, que contribuyen a un mejor anclaje y distribución de la fase activa, incrementando la actividad catalítica. Además existen claras evidencias de la influencia positiva de la presencia de átomos de N dentro de la matriz del material carbonoso que mejoran tanto la fijación del metal como la interacción electrónica entre fase activa y soporte. Finalmente, la presencia tanto de N como de S puede contribuir a aumentar sustancialmente la conductividad eléctrica del material carbonoso, propiedad fundamental para su funcionamiento como parte del electrocatalizador.

Resumen del Curriculum Vitae:

Finalicé mis estudios en Ciencias Químicas en Junio de 1999, dentro de la especialidad de Química Técnica. En Febrero de 2000 comencé a trabajar en mi Tesis Doctoral, defendida en Octubre de 2005, obteniendo el título de Doctor en Ciencias Químicas por la Universidad de Zaragoza. Dicha tesis fue llevada a cabo en las instalaciones del Instituto de Carboquímica del CSIC, bajo la dirección de los Dres. M.J. Lázaro y R. Moliner. El trabajo comprendía la preparación y estudio de diferentes catalizadores carbonosos preparados con distintos compuestos de vanadio, incluyendo las cenizas de un coque de petróleo, para su aplicación en la reducción selectiva catalítica de NOx en presencia de NH3. Paralelamente, participé en otros proyectos de investigación cuyo objetivo era la preparación de conformados de baja pérdida de carga, como briquetas carbonosas y monolitos recubiertos de carbono, para la eliminación catalítica de NOx. Tras mi etapa predoctoral, en Febrero de 2006 me incorporé al grupo del Prof. Steinfeld en el Institute of Energy Technologies en la ETH-Zurich, para la realización de una estancia post-doctoral, durante 29 meses. En este tiempo estudié diferentes reacciones involucradas en procesos termoquímicos solares para la producción de H2, gas de síntesis y otros compuestos con aplicaciones químicas/energéticas. Mi tarea era proporcionar una visión completa desde el punto de vista de la cinética e ingeniería química de estas reacciones, de cara al escalado y modelado de los diferentes procesos. Para ello se utilizaron técnicas termogravimétricas para la determinación de las cinéticas intrínsecas, junto con ensayos en simulador solar, simulando las características de la energía solar concentrada. En Julio de 2008 finalicé mi etapa post-doctoral en la ETH-Zurich y me reincorporé al Instituto de Carboquímica, primeramente con un contrato dentro del programa JAEDoc, hasta disfrutar desde Mayo de 2009 de un contrato Juan de la Cierva. A día de hoy, colaboro fundamentalmente en dos líneas de investigación. La primera de ellas se enmarca dentro de diferentes proyectos existentes en el grupo, cuyo objetivo es la síntesis de electrocatalizadores para pilas de combustible PEM, con mayor actividad, mejorada durabilidad y menor coste. En mi caso me ocupé particularmente de la utilización de soportes carbonosos sintéticos, como xerogeles de carbono, aportando mi experiencia y conocimientos en el campo de la catálisis, en la preparación y estudio de las propiedades de estos materiales. Por otra parte colaboro en una serie de proyectos que contemplan la preparación de catalizadores soportados sobre materiales filtrantes para la eliminación simultánea de hollín y NOx en gases de escape. El objetivo es la obtención de sistemas catalíticos que resulten efectivos en la eliminación de estos contaminantes en las condiciones oxidantes típicas de motores de combustión que operan en condiciones de mezcla pobre de combustible. En total he publicado 27 artículos en revistas internacionales con importante índice de impacto dentro del campo de la tecnología química (dentro del 25% de las revistas con mayor índice de impacto del área), tres capítulos en libros igualmente especializados dentro de diferentes campos de gran importancia en éste área, una patente y he participado en congresos y conferencias nacionales e internacionales, con un total de 38 comunicaciones.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: PEREZ DE LOS RIOS, ANTONIA

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Título:

NEW INTEGRATED REACTION/SEPARATION BIOTECHNOLOGY PROCESSES FOR FINE CHEMICALS PRODUCTION BASED ON THE COMBINATION OF IONIC LIQUIDS AND MEMBRANE TECHNOLOGY

Resumen de la Memoria:

The proposed research line aims to develop the more efficient and cleaner synthesis of pharmaceutical and fine chemicals through improved catalysis using benign and alternative green solvents such as ionic liquids as reaction and/or separation media, and membrane technology. Mainly driven by the pharmaceutical industry itself, the demand for enantiopure compounds has shown a dramatic increase in recent years. Efficient methodologies for the production of enantiomerically pure or enriched compounds are of great academic and industrial importance, for which purpose (bio)catalytic kinetic resolution has been found to be an attractive option. Lipase-catalyzed acylation of chiral alcohols is of particular interest as a preparative tool and as a benchmark reaction. However, the main disadvantage for its practical application lies in the need to use chromatography for separation of the alcohol and ester, which requires the use of large volumes of organic solvents. A promising alternative to overcome this disadvantage is the use of enzymatic membrane reactors. Among membrane-based processes, the use of supported liquid membranes (SLMs) based on organic solvents has numerous advantages, including the minimal amount of solvent needed and the fact that the extraction and stripping processes are combined into one single step. Nevertheless, their industrial application is still limited, mainly due to concerns about SLM stability and long-term performance. The use of room temperature ionic liquids (ILs) as an immobilized phase in a supporting membrane is particularly interesting in this respect. ILs have recently been revealed as interesting clean alternatives to classical organic solvents and they have been shown to be good solvents for a wide variety of chemical processes (e.g., extraction, reaction media, chemical catalysis, etc.). The use of these new solvents as a liquid membrane phase stabilises the SLMs. Furthermore, biocatalysts have been shown to be stable and active in ionic liquids. Therefore, the use of ILs as liquid phase in SLMs will allow the preparation of a new membrane concept, reactive membranes, in which the membrane acts as the reaction and separation medium. The aim of this research line is to push forward in our efforts in the development of new integrated reaction/separation biotechnology processes (process intensification) for pharmaceutical and fine chemicals production based on the combination of ionic liquids and membrane technology.

Resumen del Curriculum Vitae:

Graduate in Chemistry (2000) and in Chemical Engineering (2004) at the University of Murcia (UMU), she was awarded the First National Award in Chemical Engineering by the MEC. The candidate was granted an FPI fellowship from the MEC in 2003, starting her PhD degree in a project related to the design and optimization of biocatalytic processes based on the use of ionic liquids and membrane technology under the supervision of Prof. G. Villora. She has carried out four Masters related with her area of knowledge. The candidate made a short stay in the prestigious group of Prof. R.A. Sheldon at Delft University of Technology (TUDelft, The Netherlands), working in the field of ionic liquids in biocatalysis. She was chosen at international level as postgraduate student in the Excellence Campus 2006. In November 2007, she received her PhD degree in Chemical Engineering (European Doctorate) at the UMU, with the qualification "sobresaliente Cum Laude", being awarded with distinction of Extraordinary Award of Doctorate (2008). Her postdoctoral stage began in October 2007 with a research grant from the CAM in the Department of Chemical Engineering at the UMU. She carried out a post-doctoral stay in the group of Prof. R.A. Sheldon at TUDelft (2008). From January 2009 until now, she has been working in the group of Prof. C. Godínez in the Department of Chemical and Environmental Engineering at the UPCT, with a "Juan de la Cierva" contract. During this period the candidate has opened new research lines concerning the application of supported ionic liquids membranes to different processes such as separation of racemic compounds, removal of metal ions from aqueous solutions and microbial fuel cells. She was a guest in international-level laboratories, such as the laboratories of Prof. G. Stephens and Prof. P. Licence at the University of Nottingham, working on the project "Integrating bio and chemocatalysis using ionic liquids". She has published 55 papers: 32 publications in SCI journals with high impact factor (72% within the 25% best category), being the first, second and/or corresponding author in 91% of them, 6 papers in other international journals and 17 papers in national journals. She has also published 1 patent and 6 chapters of book, invited by the Editorials Springer and Nova Publishers. She has received 232 cites (H index= 8, Scopus). The candidate has contributed with 65 communications in international and 12 in national conferences, presented in oral and poster sessions. She has supervised one PhD thesis in Chemical Engineering and is currently co-supervising another Ph.D. thesis at the UPCT. She has also supervised 19 student projects. The candidate serves as regular referee for 8 SCI journals. She was involved in teaching activities for graduates and postgraduates (350h) and collaborated in activities for the promotion and divulgation of scientific knowledge at the UMU and UPCT. In January 2010 she obtained a positive assessment of "Profesor Contratado Doctor" by ANECA. During her PhD and following postdoctoral research the candidate has participated in the preparation and development of research projects: 6 national projects and 5 research contracts with private companies, being the principal researcher in two of these contracts, which are related with the research line proposed. During her career she has established her own extensive network of international academic and industry collaborations and outreach contacts covering various d



Nombre: FRANCO URIA, AMAYA

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Título:

Desarrollo de herramientas para la gestión sostenible de procesos y residuos

Resumen de la Memoria:

La creciente presión ejercida por la actividad de la industria en general y la acumulación de contaminantes en diversas matrices medioambientales están afectando de forma preocupante a la conservación del entorno natural y sus recursos. Se requiere, por tanto, el desarrollo y la aplicación urgente de herramientas específicamente orientadas hacia su gestión sostenible, que vayan más allá de la mera monitorización. La línea de investigación propuesta se centra fundamentalmente en dos campos de actuación. El primero de ellos consiste en el desarrollo de modelos multimedia de tipo mecanístico para estimar la distribución (flujos) y destino (acumulación) de contaminantes en diferentes compartimentos abióticos y bióticos (cadenas tróficas) principalmente orientados a aquellos escenarios más sensibles (zonas de vertido de aguas residuales, áreas de explotación agrícola intensiva, etc.). Se investigará especialmente el efecto de los diferentes mecanismos de emisión y transferencia de contaminantes, así como la búsqueda de nuevos mecanismos no incluidos en los modelos tradicionales, de forma que se establezcan ciclos cerrados en el medio ambiente. Estos modelos, basados en las propiedades físico-químicas del compuesto evaluado (fugacidad, índice covalente, etc.) permitirán, mediante su combinación con técnicas GIS, la creación de mapas de contaminación que pueden resultar de gran utilidad en el establecimiento de acciones reguladoras por parte de la Administración competente. Asimismo, es necesaria una explotación y gestión sostenible de los recursos, la cual se puede lograr mediante, entre otras medidas, la reducción del uso de dichos recursos y favoreciendo la reutilización o valorización de los residuos generados en diferentes actividades (tratamiento biológico de aguas, agricultura, industria, etc.) y de acuerdo con políticas promovidas por la Comisión Europea. Se propone una contribución en este campo orientada a favorecer el desarrollo de procesos sostenibles y la gestión adecuada de residuos de forma que su reutilización no suponga un impacto adicional sobre el entorno medioambiental. Para ello, se proponen herramientas de diseño y optimización de dichos procesos que integren criterios tanto operacionales como ambientales y socio-económicos en un sistema de apoyo a la toma de decisiones que permita manejar diferentes escenarios. Desde el punto de vista ambiental, es importante tener en cuenta la presencia de sustancias tóxicas o de carácter persistente en la fabricación de muchos productos de uso cotidiano, así como su acumulación en residuos potencialmente reutilizables. Teniendo en cuenta esta premisa, se propone la evaluación de riesgo ambiental como criterio de integración horizontal que permita la complementariedad entre la modelización ambiental y el uso de indicadores medioambientales empleados en la ingeniería de procesos y productos sostenibles.

Resumen del Curriculum Vitae:

Me licencié en CC Químicas por la Universidad de Santiago de Compostela, en la Especialidad de Química Industrial. A continuación me incorporé al Departamento de Ingeniería Química de esta misma Universidad, donde defendí mi Tesis Doctoral en el año 2004 bajo la dirección de los Prof. Juan M. Lema Rodicio y Enrique Roca Bordello, en el Grupo de Ingeniería Ambiental y Bioprocesos. Mi trabajo de doctorado, Biorreactores pulsantes para el tratamiento anaerobio/anóxico de aguas residuales de alta carga, estuvo centrado en la optimización de sistemas de alta carga, orientada a mejorar las propiedades de biomasa floculenta y granular, así como mejorar la eficacia, facilitar la operación y reducir significativamente la duración de la puesta en marcha de este tipo de reactores mediante la aplicación de flujo pulsante. También colaboré de forma activa durante esta etapa en varios proyectos (nacionales y europeos) relacionados con la monitorización, supervisión y control de digestores anaerobios. Como resultado de mi etapa predoctoral, se han publicado 7 artículos de investigación en publicaciones del SCI (5 como primera autora) y 2 capítulos de libro. Aunque me fue concedido un contrato Postdoctoral de la USC para continuar mi investigación predoctoral, renuncié a él para poder abordar un nuevo tema de investigación, la Evaluación de Riesgo Ambiental (ERA), y con una beca de la Xunta de Galicia, realicé una estancia de con la Dra. Marta Schuhmacher, iniciadora de esta línea a nivel nacional, en la Universitat Rovira i Virgili, donde me centré en el estudio de modelos dinámicos de acumulación y distribución de metales pesados, así como de exposición, con la idea de estimar el riesgo sobre la salud. Otra estancia en el año 2006 en el Fate and Exposure Modelling Group, del ITM, en la University of Stockholm, Suecia, bajo la supervisión del Dr. Ian Cousins, me permitió profundizar en el uso de modelos ambientales multimedia para la predicción de la distribución de contaminantes orgánicos en diferentes matrices ambientales y también en el uso de modelos integrales de ERA. De forma complementaria durante mi etapa postdoctoral, amplí mis conocimientos sobre otro tipo de herramientas de gestión ambiental (ACV y Huella Ecológica, HE) y su integración con ERA, aplicados fundamentalmente al sector textil, participando en dos contratos de investigación con INDITEX. En el año 2007, realicé una estancia en IIM-CSIC para la aplicación de indicadores medioambientales como criterios adicionales para el diseño y la optimización de procesos de valorización de residuos procedentes de las actividades pesqueras, de forma que estos procesos sean sostenibles y no supongan un impacto adicional. De hecho, estoy contratada desde el 1 de Enero de 2008 bajo la supervisión del Dr. Antonio Álvarez Alonso en el IIM con un contrato Juan de la Cierva. De mi labor investigadora postdoctoral, han resultado 22 publicaciones, la mayoría en el SCI, y en el primer cuarto del área correspondiente, y 6 capítulos de libro. He codirigido 11 proyectos de fin de carrera, y un DEA. Estoy codirigiendo actualmente dos tesis doctorales y he colaborado en la puesta en marcha y docencia del curso de 3er ciclo Evaluación de Riesgo Ambiental, de 30 créditos, en el programa Ingeniería Química y Ambiental de la Universidad de Santiago de Compostela.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

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Título:

SYNTHESIS, CHARACTERIZATION AND TECHNOLOGICAL VIABILITY OF NEW MEMBRANES FOR GAS SEPARATION

Resumen de la Memoria:

Membrane technology is recognised as one of the best available techniques for many useful scientific and technological fields. One of their functions is the fast transport of molecules, saving energy and cost. Membrane materials are expected to meet the requirements of potential separation applications under harsh conditions, such as hydrogen purification for steam reforming or carbon dioxide capture. Everyday, materials with potential in multiple functions are investigated in laboratory research. However, they do not often go beyond. So far, research groups study the influence of the experimental variation of old recipes for a specific material on its structural properties or the viability of a certain material is studied for a target application. This is a time-consuming process limited to isolated recipes. It often occurs that materials and process engineering groups working in parallel are not related. The aim of this research line is establishing an integrated cycle linking synthesis conditions, structural and dynamic functional characterization of those materials that have not been developed out of laboratories but may show potential in target problems, i.e. H₂ and hydrocarbon purification, CO₂ removal from flue gas, by using mixed matrix membrane technology. Mixing novel inorganics and polymers ease the transfer from materials to membranes, allowing the exploration of new materials as clean challenging separations solutions, as well as setting up a correlation between materials and their functional characterization, deepening knowledge of novel inorganic materials and polymers. This will allow choosing a material as a function of an application, avoiding time-consuming and inflexible experiments. The work could be divided into: (1) literature survey of industrial and environmental applications where membrane technology may be an energy-efficient alternative; (2) synthesis and functionalization of selected inorganic materials regarding their compatibility and adhesion with various polymers to give homogeneous membranes; (3) characterization of the materials by analytical techniques and the membranes in separation; (4) modelling and validation, to design new synthesis and characterization methods, beyond the timeline of the project. Once the structure-transport properties correlation has been succeeded for one material, it will be applied to other materials with interesting properties. Materials for gas separation could be extrapolated to other fields: catalysis, sensors, biomedicine... The project might thus be extended to the areas of physics, chemistry, biotechnology, as well as chemical and process engineering.

Resumen del Curriculum Vitae:

Ingeniera química por la Universidad de Cantabria en 2000, habiendo superado el 5º curso en la Rijksuniversiteit Gent (Bélgica) mediante el programa Sócrates-Erasmus. Realizó prácticas en la empresa Nestlé España, y un master en Gestión Ambiental organizado por el Colegio Oficial de Químicos de Cantabria antes de incorporarse al Departamento de Ingeniería Química y Química Inorgánica de la Universidad de Cantabria, como ingeniera contratada en un proyecto financiado por la Comisión Interministerial de Ciencia y Tecnología (FEDER 1FD97-1/89) para el desarrollo de procesos de deshidratación de mezclas agua/acetona y agua/isoamilcetona mediante pervaporación, hasta la concesión de la beca FPI para realizar la tesis doctoral, dirigida por las profesoras I. Ortiz y A. M. Urriaga y defendida el 7 de junio de 2005, que obtuvo la máxima calificación y mención europea. Durante el doctorado realizó 2 estancias en prestigiosos centros del campo de la tecnología de las membranas: de tres meses en el Institut Européen des Membranes (Montpellier, Francia) con la Dr. A. Julbe, y de diez meses en el Laboratorio de Tecnología de Membranas del departamento de Ingeniería Química de la Universidad de Hiroshima (Japón), con el profesor M. Asaeda. Al finalizar la etapa predoctoral, se incorporó inmediatamente a éste último como investigadora financiada por la Japan Society for the Promotion of Science para desarrollar membranas cerámicas selectivas a la separación de CO₂ de otros gases a temperaturas de hasta 200 °C (, durante 10 meses). A su regreso a Europa, se incorporó como investigadora postdoctoral contratada en el European Membrane Institute de la Universidad de Twente, con los Drs. A. Kemperman y M. Wessling, estudiando la estabilidad química de membranas compuestas de pervaporación a elevadas temperaturas. En 2007, gracias al programa ¿Juan de la Cierva¿ se incorporó al Departamento de Ingeniería Química y Tecnologías del Medio Ambiente de la Universidad de Zaragoza (UZ), con el profesor J. Coronas, en una nueva línea de investigación sobre el desarrollo de materiales híbridos polímero-zeolita y membranas mixtas para separación moleculares. La última estancia postdoctoral, de tres meses?, la realizó en 2009, mediante la concesión de una ayuda de la Dirección General de Aragón para la movilidad de investigadores, en el Instituto de Tecnología Química del CSIC en Valencia, preparando membranas cuya capa activa está formada por la zeolita de sílice pura ITQ-29, para separación de hidrocarburos, continuando así la colaboración entre grupos de investigación. Los trabajos de investigación realizados han resultado en la publicación de 17 artículos en revistas internacionales, 5 como primera autora, 2 capítulos de libro, uno de ellos como primera autora, 3 artículos en preparación, así como 2 patentes españolas con el grupo de la UZ. Además, ha participado en 28 contribuciones a congresos internacionales, con 9 comunicaciones orales. Ha sido investigadora colaboradora en 9 proyectos de investigación y responsable en 1 proyecto de medida en el ESRF (Grenoble), 2 de ellos en ejecución y 1 de reciente concesión. Ha codirigido 5 proyectos fin de carrera y está dirigiendo otros 3; posee la evaluación positiva de la ANECA como Profesor Contratado Doctor. Durante el período ¿Juan de la Cierva¿, ha realizado 80 horas de colaboración de docencia en asignaturas del Departamento. Hoy, está contratada como Prof. Ayudante Doctor en la Universidad de Zaragoza.



Nombre: RINCON LLORENTE, BARBARA MARIA

Referencia: RYC-2011-08783

Area: Tecnología Química

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Título:

Co-digestion of alperujo and microalgae for a more sustainable olive oil mill industry

Resumen de la Memoria:

The main research line developed by the candidate is the alperujo treatment. The proposed project is focused on the treatment of Alperujo, highly polluted agro-waste, through anaerobic co-digestion together with microalgae to produce biogas (mixture methane (60-70%) and carbon dioxide (40-30%)) as renewable energy. The co-digestion effluent and the carbon dioxide of the produced biogas are recycled to grow microalgae for a more sustainable olive oil industry. This project is aligned with one of the main targets of the European Union to reduce greenhouse gas emissions by 20% and ensure 20% of renewable energy sources within the Community by 2020. The olive oil mills produce high quantities of highly polluted wastes, i.e. wastewaters of olive and oil cleaning and solid waste. The annual worldwide production of edible oils and olive oil has been estimated at 8 million metric tons and 1.75 million metric tons respectively, from 25,000 olive-mills. Currently the main waste generated in the olive oil extraction process is the solid waste: alperujo. This waste is produced in a proportion of 800 kg per ton of olives processed. In Spain, 2-4 million tons of this waste are produced every year generating large-scale environmental problems. Its characteristics (high humidity, low pH, high content in solids/organic matter, presence of inhibitory compounds as poly-phenols, etc.) make of it a very pollutant waste. There are different alternatives for its treatment but the low quantities used in these treatments are unable to solve the problem. The proposed research project will study the feasibility of alperujo co-digestion, a poor nitrogen content substrate, together with microalgae, with high nitrogen content. This approach takes advantage of the positive synergy between both substrates for an optimized co-digestion. After the co-digestion process, the effluents keep all elemental nutrients (N, P, K) and the obtained biogas contains 30-40 % of carbon dioxide. The nutrients from the digestate and the CO₂ from the biogas will be recycled to growth microalgae, minimizing the needed post-treatment for such effluents and decreasing the greenhouse gas emissions. From a waste, alperujo; with no value and problematic disposal we are producing renewable energy i.e biogas of high calorific value (5000-6000 kcal/m³). Furthermore the production of microalgae is a promising technology to produce added value products as carotenoids, food additives, colorants or biodiesel which can be extracted from the grown microalgae. The exhausted microalgae will be used as the proposed substrate for co-digestion with alperujo towards a closed loop technology for olive mill industries.

Resumen del Curriculum Vitae:

The candidate interest in environmental problems drove her to carry out 3 different stays in Spain about environmental studies when she was undergraduate student in CEPSA (Huelva), Department of Vegetable Biochemistry and Molecular Biology (University of Sevilla) and Confederación Hidrográfica del Guadalquivir (Ministerio de Medio Ambiente). The candidate obtained her degree in Chemical Sciences at the University of Sevilla in 2000. The candidate started her PhD with Dr. Rafael Borja at Instituto de la Grasa, Consejo Superior de Investigaciones Científicas (CSIC), Sevilla. Her work was focused in a comparative study of the anaerobic digestion process in one and two stages of the solid olive oil mill waste, a pollutant waste of problematic disposal and management. In June 2006 she finished her PhD in Chemical Sciences with honours *¿cum laude¿* at University of Sevilla. The results obtained for this work generated a high number of ISI publications. The doctoral dissertation was awarded with the XXV San Alberto Magno de Tesis Doctorales Prize by the Ilustre Colegio Oficial de Químicos de Sevilla for the most outstanding PhD thesis dissertation in Chemistry and its applications in the regions of Andalucía and Extremadura. After her PhD, the candidate joined an European Project: *¿Renewable energy from crops and agrowastes¿*, for the study of the hydrolytic-acidogenic step of the process of anaerobic digestion of sunflower oil wastes. Subsequently the candidate gained two years postdoctoral Fellowship of the Spanish Ministerio de Educación y Ciencia and a contract with the Fundación Española de Ciencia y Tecnología to work abroad. She was working at the University of Southampton with Professor Charles J. Banks at the School of Civil Engineering and the Environment (United Kingdom). During this postdoctoral period the candidate worked on the anaerobic digestion of winter and spring wheat as energy crop, contributing to the project 'Integrated systems for farm diversification into energy production by anaerobic digestion: implications for rural development, land use & environment' funded by the UK Joint Research Councils. The results she obtained were of great interest, both from the scientific viewpoint and due to their significance in terms of the design of full-scale plant for anaerobic digestion of this substrate and of other similar energy crops. The candidate started a second postdoctoral stay (October 2009) with a contract *¿Junta de Ampliación de Estudios¿* at Instituto de la Grasa, Sevilla, to work in the treatment of sunflower oil industry wastes through different pre-treatments plus anaerobic digestion. She has worked in the determination of the microbial communities into the anaerobic reactors by Molecular Biology techniques. She was actively collaborating with the Instituto de Recursos Naturales y Agrobiología, CSIC (Seville). Currently the candidate has different publications regard to this subject. The candidate has published one book chapter and participated in 5 project. She has attended to 15 international congresses. The candidate has 29 peer-reviewed publications up to date, all of them included in the Journal Citation Reports. Some of them account with more than 30 citations, and 253 times cited in total. The candidate has an h-index 10, which shows the high impact that her research has achieved in the scientific community.



MINISTERIO
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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: HERNANDEZ ALONSO, MARIA DOLORES

Referencia: RYC-2011-07719

Area: Tecnología Química

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Título:

TOWARDS MORE EFFICIENT SOLAR PHOTOCATALYTIC SYSTEMS FOR AIR TREATMENT APPLICATIONS

Resumen de la Memoria:

Solar Photocatalysis is an area of utmost interest within the renewable sources scenario. Photocatalytic oxidation of pollutants constitutes a viable decontamination process that can be applied to both water and air purification. Nevertheless, most of the research in this field is devoted to elimination of pollutants in aqueous phase and surprisingly, in the case of air applications, the number of studies is very limited. This is mainly due to technical difficulties associated to this particular application. On one hand, the use of continuous operating systems, in contrast to recirculation systems generally used in water applications, are required due to the impracticality of storing large gas volumes. On the other hand, fixation of the photocatalyst to a solid support is crucial to avoid losses of the active component or expensive filtration processes. However, there are some drawbacks of using immobilized systems, related to the decreased photocatalytic efficiency due to the poor contact between the pollutant and the photoactive material, and to problems associated to inefficient irradiation of the semiconductor particles. Thus, despite the advantages of this environmentally friendly process, several issues have to be overcome in order to implement successfully this technology for the treatment of polluted air in real conditions, being important to deepen in the development of more efficient systems in terms of the photoactive materials, reactor design and photocatalyst configuration. The aim of the proposed research is to develop commercially competitive photocatalytic systems, able to compete with other degradation technologies, for polluted air treatment. Firstly, achieving a strict control of the nanoarchitecture of the photocatalysts during the synthesis and searching for the optimum technology to deposit a photocatalyst coating on the appropriate substrate for each particular application are necessary tasks for this research. These coatings can be employed on other practical applications such as self-cleaning products (e.g. construction and building materials or photocatalytic systems for indoor air purification and disinfection). A parallel goal will be to develop feasible, easy to handle structured-shaped hybrid composites (adsorbent/photocatalyst), endowed with improved properties as compared to standard photocatalysts due to the synergetic effect between the adsorption capacity of the adsorbent and the photoactive material. Finally, other important aspect of the research line will be the design of adequate photocatalytic reactors for these structured photocatalysts. The experience of the candidate matches perfectly the requirements of the project and can be fully identified with the objectives of the proposed research line. Besides, the candidate possesses the technical skills and the background in photocatalysis, catalysts preparation and reactor design necessities to ensure the success of the project.

Resumen del Curriculum Vitae:

The candidate has been awarded during her career with different predoctoral fellowships and postdoctoral contracts (Comunidad de Madrid, FPU, Posdoctoral MICINN, Juan de la Cierva). At present, she is working at CIEMAT-PSA with a Juan de la Cierva contract, about to start its last year. She is co-author of 23 published articles in SCI journals (another 2 manuscripts currently under review), 11 of them with an impact factor higher than 5.0 (ca. 90% with an impact factor higher than 3.0) which place them amongst the top ranked journals in the Chemical Engineering and Environmental Engineering area. These publications accumulate more than 400 citations, being her h index = 12. Some of these articles are listed as Most-Downloaded and in ScienceDirect TOP25 Hottest Articles. Her work has given rise to more than 40 contributions to national and international conferences (18 as presenting author). The researcher has participated in 12 projects, 5 of them currently active, including a CONSOLIDER, awarded with the IWA prize 2010 for innovation in the practical realisation of sustainable urban water management. The candidate is the Principal Investigator of one of them (MAT2008-01094/MAT), funded with 76.000 euros. Four of the projects were/are financed or promoted by companies (EASTMAN, COMSA, Aire Limpio, and ELCOGAS), which have generated different confidential reports and technology transference activities (e.g. TRACE, TRA2009_0262_01). The applicant has proved her mobility working in international reference laboratories in USA (Environmental Chemistry and Technology Program, University of Wisconsin-Madison, 7 months) and The Netherlands (Catalysis Engineering Department, Delft University of Technology, Delft, 2 years), and national research centres such as UCM, ICP-CSIC and CIEMAT-PSA. She has being involved in different educational and supervision tasks, which include the supervision of 2 Master Thesis Projects, and has being invited to review articles for Chemistry of Materials, Chemical Communications or Catalysis Today, among others.



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**SUBPROGRAMA RAMON Y CAJAL
CONVOCATORIA 2011**

Nombre: LOPEZ-SUEVOS FRAGUELA, FRANCISCO

Referencia: RYC-2011-09052

Area: Tecnología Química

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Título:

Eco-efficient bio-based tannin adhesives for exterior-grade wood-based composites

Resumen de la Memoria:

The first goal of this research line is to develop tannin adhesives from renewable raw materials (bio-based) that are efficient regarding to both ecological and economical aspects (eco-efficient) and that can be used to reproduce the behaviour and performance of synthetic resins. The second goal is to apply the resulting eco-efficient bio-based adhesives to the manufacture of wood-based composites for non-load bearing exterior-grade use. In order to reach these goals the following steps are proposed:1. Lignocellulosic materials from various sources will be processed to obtain tannin-rich extracts that will be characterized by GPC and MALDI-TOF-MS to determine their characteristic average size and polydispersity.2. Tannin adhesives will be formulated with the addition of hardeners that are not formaldehyde-yielding compounds under the conditions of use, such as hexamine or methylolated nitroparaffins.3. The resulting tannin adhesives will be thoroughly characterized in terms of their rheological, thermal, structural and stability behaviour by using different techniques, including but not limited to, rheometry, contact angle measurements, TGA, DSC, DMA and ¹³C NMR.4. Wood-based composites such as plywoods, particleboards and medium density fiberboards will be prepared with the tannin adhesives and with available commercial adhesives as controls. The tannin adhesives will be tailored to fit the requirements needed for the different types of boards. The wood bonding performance of the panels for outdoor-grade use will be evaluated according to the relevant European standards.If, in the light of the obtained results, it can be concluded that tannin adhesives can successfully lead to wood-based composites for non-load bearing exterior-grade use, the candidate will move to attract industrial partners to test the developed adhesives in an industrial scale. And, optimally, this will lead to the start up of a production facility for tannins extraction and adhesive preparation using the developed technology.

Resumen del Curriculum Vitae:

Currently, Francisco López-Suevos Fraguela is an Isidro Parga Pondal researcher (Xunta de Galicia) at the Centro de Innovación y Servicios Tecnológicos de la Madera (CIS-Madeira), Spain, from where he runs a program on Wood Chemistry, wood adhesives, wood-based composites and thermal analysis and provides technical assistance to the R+D Departments of different National Timber/Adhesives companies. Bachelor of Science (B.S.) in Chemistry in 1998, B.S. Thesis in Chemistry in 1999, Masters degree in Chemical Engineering in 2001 (DEA), all diplomas obtained from the University of Santiago de Compostela (USC), Spain. PhD in Chemical Engineering in 2003 from the USC with a research thesis titled "Preparation of industrial adhesives using tannins from the Pinus pinaster bark". Among the awarded fellowships, the most relevant are: Segundo Gil Dávila Foundation and Galician Government PhD fellowships (1999-2003) and a Fulbright-MECD postdoctoral fellowship (2003-2005). The candidate has also held postdoctoral research positions at the Paffenbarger Research Center (American Dental Association Foundation) in Gaithersburg, MD, USA (2006-2007) and at the Swiss Federal Laboratories for Materials Testing and Research (Empa, 2007-2009). He has 420h of teaching experience at the Chemical Engineering Department of the USC (Spain) and he actively contributed to the training of PhD students in Virginia Tech (USA) and in Empa (Switzerland), and since 2010 he is co-advising a Ph.D. Thesis. The candidate has been involved in 12 national and International research projects and in two technological transfer activities. He has also been selected to participate in industrial internships in several wood-based and wood adhesives companies (Grupo Losán, Foresa and Finsa). As a result of his research activity, he has co-authored 19 peer-reviewed papers in International journals of high impact factor (rated in the Science citation index) in the subject category that relates to this application. In addition, 19 abstracts were accepted in various international and national conferences. The candidate also regularly contributes as reviewer to the Journal of Adhesion Science and Technology.



Nombre: BERRUECO MORENO, CESAR

Referencia: RYC-2011-09202

Area: Tecnología Química

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Título:

PREPARATION AND CHARACTERISATION OF BIOMASS-DERIVED CHAR AND ITS APPLICATION AS SUSTAINABLE ENERGY MATERIAL

Resumen de la Memoria:

The substitution of fossil fuels by biomass in energy production is an important route for the abatement of CO₂ emissions and for reducing fossil resource utilisation. Although biomass is currently co-combusted and co-gasified with coal in several large-scale plants around the world, its widespread use still faces some barriers. One of them is the low energy density of biomass feedstocks, which makes them expensive to transport over long distances. One approach to overcome these drawbacks consists in increasing the energy density of the feedstock prior to its transportation by producing a carbonaceous solid material, or char, which could subsequently be transported and used for energy purposes. In this context, the present proposal has been formulated with the aim of getting a better understanding of the processes of pyrolysis and gasification of biomass for the preparation of carbonaceous solid materials and the evaluation of such materials for energy uses, in order to implement these processes and assess their feasibility from an operational, energetic and environmental point of view. Two different technologies have been considered for the application of the produced char in the field of energy production, namely, gasification and direct carbon fuel cells. Regarding gasification, the benefit of the proposed technology lies in the fact that a central gasifier could be fed with chars produced in relatively small-scale units in locations where the biomass is readily available. The approach is promising at the conceptual stage, but requires a detailed study of the char reactivity to optimise the amount and calorific value of the gas product from the gasifier. Direct carbon fuel cells represent a promising alternative to directly converting carbon-rich solid materials into electricity, due to its high efficiency (around 80%). Biomass-derived char as feedstock for direct carbon fuel cells needs to fulfil specific requirements (in terms of composition and chemical structure), which could be customized by controlling the conditions for char production. In order to achieve the final objective, the following partial objectives are defined: 1) Study of the factors affecting the production of the biomass-derived chars. It will be necessary to carefully select the conditions to be used in the char production process by evaluating the behaviour of the feedstocks under conditions likely to prevail in this stage. In particular, it will be investigated the potential yields that can be formed from a range of selected biomass feedstocks over a wide range of process conditions. The data produced will be used for identifying the more suitable feedstocks and operating parameters for the pyrolysis char production stage. 2) Evaluation of the char properties in relation to its final use. The characterization results of the produced chars will be related to the specific requirements for each particular application, including production of energy through gasification and use in direct carbon fuel cells, in order to assess the suitability of these materials. This project aims to develop the technology for the utilization of biomass for energy purposes, introducing a novel approach: the separation of two stages, i.e. biomass-derived char production and char gasification/use in fuel cells. Moreover, this research line is of great interest (technologically and environmentally) to the scientific community in the search for a sustainable energy model.

Resumen del Curriculum Vitae:

The applicant is a senior researcher that has worked in the thermochemical conversion processes field since 2000, when he graduated in Chemical Engineering at the University of Zaragoza. In November 2000, he joined the Thermochemical Processes Group of the Department of Chemical and Environmental Engineering of the University of Zaragoza, where he received the PhD with honours in July 2005. During this period, he was actively involved in different research projects that were being carried out by the Research Group and were either publicly (C.I.C.Y.T., M.E.C.) or privately (GUASCOR I+D) financially supported. After finishing his PhD he was given a contract associated with the Project ζ Catalytic degradation of polyolefins and application to the catalytic reforming to obtain hydrogen ζ . In November 2005 he became a member of the University of Zaragoza academic staff, as Assistant Professor in the area of Chemical Engineering, thus he combined the teaching assignment with the research activities. In 2007 he incorporated into the Energy Engineering Group at Imperial College London, thus starting his postdoctoral stage abroad, under the supervision of Prof. Rafael Kandiyoti. Until February 2009 he held a fellowship from the Spanish Ministry of Education and Science as a Postdoctoral fellow, to carry on the Project ζ Characterisation of asphaltenes and of deposited foulants ζ , a sub-project of the ζ Crude oil fouling ζ project, that brings together several researcher groups from Imperial College London, other UK Universities as well as important industries in the petrochemical sector. After the Postdoctoral fellowship, and thanks to his experience both in the field of gasification and in the treatment of petroleum derived materials, he was contracted as Research Associate, continuing his collaboration in the Energy Engineering Group involved in the research project: ζ In-situ production of tar sands and heavy oils ζ . The contractual situation at Imperial College London continued until January 2011 as Research Associate, being involved in several projects (FLEXGAS, Eurofibres, Green EAF, FECUNDUS) with an increase in responsibility, taking part in project meetings and research decisions. In January 2011 he was offered a contract as researcher at the Bioenergy and Biofuels Area of the ζ Catalonia Institute for Energy Research ζ (IREC) in the frame of the project COMBOX. The contract started with a three month stay at Imperial College London as Academic visitor, in order to design and develop a series of tasks related to the project. The research work developed during his doctoral and Postdoctoral stages resulted in the publication of 12 articles in peer-reviewed journals of high scientific level and impact factor (Energy and Fuels, Bioresources Technology, Journal of Analytical and Applied Pyrolysis), being the first author of five of them. His work has been also spread in a large number of national and international conferences, with a total of 25 communications, two of them appearing as publication in a scientific collective volume, apart from several private seminars. Furthermore, he has been the director of three Final Project Works at the University of Zaragoza, and has been involved in the tutoring of several Masters and PhD students at Imperial College London. He has also fulfilled the requirements to obtain the ANECA accreditation for several teaching figures. His current h-index is 6.