ICMS

Instituto de Ciencia de Materiales de Sevilla

Memoria de Actividades
Annual Report

Consejo Superior de Investigaciones Científicas

Universidad de Sevilla

Junta de Andalucía

2023

Consejo Superior de Investigaciones Científicas
Universidad de Sevilla
Junta de Andalucía

INSTITUTO DE CIENCIA DE MATERIALES DE SEVILLA

Memoria de Actividades
Annual Report
2023

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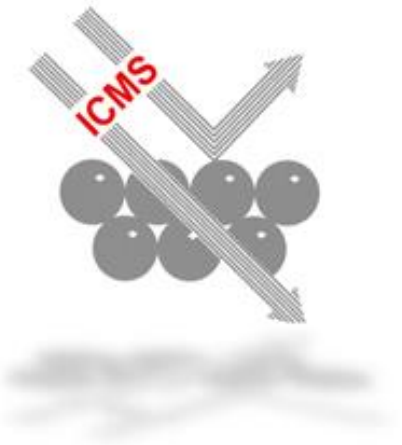

EDITA

Instituto de Ciencia de Materiales de Sevilla (ICMS)
Centro Mixto entre el Consejo Superior de Investigaciones
Científicas y la Universidad de Sevilla
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DISEÑO Y MAQUETACIÓN
José Carlos Rivero Cabello

COMISIÓN MEMORIA-ICMS
Gerardo Colón Ibáñez - Francisco José Gotor Martínez – Svetlana Ivanova - Pedro José Sánchez Soto

COORDINADORA DE DIVULGACIÓN CIENTÍFICA ICMS
T. Cristina Rojas Ruiz

EL CONTENIDO DE LA PRESENTE MEMORIA TIENE UN CARÁCTER EXCLUSIVAMENTE INFORMATIVO

INDICE

TABLE OF CONTENTS

Presentación

A través de esta Memoria 2023, el Instituto de Ciencia de Materiales de Sevilla (ICMS) pretende comunicar lo mejor de las actividades científicas realizadas a lo largo del pasado año. El ICMS es un centro mixto del Consejo Superior de Investigaciones Científicas (CSIC) y la Universidad de Sevilla (US), cofinanciado por la Junta de Andalucía. Fue creado en 1986 y está integrado por personal científico de la Universidad de Sevilla y el CSIC. A finales de 2023, contaba con 141 empleados, de los cuales 62 eran científicos permanentes.

De acuerdo con la estructura establecida en el vigente Plan Estratégico 2022-2025, nuestro centro se organiza en torno a 5 departamentos, cuyos miembros abordan temáticas tanto fundamentales como aplicadas. Así, nuestras investigaciones abordan problemas candentes de la Química y Física del Estado Sólido, la Catálisis Heterogénea, la Cerámica, la Óptica, la Ciencia de Superficies, las Energías Renovables y el Medio Ambiente, etc. Entre ellas, podemos resaltar el aprovechamiento de las energías solar y de biomasa, la generación de H_2 y otros combustibles limpios y de origen renovable, el aprovechamiento y conversión química del CO_2, la depuración de efluentes químicos, el secuestro de residuos radioactivos, la mejora de la selectividad y rendimiento de reacciones químicas básicas, el aumento de la eficiencia de los dispositivos generadores de energía renovable (celdas fotovoltaicas, electrodos, generadores piezoeléctricos, celdas de combustible o baterías) y de los emisores de luz (LEDs), el desarrollo y la mejora de sensores químicos y agentes de contraste radiológico, de materiales biocompatibles para implantes quirúrgicos, de pigmentos cerámicos, de recubrimientos hidrofóbicos o hidrofílicos, recubrimientos hielofóbicos,… y un largo etcétera.

Nuestros principales empeños para los años venideros son realizar investigaciones que se sitúen en la vanguardia de la Ciencia e Ingeniería de Materiales y que éstas sirvan de apoyo al desarrollo en Andalucía de un nuevo sistema económico, en el que las bases científica y tecnológica pasen a ser pilares fundamentales.

Dr. Juan Pedro Espinós Manzorro
Director del Instituto de Ciencia de Materiales de Sevilla

Presentation

Through this Activity Report 2023, the Institute of Materials Science of Seville (ICMS) is communicating the best of its scientific activities carried out for the last year. The ICMS is a joint centre of the Spanish Research Council (CSIC) and the University of Seville (US), also funded by the Junta de Andalucía. It was founded in 1986, and integrated by scientific staff of the University of Seville and the CSIC. At the end of last year, it includes 141 people, 62 of them as permanent scientific staff.

The current Strategic Plan 2022-2025 organizes our Centre in 5 departments, which personnel address both fundamental and applied research. Thus, our researchers address hot topics related with disciplines of Solid State Chemistry and Physics, Heterogeneous Catalysis, Ceramics, Optics, Surface Science, Renewable Energy and Environment, etc. Among them, we could mention the exploitation of solar energy and biomass, the generation of H_2 and other clean and renewable fuels, the exploitation and chemical conversion of CO_2, the removal of pollutants, the storage of radioactive wastes, the improvement of the selectivity and yield of basic chemical reactions, the efficiency of renewable energy generators (photovoltaic cells, electrodes, piezoelectric devices, fuel cells and batteries) and light emitting devices (LEDs), the development and improvement of chemical sensors and radiological contrast agents, the production of biocompatible scaffolds for surgical implants, the production of ceramic pigments, many different coatings and thin films, … and a long etcetera.

Our main efforts for near future are to cover the most modern and innovative aspects of the current Material Science and Material Engineering, as well as to support in the region of Andalusia, the development of a new economic system, in which scientific and technological basis should become fundamental pillars.

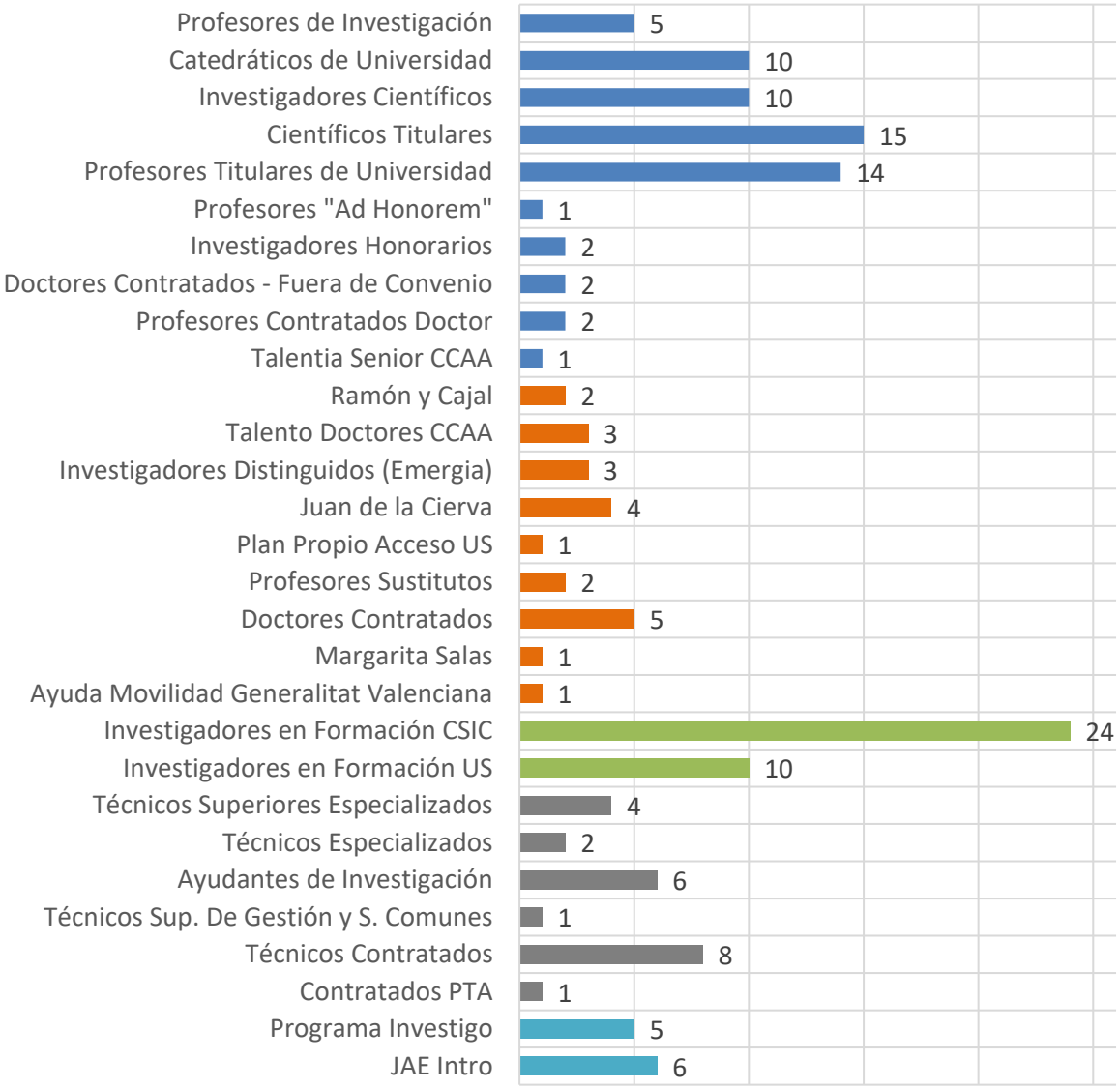
Dr. Juan Pedro Espinós Manzorro
Director of the Institute of Materials Science of Seville

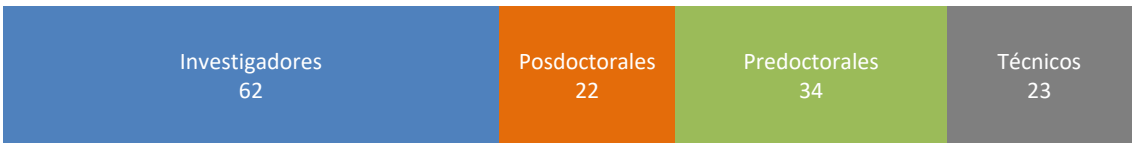
El ICMS en 2023
ICMS in 2023

Datos Estadísticos del ICMS
Statistical Data of ICMS

RECURSOS HUMANOS / HUMAN RESOURCES

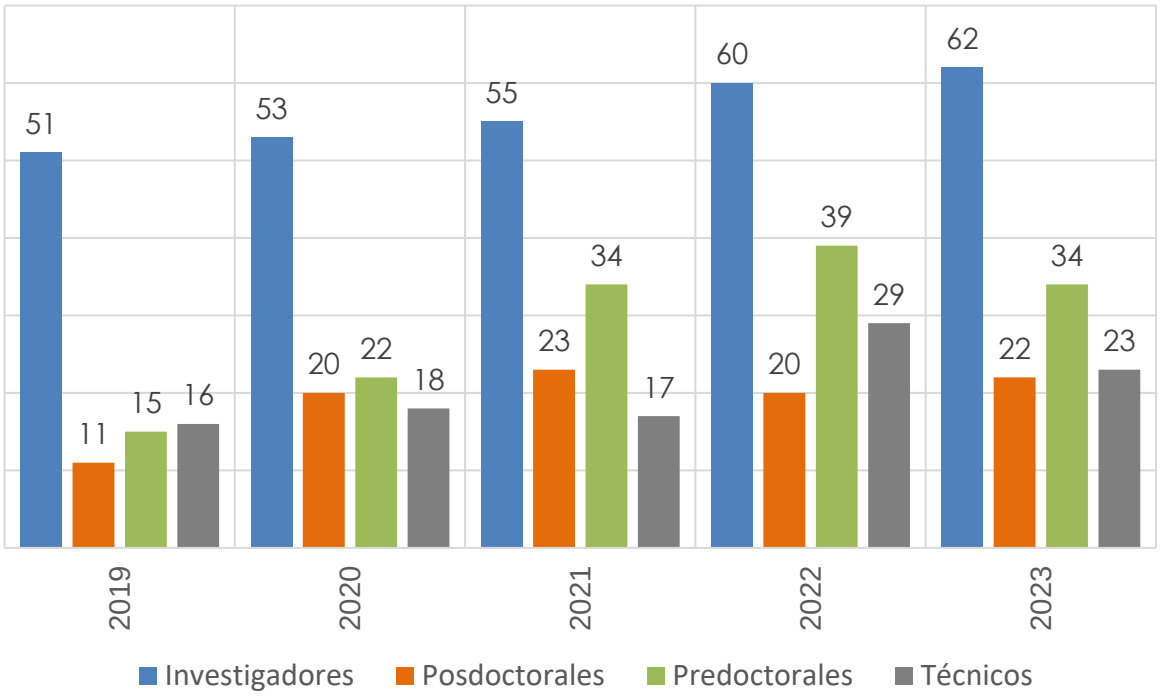
Distribución del personal por categorías
Distribution by professional category



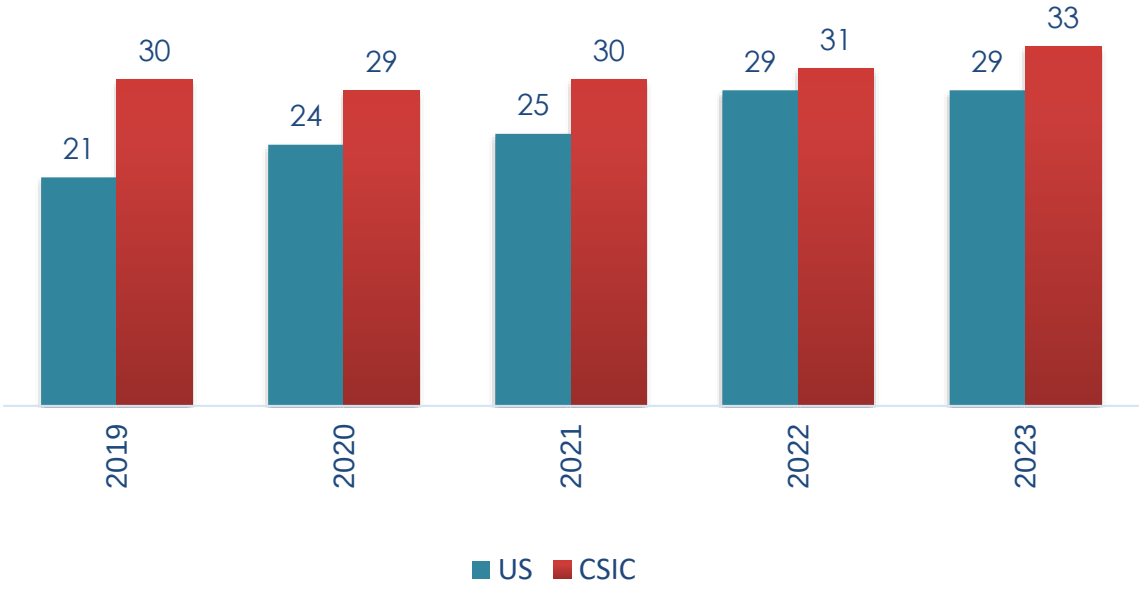


*Datos a 31 de Diciembre de 2023

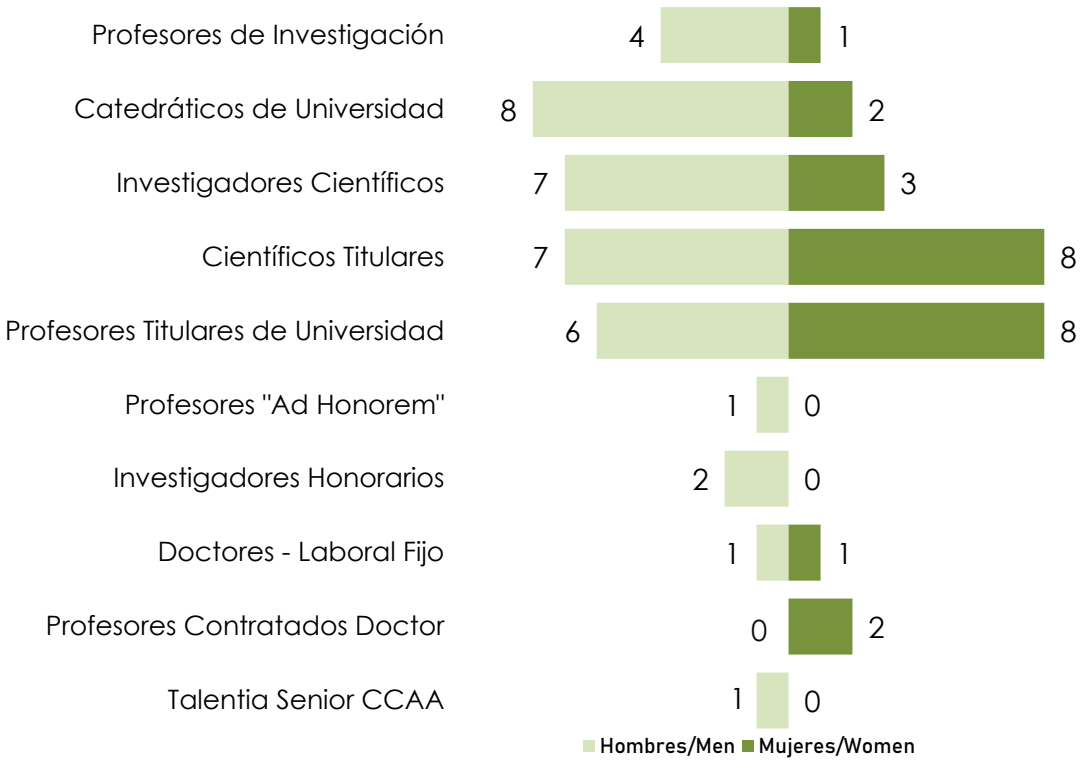
Evolución 2019-2023 del personal
Evolution of staff

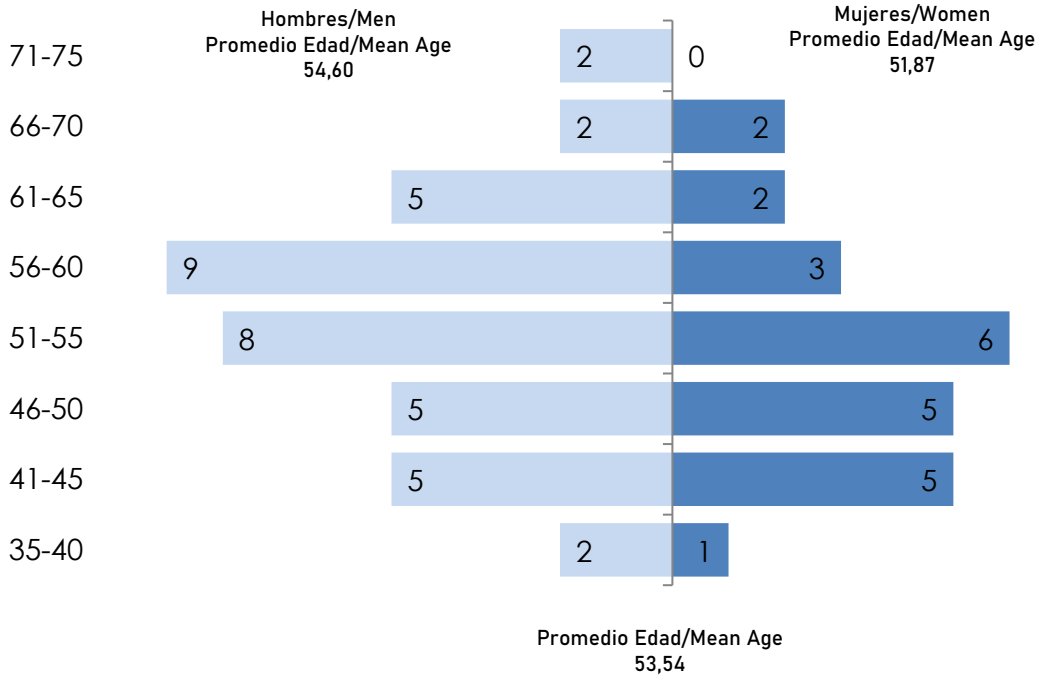


Evolución 2019-2023 del personal investigador
Evolution of research staff



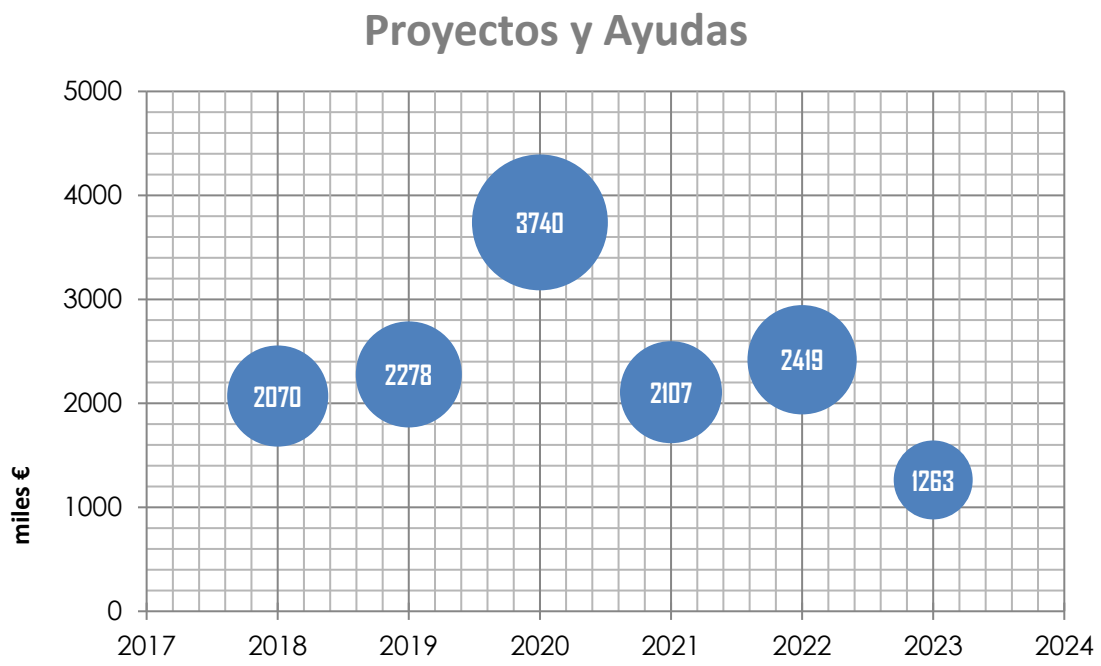
Distribución del personal investigador (sexo y edad)
Distribution by scientific staff (gender and age)





FINANCIACIÓN / FUNDING

Financiación conseguida por año (miles€)
Evolution of the funding of the ICMS



PRODUCCIÓN CIENTÍFICA / SCIENTIFIC PRODUCTION

Revistas SCI en las que se ha publicado algún artículo, por orden de Factor de Impacto (WoS)
Number of scientific papers published in a specific journal arranged by their Impact Factor

Revista Journal	Artículos Papers	Factor De Impacto Impact Factor (*)	Mejor PCT	
Advanced Composites and Hybrid Materials	1	23,2	D1	Q1
Applied Catalysis B-Environmental	1	20,2	D1	Q1
Advanced Functional Materials	3	18,5	D1	Q1
Nature Physics	1	17,6	D1	Q1
Nano Energy	1	16,8	D1	Q1
Renewable & Sustainable Energy Reviews	2	16,3	D1	Q1
Environmental Chemistry Letters	1	15	D1	Q1
Chemical Engineering Journal	2	13,3	D1	Q1
ACS Catalysis	2	11,3		Q1
Food Hydrocolloids	1	11	D1	Q1
Green Energy & Environment	1	10,7	D1	Q1
Journal of Materials Chemistry A	1	10,7	D1	Q1
Journal of Cleaner Production	2	9,7	D1	Q1
Rare Metals	1	9,6	D1	Q1
Journal of Colloid and Interface Science	2	9,4		Q1
NPJ 2D Materials and Applications	1	9,1		Q1
Energy	3	9	D1	Q1
Renewable Energy	1	9		Q1
Journal of Energy Storage	1	8,9		Q1
Food Chemistry	1	8,5	D1	Q1
ACS Applied Materials & Interfaces	3	8,3		Q1
Acta Materialia	1	8,3	D1	Q1
Science of the Total Environment	1	8,2	D1	Q1
Chemosphere	1	8,1	D1	Q1
International Journal of Hydrogen Energy	4	8,1		Q1
Separation and Purification Technology	1	8,1	D1	Q1
Materials & Design	1	7,6		Q1
Journal of Environmental Chemical Engineering	3	7,4		Q1
Chemistry of Materials	1	7,2		Q1
Fuel Processing Technology	2	7,2		Q1
Journal of CO2 Utilization	2	7,2		Q1
ACS Sustainable Chemistry & Engineering	1	7,1		Q1
Fuel	2	6,7		Q1
Advanced Materials Technologies	1	6,4		Q1

Revista Journal	Artículos Papers	Factor De Impacto Impact Factor (*)	Mejor PCT	
Applied Surface Science	2	6,3		Q1
Journal of Materials Research and Technology-JMR&T	1	6,2	D1	Q1
Applied Thermal Engineering	1	6,1	D1	Q1
Inorganic Chemistry Frontiers	1	6,1	D1	Q1
Journal of Alloys and Compounds	2	5,8	D1	Q1
Journal of The European Ceramic Society	2	5,8	D1	Q1
Nanoscale	3	5,8		Q1
ACS Applied Energy Materials	2	5,4		Q2
ACS Applied Nano Materials	1	5,3		Q2
Surface & Coatings Technology	1	5,3		Q1
Catalysis Today	3	5,2		Q1
Energy & Fuels	3	5,2		Q1
Materials Advances	1	5,2		Q2
Ceramics International	5	5,1	D1	Q1
Sustainable Energy & Fuels	1	5		Q2
Colloids and Surfaces A-Physicochemical and Engineering Aspects	1	4,9		Q2
Microporous and Mesoporous Materials	2	4,8		Q1
Polymers	1	4,7		Q1
Batteries	1	4,6		Q2
Catalysis Science & Tecnology	1	4,4		Q2
Nanomaterials	5	4,4		Q2
Chemical Communications	1	4,3		Q2
Materials Chemistry and Physics	1	4,3		Q2
Advanced Powder Technology	1	4,2		Q2
Materials Science in Semiconductor Processing	1	4,2		Q1
Molecules	2	4,2		Q2
RSC Advances	1	3,9		Q2
Catalysts	4	3,8		Q2
Advanced Photonics Research	1	3,7		Q2
Energy Technology	1	3,6		Q3
ChemElectroChem	1	3,5		Q2
Journal of the American Ceramic Society	2	3,5		Q1
Heliyon	1	3,4		Q2
Journal of Non-Crystalline Solids	3	3,2		Q1
Journal of Solid State Chemistry	1	3,2		Q2
Optics Express	1	3,2		Q2
Physical Review B	1	3,2		Q2

Revista Journal	Artículos Papers	Factor De Impacto Impact Factor (*)	Mejor PCT	
Journal of Chemical Physics	1	3,1		Q1
Lubricants	1	3,1		Q2
Materials	6	3,1		Q1
Photochemical & Photobiological Sciences	1	3,1		Q2
Thermochimica Acta	1	3,1		Q2
Journal of Thermal Analysis and Calorimetry	3	3		Q2
Coatings	2	2,9		Q2
Nanotechnology	1	2,9		Q2
Physical Chemistry Chemical Physics	1	2,9		Q1
Plos One	1	2,9		Q1
Journal of Chemical Technology and Biotechnology	1	2,8		Q2
Journal of the Spanish Ceramic and Glass Society	1	2,7		Q1
Frontiers in Energy Research	1	2,6		Q3
Plasma Chemistry and Plasma Processing	1	2,6		Q2
Journal of Chemical Education	1	2,5		Q2
ACS Agricultural Science & Technology	1	2,3		Q1
Journal of Nanoparticle Research	1	2,1		Q3
Physica Status Solidi A-Applications and Materials Science	1	1,9		Q3
International Journal of Applied Ceramic Technology	1	1,8		Q2
Revista Facultad de Ingeniería-Universidad de Antioquia	2	0,9		Q3
Nuovo Cimento C-Colloquia and Communications in Physics	1	0,3		Q4
Total	146	6,36		

Mejor PCT									
D1		Q1		Q2		Q3		Q4	
38	26,03 %	97	66,44 %	42	28,77 %	6	4,11 %	1	0,68 %

(*) Factor de Impacto correspondiente al año 2023
Journal Citation Reports of 2023

Composición y Estructura
Structure and Organisation

EL INSTITUTO / THE INSTITUTE

El Instituto de Ciencia de Materiales de Sevilla (ICMS) fue creado en 1.986. En 1996 se trasladó a unos nuevos locales en la Isla de la Cartuja, integrándose, junto con otros dos Institutos Mixtos, en el Centro de Investigaciones Científicas Isla de la Cartuja (Consejo Superior de Investigaciones Científicas - Universidad de Sevilla - Junta de Andalucía). El ICMS se estructura en cinco Unidades de Investigación ubicadas en el edificio de la Isla de la Cartuja y una Unidad Externa en el Campus Universitario de Reina Mercedes, Facultad de Física. En la actualidad, el Instituto está formado por grupos de investigación del CSIC y de la Universidad de Sevilla. Estos grupos tratan de aunar sus esfuerzos en diversas áreas de la física y química del estado sólido, físico-química de superficies y otras disciplinas relacionadas con la Ciencia de Materiales. Esta actividad persigue contribuir al desarrollo científico dentro de los Planes de Investigación tanto Autonómicos como Nacionales en el área de la Ciencia y Tecnología de Materiales, así como de las equivalentes de la UE.

The Institute of Materials Science of Seville (ICMS) was created in 1986. In 1996, it moved to new premises at the Isla de la Cartuja, combining with two other Mixed Institutes to make up the Isla de la Cartuja Scientific Research Centre (Consejo Superior de Investigaciones Científicas - Universidad de Sevilla - Junta de Andalucía). The Institute comprises three research units housed in the building at the Isla de la Cartuja and an external unit at the Physics Faculty on the Reina Mercedes University Campus. Today it incorporates research groups of CSIC and the University of Seville. The aim of these groups is to unite efforts in various areas of solid-state physics and chemistry, physical chemistry of surfaces, and other related disciplines of materials science. Such activity seeks to contribute to scientific development within the Research Plans of both regional and state authorities, and their EU equivalents, in the field of materials science and technology.

ORGANIGRAMA / ORGANIZATION CHART

Grupos de Investigación

Fotocatálisis Heterogénea: Aplicaciones Materiales y Procesos Catalíticos de Interés Ambiental y Energético
Química de Superficies y Catálisis
Materiales de Diseño para la Energía y Medioambiente
Materiales Avanzados
Propiedades Mecánicas, Modelización y Caracterización de Cerámicos Avanzados
Reactividad de Sólidos
Nanotecnología en Superficies y Plasma
Materiales Nanoestructurados y Microestructura
Materiales para Bioingeniería y Regeneración Tisular
Tribología y Protección de Superficies
Materiales Coloidales
Materiales Ópticos Multifuncionales
Materiales Semiconductores para la Sostenibilidad

Servicios Científicos Técnicos

Análisis Químico de Superficie por Fotoemisión
Análisis Textural y Térmico
Caracterización Tribológica y Mecánica de Superficies
Determinación del Mojado en Superficie
Difracción de Rayos X
Espectroscopía de Electroluminiscencia
Espectrometría de Emisión Atómica
Espectroscopía Ultrarápida
Espectroscopía Ultravioleta-Visible-Infrarrojo Cercano
Espectroscopías Vibracionales
Mecanizado
Microscopía Electrónica
Preparación y Caracterización de Sistemas Catalíticos Heterogéneos

DIRECCIÓN / DIRECTORATE

Director / Director: Dr. **Juan Pedro Espinós Manzorro**
Vicedirectora / Vicedirector: Dra. **Ana María Gómez Ramírez**
Dra**. Anna Penkova** hasta el 20 de julio

JUNTA DE INSTITUTO / INSTITUTE BOARD

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Dra**. Anna Penkova** hasta el 20 de julio
Secretario / Secretary: Dª. **María Teresa Zaragoza Benítez**
D. **Enrique Díaz Ruíz** hasta el 18 septiembre

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Dr. **Tomás Ramírez Reina** (Dr. **Juan Pedro Holgado Vázquez** hasta el 23 de junio)

Representante U.I. Ingeniería de Cerámicos para Ambientes Extremos
Dr. **Joaquín Ramírez Rico** (Dra. **María Dolores Alba Carranza** hasta el 23 de junio)

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Dr. **Luis A. Pérez Maqueda**

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Dr. **Ángel Barranco Quero**

Representante U.I. Materiales Ópticos
Dr. **Hernán R. Míguez García**

Representante U.E.I. Física de Materiales
Dr. **Jhon Jairo Ipus Bados**

Representante del Profesorado de plantilla de la Universidad de Sevilla
Dra. **Leidy Marcela Martínez Tejada** (Dra. **Svetlana Ivanova** hasta el 23 de junio)

Representante del Personal Científico de plantilla del CSIC
Dr. **Gerardo Colón Ibáñez** (Dr. **Juan Carlos Sánchez López** hasta el 23 de junio)

Representante del Personal No Científico y No Profesorado de plantilla
D. **Juan Carlos Martín Sánchez**

CLAUSTRO CIENTÍFICO / SCIENTIFIC BOARD

Presidente / Chairman Espinós Manzorro, Juan Pedro

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A
Alba Carranza, María Dolores
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Álvarez Molina, Rafael
Anaya Martín, Miguel
Aparicio Rebollo, Francisco J.
Avilés Escaño, Miguel Ángel
Ayala Espinar, María Regla

B
Barranco Quero, Ángel
Becerro Nieto, Ana Isabel
Benítez Jiménez, José Jesús
Blázquez Gámez, Javier S.
Bobadilla Baladrón, Luis F.
Borrás Martos, Ana Isabel
Borrego Moro, Josefa
Bravo León, Alfonso

C
Caballero Flores, Rafael
Caballero Martínez, Alfonso
Caliò, Laura
Calvo Roggiani, Mauricio E.
Castaing, Víctor
Castro Arroyo, Miguel Ángel
Centeno Gallego, Miguel Ángel
Colón Ibáñez, Gerardo
Conde Amiano, Clara F.
Córdoba Gallego, José Manuel
Cotrino Bautista, José
Criado Vega, Alberto

D
Díaz Cuenca, María Aránzazu
Domínguez Leal, María Isabel

E
Esquivias Fedriani, Luis

F
Fernández Camacho, Asunción
Fernández Carrión, Alberto J.
Fortio Godinho, Vanda
Franco García, Victorino

G
Galisteo López, Juan Francisco
Gallardo Cruz, Carmen
Gallardo López, Ángela María
Gil González, Eva
Gil Rostra, Jorge
Gómez García, Diego
Gómez Ramírez, Ana María
González Arias, Judith
González Castaño, Miriam
Gotor Martínez, Francisco José
Gutiérrez Mora, Felipe

H
Hidalgo López, M. Carmen
Holgado Vázquez, Juan Pedro

I
Ipus Bados, Jhon Jairo
Ivanova, Svetlana Lyubomirova

J
Jiménez de Haro, M. Carmen
Jiménez Melendo, Manuel
Jurado Fuentes, Dolores

L
López Flores, Víctor
López Santos, Carmen
Lozano Barbero, Gabriel
Luque Centeno, José Manuel

M
Malet Maenner, Pilar
Manchón Gordón, Alejandro F.
Martín Olalla, José María
Martínez Fernández, Julián
Martínez Tejada, Leidy Marcela
Mesquita Coelho, Joâo Carlos
Míguez García, Hernán Ruy
Morales Flórez, Víctor
Morales Rodríguez, Ana
Moriche Tirado, Rocío
Moshtaghion Enterazi, Bibi Malmal
Muñoz Bernábé, Antonio

N
Navío Santos, José Antonio
Nawaz, Muhammad Asif
Núñez Álvarez, Nuria Ofelia

O
Ocaña Jurado, Manuel
Odriozola Gordón, José Antonio
Oliva Ramírez, Manuel

P
Pastor Pérez, Laura
Pavón González, Esperanza
Palmero Acebedo, Alberto
Penkova, Anna Dimitrova
Perejón Pazo, Antonio
Pereñíguez Rodríguez, Rosa M.
Pérez Maqueda, Luis Allan
Platero Moreno, Francisco J.
Poyato Galán, Rosalía

R
Ramírez de Arellano-López, Antonio
Ramírez Rico, Joaquín
Ramírez Reina, Tomás
Real Pérez, Concepción
Rico Gavira, J. Víctor
Rodríguez González-Elipe, Agustín
Rojas Ruiz, T. Cristina
Romero Landa, Francisco Javier
Romero Sarria, Francisca

S
Sánchez Jiménez, Pedro E.
Sánchez López, Juan Carlos
Sánchez Soto, Pedro José
Sánchez Valencia, Juan Ramón
Sayagués De Vega, M. Jesús

T
Thi Tuyen, Ngo

V
Vattier Lagarrigue, Florencia
Villora Picó, Juan José

Y
Yubero Valencia, Francisco

DIRECTORIO / DIRECTORY

UNIDAD DE INVESTIGACIÓN RESEARCH UNIT: CATÁLISIS PARA EL MEDIOAMBIENTE Y LA ENERGÍA CATALYSIS FOR ENVIROMENT AND ENERGY

Catedráticos de Universidad	Alfonso Caballero Martínez Svetlana Ivanova José Antonio Odriozola Gordón
Investigadores Científicos	Miguel Ángel Centeno Gallego Gerardo Colón Ibáñez
Científicos Titulares	María del Carmen Hidalgo López Juan Pedro Holgado Vázquez
Profesores Titulares de Universidad	Luis Francisco Bobadilla Baladrón José Manuel Córdoba Gallego María Isabel Domínguez Leal Leidy Marcela Martínez Tejada Anna Dimitrova Penkova Rosa María Pereñíguez Rodríguez Tomás Ramírez Reina Francisca Romero Sarria
Investigadores Honorarios	José Antonio Navío Santos
Doctores Contratados	Dolores Jurado Fuentes Miriam González Castaño Judith González Arias Muhammad Asif Nawaz Laura Pastor Pérez Francisco Jesús Platero Moreno Estela Ruiz López Juan José Villora Picó
Investigadores en Formación	Débora Álvarez Hernández José Rubén Blay Roger Sergio Carrasco Ruiz Gabriel Delgado Martín Ligia Amelia Luque Álvarez Daniela Aielen Oreggioni Gadea María Saif Guillermo Torres Sempere
Técnicos Contratados	Ana María Fernández Sánchez
Programa Investigo	María Escamilla Rebollo Juan Carlos Ibáñez Rodríguez Melania Serrano Cruz

UNIDAD DE INVESTIGACIÓN RESEARCH UNIT: INGENIERÍA DE CERÁMICAS PARA MEDIOAMBIENTES AGRESIVOS ENGINEERED CERAMICS FOR EXTREME ENVIRONMENTS

Catedráticos de Universidad	Miguel Ángel Castro Arroyo Manuel Jiménez Melendo Pilar Malet Maenner Julián Martínez Fernández Antonio Ramírez de Arellano-López Joaquín Ramírez Rico
Investigadores Científicos	María Dolores Alba Carranza
Científicos Titulares	José Jesús Benítez Jiménez
Profesores Titulares de Universidad	Alfonso Bravo León
Doctores Contratados	Joâo Carlos Mesquita Coelho Esperanza Pavón González

UNIDAD DE INVESTIGACIÓN RESEARCH UNIT: MECANOQUÍMICA Y REACTIVIDAD DE MATERIALES MECHANOCHEMISTRY AND REACTIVITY OF MATERIALS

Profesores de Investigación	Luis Allan Pérez Maqueda
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FÍSICA DE MATERIALES PHYSICS OF MATERIALS

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Unidades de Investigación
Research Units

Catálisis para el Medioambiente y la Energía
Catalysis for Environment and Energy

Grupos de Investigación

Fotocatálisis Heterogénea: Aplicaciones |642005
Heterogeneus Photocatalysis: Applications
http://materphotocat.ciccartuja.es

Materiales y Procesos Catalíticos de Interés Ambiental y Energético |642004
Materials and catalytic processes for environment and energy
http://matproner.icms.us-csic.es

Química de Superficies y Catálisis |642006
Surface Chemistry and Catalysis
http://surfcat.icms.us-csic.es

PERSONAL / PERSONNEL

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PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Reactores estructurados no convencionales para el craqueo catalítico de metano libre de CO2
STructured unconventional reactors for CO2-fRee Methane catalytic crackING

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
EU240226_01	01-09-2022 31-08-2025	Comisión Europea	246.285 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

STORMING desarrollará reactores estructurados innovadores calentados con electricidad renovable, para convertir CH_4 fósil en H_2 libre de CO_2 y en nanomateriales de carbono de alto valor para aplicaciones de baterías. Más específicamente, se desarrollarán catalizadores innovadores basados en Fe, altamente activos y fácilmente regenerables mediante procesos que no generen residuos, a través de un protocolo de diseño racional de catalizadores, que combina estudios teóricos (Teoría del Funcional de la Densidad y Cálculos de Dinámica Molecular) y experimentales (cluster), todos de ellos asistidos por caracterización in situ y operando y herramientas de Machine Learning. La electrificación (con calentamiento por microondas o por efecto joule) de reactores estructurados, diseñados por fluidodinámica computacional y preparados mediante impresión 3D, permitirá un control térmico preciso que dará como resultado una alta eficiencia energética. El proyecto validará, en un nivel 5 de TRL, la tecnología catalítica más prometedora (elegida con criterios tecnológicos, económicos y ambientales) para producir H_2 con eficiencia energética (> 60 %), cero emisiones netas y con un coste hasta un 10 % menor al del proceso convencional. La difusión y comunicación de los resultados impulsará la aceptación social de las tecnologías relacionadas con el H_2 y la participación de las partes interesadas en la explotación y el despliegue de procesos a corto plazo. La clave para alcanzar los desafiantes objetivos de STORMING es el muy alto grado de complementariedad e interdisciplinaridad de los grupos que forman el consorcio, donde las ciencias básicas y aplicadas se fusionan con la ingeniería, la informática y las ciencias sociales. El Grupo del ICMS implicado llevará a cabo el desarrollo del catalizador desde la preparación de los catalizadores en polvo hasta su washcoating sobre soportes estructurados. CSIC participa como miembro del consorcio, participando la Universidad de Sevilla como entidad asociada.

STORMING will develop breakthrough and innovative structured reactors heated using renewable electricity, to convert fossil and renewable CH_4 into CO_2-free H_2 and highly valuable carbon nanomaterials for battery applications. More specifically, innovative Fe based catalysts, highly active and easily regenerable by waste-free processes, will be developed through a smart rational catalyst design protocol, which combines theoretical (Density Functional Theory and Molecular Dynamics Calculations) and experimental (cluster) studies, all of them assisted by in situ & operando characterisation and Machine Learning tools. The electrification (microwave or joule-heated) of structured reactors, designed by Computational Fluid Dynamics and prepared by 3D printing, will enable an accurate thermal control resulting in high energy efficiency. The project will validate, at TRL 5, the most promising catalytic technology (chosen considering technological, economic, and environmental assessments) to produce H_2 with energy efficiency (> 60%), net-zero emissions, and decreasing (ca. 10 %) the costs in comparison with the conventional process. The dissemination and communication of the results will boost the social acceptance of the H_2-related technologies and the stakeholder engagement targeting short-term process exploitation and deployment. The key to reach the challenging objectives of STORMING is the highly complementary and interdisciplinary consortium, where basic and applied science merge with engineering, computer and social sciences. The ICMS Group involved in the project will carry out the development of the catalyst from the preparation of powder catalysts to their washcoating on structured supports. CSIC participates as member of the consortium, with the University of Seville participating as an associated entity.

Valorización de CO_2 mediante procesos catalíticos y termofotocatalíticos: reducción de emisiones y obtención de metano y otros hidrocarburos ligeros

CO_2 recovery though catalytic and thermophotocatalytic processes: reduction of emissions and obtaining methane and other light hydrocarbons (CO2MET)

MINISTERIO DE CIENCIA E INNOVACIÓN

AGENCIA ESTATAL DE INVESTIGACIÓN

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2020-119946RB-I00	01-09-2021 31-08-2024	Ministerio de Ciencia e Innovación	181.500 €

Investigador Principal Research Head	Componentes Research Group
Alfonso Caballero Martínez Gerardo Colón Ibáñez	Juan Pedro Holgado Vázquez Rosa María Pereñíguez Rodríguez

RESUMEN / ABSTRACT

En este proyecto se llevarán a cabo diversos estudios y desarrollos relacionados con la reacción de hidrogenación de CO_2 para la producción de Gas Natural Sintético (GNS) e hidrocarburos ligeros. Así, la metanación y las denominadas reacciones modificadas de Fischer-Tropsch a olefinas (FTO) se están convirtiendo en procesos muy interesantes desde el punto de vista económico, energético y medioambiental. Por otra parte, el uso de hidrógeno verde como agente reductor, obtenido a su vez a partir de fuentes renovables, representa, además de la reducción de las emisiones de gases de efecto invernadero, una forma de almacenar la energía procedente de fuentes renovables, muchas de las cuales son intermitentes y, por tanto, difíciles de ajustar a las necesidades de consumo.

Con todo ello, este proyecto persigue un enfoque multicatalítico que comprende la termocatálisis y la fotocatálisis térmica con el fin de conseguir altos rendimientos, alta sostenibilidad y con los menores costes de producción, orientados en todo caso a una aplicación industrial final. Por otro lado, el desarrollo y optimización de los materiales catalíticos, considerando nuevos sistemas catalíticos heterogéneos basados en Ni, Fe, Co, Ru, Au, Pd entre otros metales, que han mostrado un gran potencial para estas reacciones de hidrogenación en los últimos años. En cuanto a los materiales catalíticos, se seleccionarán soportes micro y mesoporosos de composición variable (zeolitas, SBA-15, etc.), así como otros basados en óxidos y perovskitas ABO_3. Para ello se utilizarán una serie de técnicas de preparación recientemente descritas (cristalización por microondas, proceso de autocombustión, mesoestructuración por nanocasting y porosidad jerárquica) que permiten obtener sistemas de alta superficie específica y nanoestructura controlada. La combinación de diferentes elementos en las posiciones A y B de la estructura de la perovskita, que actúan tanto como promotores de sistemas catalíticos como precursores de aleaciones metálicas en sistemas catalíticos reducidos, permitirá obtener materiales con propiedades catalíticas sintonizables, muy variadas y versátiles.

This project will carry out various studies and developments related to the CO_2 hydrogenation reaction for Synthetic Natural Gas (SNG) and light hydrocarbons production. Thus, methanation and the so-called modified Fischer-Tropsch to olefins (FTO) reactions are becoming very interesting processes under an economic, energy and environmental point of view. Furthermore, the use of green hydrogen as a reducing agent, obtained in turn from renewable sources, represents, in addition to the reduction of greenhouse gas emissions, a way of storing energy from renewable sources, many of which are intermittent and therefore difficult to match with consumption needs.

With all this in mind, this project pursues a multi-catalytic approach comprising thermal-catalysis and thermal photocatalysis in order to achieve high performances, high sustainability and with the lowest costs of production, oriented in all case to a final industrial application. On the other hand, development and optimization of the catalytic materials, considering new heterogeneous catalytic systems based on Ni, Fe, Co, Ru, Au, Pd among other metals, which have shown great potential for this hydrogenation reactions in recent years. Regarding to the catalytic materials, micro and mesoporous supports of variable composition (zeolites, SBA-15, etc.) will be selected, as well as others based on oxides and ABO_3 perovskites. For this purpose, a series of recently described preparation techniques will be used (microwave crystallization, autocombustion process, mesostructuring by nanocasting and hierarchical porosity) that allow to obtain high specific surface systems and controlled nanostructure. The combination of different elements in positions A and B of the perovskite structure, which act both as promoters of catalytic systems and as precursors of metal alloys in reduced catalytic systems, will make it possible to obtain materials with tunable, highly varied and versatile catalytic properties.

Acido fórmico como vector de energía: de la biomasa al hidrógeno verde
Formic acid as energetic vector: from biomass to green hydrogen

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2020-113809RB-C32	01-09-2021 31-08-2024	Ministerio de Ciencia e Innovación	263.780 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El presente proyecto forma parte del proyecto coordinado ENERCATH2 que pretende integrar una estrategia que involucra múltiples reacciones para la producción y uso de hidrógeno verde a partir de la biomasa. El objetivo último es contribuir al desarrollo de tecnologías energéticas sostenibles que sustituyan a las actuales, derivadas de las fuentes fósiles. Específicamente, el proyecto del ICMS se centra en el uso del ácido fórmico como vector energético de hidrógeno, dado que es un compuesto químico líquido con una alta densidad gravimétrica de energía, que puede ser almacenado, transportado y manipulado de manera segura usando la infraestructura existente de distribución de hidrocarburos.

El objetivo principal del proyecto es la generación de ácido fórmico a partir de biomasa lignocelulósica y la posterior obtención de corrientes de hidrógeno a partir de éste. Para este fin, se pretenden desarrollar catalizadores novedosos, preferiblemente basados en carbones derivados de la biomasa y/o en metales de transición, no nobles, (V, Ni, Cu, Co, etc.), activos, selectivos y estables, para: i) la oxidación directa y selectiva de la biomasa lignocelulósica, e.g. glucosa, bien hacia la producción masiva de ácido fórmico, bien hacia la producción de una mezcla de ácido fórmico con otros co-productos, tales como el ácido levulínico, que pueden servir como punto de partida para la generación de productos plataforma de interés industrial, intermedios en la producción de combustibles y ii) la deshidrogenación de ácido fórmico, tanto en fase líquida como gaseosa, para la producción de corrientes de hidrógeno libres de CO.

Los catalizadores preparados serán caracterizados estructural y químicamente por una gran variedad de técnicas (DRX, XPS, SEM, HRTEM, Raman, DRIFTS, TPR/TPD, UV-Vis, Análisis textural), tanto pre- como post-reacción, para evaluar las posibles modificaciones ocurridas en el transcurso de la misma. Igualmente, se realizarán estudios en condiciones de reacción (in-situ y operando) por espectroscopias DRIFTS y ATR, lo que, junto con los resultados de actividad y de caracterización, permitirá analizar el mecanismo de las reacciones y así poder establecer la relación estructura-actividad en cada caso. El conocimiento de esta relación permitirá optimizar el catalizador diseñado y, en última instancia, cada proceso catalítico de producción de vectores sostenibles de energía propuesto en el proyecto.

This project is part of the ENERCATH2 coordinated project that aims to integrate a multi reaction catalytic strategy for green-hydrogen and energy related vectors production and use from biomass in order to contribute to the development of sustainable energy technologies that replace current ones derived from fossil sources. Specifically, ICMS project focuses on the production of formic acid as hydrogen related vector Formic acid is a liquid chemical compound with a high gravimetric energy density, which can be safely stored, transported and manipulated using existing hydrocarbon distribution infrastructure.

The main objective of the project is formic acid generation from lignocellulosic biomass and its subsequent dehydrogenation to green hydrogen. For this purpose, it will be intended to develop a series of novel catalysts, preferably based on biomass-derived carbons and/or on non-noble transition metals (V, Ni, Cu, Co, etc.), active, selective and stable for i) direct and selective oxidation of lignocellulosic biomass, using glucose as representing molecule, either towards the massive production of formic acid, or towards the production of a mixture of formic and co-product levulinic acid, which serves as a starting point for the generation of intermediate platform products and commodities of industrial interest in the production of fuels and polymers and for ii) the dehydrogenation of formic acid, both in liquid and gas phase, for the production of CO-free hydrogen streams.

After the stages of preparation-functionalization and reaction, the catalysts will be structurally and chemically characterized using a wide variety of techniques available by the whole consortium (XRD, XPS, SEM, HRTEM, Raman, DRIFTS, TPR/TPD, TGA, UV-Vis, Textural Analysis). These results, in addition to the in-situ/operando DRIFTS and ATR spectroscopic ones will give us fundamental information of the reaction mechanisms, allowing to establish structure-activity relationships for the studied reactions. The knowledge of these relationships will contribute to the understanding and optimization of the designed catalysts, and the catalytic process involved on the production of sustainable energy vectors proposed in the project.

Avanzando hacia la economía circular: Biocombustibles para el transporte pesado, a partir del reciclado de residuos (NICER BIOFUELS)

steppiNg towards Circular EConomy: REcycling bio-waste into heavy tRansport BIOFUELS (NICER-BIOFUELS)

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PLEC2021-008086	01-09-2021 31-08-2024	Ministerio de Ciencia e Innovación	278.900 €

Investigador Principal Research Head	Componentes Research Group
José Antonio Odriozola Gordón Tomás Ramírez Reina	María Isabel Domínguez Leal Laura Pastor Pérez

RESUMEN / ABSTRACT

Financiado por el programa RETOS-COLABORACION PUBLICO-PRIVADA del Ministerio de Ciencia e Innovación con fondos EU bajo el marco Next Generation Europe, NICER BIOFUELS es fruto de la colaboración entre las Universidades de Zaragoza y Sevilla y la multinacional URBASER. En el contexto de la economía circular y el desarrollo de combustibles sostenibles que permitan descarbonizar el transporte y avanzar hacia una sociedad libre de emisiones, NICER-BIOFUELS representa un paso adelante para combatir el cambio climático combinando ciencia fundamental e ingeniería aplicada.

NICER-BIOFUELS aims to create a unique knowledge infrastructure that supports the decentralised, sustainable and cost-efficient conversion of biowastes and textile residues to sustainable Heavy Transport Biofuels (HTB) to contribute towards full transport system decarbonisation. The project targets the development of disruptive technologies that overcome critical technological barriers, increase process efficiency and reduce marginal costs in the bio-waste to HTB conversion process. Following the spirit of circular economy, the overriding idea of NICER-BIOFUELS is to combine CO_2 emissions with bio-waste as a carbon pool to produce the next generation of HTB. Such an ambitious goal will be achieved by integrating advanced gasification strategies, unique catalytic technologies and digital tools to deliver fuel processors which are adaptable to feedstock input and HTB demands.

Conversión Avanzada de Biogas a Ácido Acético: Soluciones Catalíticas para una Sociedad con Bajas Emisiones de Carbono

ADVanced convErsioN of biogas To acetic acid: catalytic solUtions for a low caRbon sociEty (ADVENTURE)

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2019-108502RJ-100	01-10-2020 30-09-2023	Ministerio de Ciencia e Innovación	170.080 €

Investigador Principal Research Head
Laura Pastor Pérez

RESUMEN / ABSTRACT

En ADVENTURE se presenta un nuevo concepto para convertir biogás, procedente de desechos orgánicos, en productos químicos de alto valor industrial, como es el ácido acético (AA), de una manera tanto amigable con el medio ambiente como viable económicamente. El AA se emplea

como precursor de muchos productos procedentes de la química fina, con numerosas aplicaciones, como son la fabricación de pinturas y recubrimientos, la producción de plásticos y adhesivos basados en agua, entre muchos otros, siendo una molécula plataforma muy versátil para la industria química. Tradicionalmente el AA se produce a escala comercial a través de una ruta indirecta produciendo una considerable huella global de CO_2. Por ello, el objetivo principal de ADVENTURE es rediseñar el proceso de producción de AA introduciendo biogás como principal materia prima - un enfoque completamente nuevo que provoca una sinergia entre la utilización de CO_2 y la síntesis de química fina.

En este contexto AVENTURE abordará tres desafíos principales: (i) un desafío global: las preocupaciones ambientales asociadas con la emisión de gases de efecto invernadero; (ii) una oportunidad industrial: abordará el problema de la sostenibilidad económica de la industria del biogás ofreciendo alternativas viables para la conversión de materia prima de bajo valor en bioquímicos de alto valor añadido a escala industrial; y (iii) un desafío a escala científica fundamental: se presentan dos propuestas, la intensificación de una ruta indirecta usando reactores de microcanales y una ruta directa llevada a cabo con catálisis por plasma. Para lograr estos ambiciosos objetivos, se diseñará una nueva generación de catalizadores avanzados multifuncionales capaces de proporcionar los productos específicos deseados con alta actividad, selectividad y durabilidad a largo plazo para garantizar el éxito de ADVENTURE.

ADVENTURE represents a new concept to convert biogas from organic waste into high-value industrial chemicals such as acetic acid (AA) in an environmentally and economically viable manner. AA is a precursor for many fine chemical compounds with a wide range of applications including paints and coatings manufacturing, plastics and water-based adhesives production among many others, representing a very versatile platform molecule for the chemical industry. Traditionally, AA is produced at a commercial scale through an indirect route with a considerable global CO_2 footprint. In this regard, the main target of ADVENTURE is to re-design the AA production route introducing biogas as initial feedstock - a completely new approach that synergises CO_2 utilisation with fine chemicals synthesis.

In this context, ADVENTURE will tackle three main challenges: (i) A global challenge the environmental concerns associated with the emission of Greenhouse Gases (GHG); (ii) An industrial opportunity the problem of economic sustainability of the biogas industry by offering viable pathways for conversion of low-value feedstock into added-value biochemicals at industrial scale; and (iii) A fundamental scientific challenge the inexistence of AA production from biogas, by introducing two new revolutionary routes for AA production: an intensified indirect route using microchannel reactors and a direct route enabled by plasma catalysis. In order to accomplish these ambitious goals, a new generation of advanced multifunctional catalysts able to deliver the targeted products with high activity, selectivity and long-term durability will be designed to guarantee the success ADVENTURE.

Desarrollo de materiales heteroestructurados basados en biocarbones con propiedades fotofuncionales para aplicaciones en procesos de descontaminación de aguas y desinfección Development of biochar based heterostructured materials with photofuntional properties for applications in water decontamination and disinfection processes

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2021-122413NB-I00	01-09-2022 31-08-2025	Ministerio de Ciencia e Innovación	145.200 €

Investigador Principal Research Head	Componentes Research Group
María del Carmen Hidalgo López Francisca Romero Sarria	José Manuel Córdoba Gallego Concepción Real Pérez María Dolores Alcalá González José Antonio Navío Santos Rosa Mosteo Abad (UNIZAR)

RESUMEN / ABSTRACT

En el presente proyecto de investigación se propone el desarrollo de sistemas fotocatalíticos heteroestructurados ($ZnWO_4/ZnO$, $WO_3/AgBr$, WO_3/TiO_2, Bi_2WO_6/TiO_2, $ZnBi_2O_4/ZnO$, BixTiyOz) acoplados o soportados sobre biocarbones (procedentes de la pirólisis de restos de poda de olivo, cascarilla de arroz y hueso de aceituna y que permiten una vía de revalorización de estos residuos), el estudio de las diferentes variables y métodos de síntesis, su optimización, y su comportamiento fotocatalítico evaluado en la desinfección de aguas y eliminación de contaminantes emergentes. En los últimos años se han estudiado nuevos fotocatalizadores basados en materiales heteroestructurados, donde se desarrollan heterouniones de semiconductores para conseguir una mejor separación espacial de electrones y huecos fotogenerados, obteniendo mayores tiempos de vida de estos portadores, aumentando así la eficiencia de los sistemas. Aunque estos materiales han mostrado buena actividad fotocatalítica en diferentes sustratos estudiados, generalmente presentan valores de superficie específica moderados o bajos, y algunos tienen problemas de estabilidad tras pocos ciclos de reacción.

El proyecto propone el acoplamiento o soporte de estos fotocatalizadores heteroestructurados con biocarbones de diferentes características, con el objetivo de dotarlos de mayor área superficial y aumentar su eficacia y estabilidad para sus aplicaciones como fotocatalizadores; mejorando la capacidad de absorción, estrechando el band-gap donde el biocarbón puede actuar como fotosensibilizador, mejorando el transporte de electrones, permitiendo una mejor separación de los portadores fotogenerados prolongando su vida útil y proporcionando estabilización y fotoestabilización a los sistemas.

Los biocarbones son materiales ricos en carbono que se obtienen mediante la calcinación de la biomasa en ausencia de oxígeno (pirólisis) y presentan interesantes propiedades, como gran área superficial y alta porosidad, y pueden ser modulados, mediante el control de las condiciones de operación, para obtener la cantidad y el tipo de grupos funcionales deseados en la superficie, hidrofobicidad o hidrofilicidad o diferentes pH superficial.

Los objetivos del proyecto incluyen la caracterización físico-química completa y la optimización de los fotocatalizadores heteroestructurados/biocarbón para las aplicaciones propuestas bajo diferentes condiciones de operación, como iluminación solar o visible. Se evaluará la eficacia de cada sistema en la eliminación de contaminantes emergentes (antibióticos) y en la inactivación de microorganismos potencialmente patógenos habitualmente presentes en aguas.

La presencia de microorganismos patógenos en las aguas es un tema de especial preocupación debido al riesgo potencial de transmisión de enfermedades y, en consecuencia, es necesario el control microbiano en las aguas. Asimismo, los productos farmacéuticos y de higiene son ampliamente usados hoy en día, llegando hasta las aguas. Sus potenciales efectos adversos sobre la salud humana han llevado a catalogarlos como contaminantes ambientales relevantes de la clase de contaminantes emergentes El proyecto se aborda desde un punto de vista interdisciplinar y en el contexto de la economía circular, revalorizando un residuo (biomasa) para desarrollar fotocatalizadores que den solución a un problema (descontaminación y desinfección de aguas) mediante procesos respetuosos con el medio ambiente (fotocatálisis heterogénea).

In the present research project we propose the development heterostructured photocatalyst systems ($ZnWO_4/ZnO$, $WO_3/AgBr$, WO_3/TiO_2, Bi_2WO_6/TiO_2, $ZnBi_2O_4/ZnO$, $Bi_4Ti_3O_{12}/Bi_{20}TiO_{32}$) coupled or supported on biochars (coming from the pyrolysis of olive pruning waste, rice husk and olive stones and allowing a path of revalorization of these wastes), the study of the different synthesis variables and methods, their optimization, and their photocatalytic behavior evaluated in the disinfection of water and degradation of emerging pollutants.

In the last years, new photocatalysts based on heterostructured materials are arising, where semiconductor heterojunctions have been developed to achieve the spatial separation of electrons and holes providing appropriate separation pathways, thus obtaining benefits for prolonged charge carriers lifetime, broadening light absorption and increasing the efficiency of the system. Although these materials have shown good behavior in the visible on the different substrates studied, they generally present moderate or low specific surface area values, and some of them have stability problems after few reaction cycles.

The project proposes the coupling or support of these heterostructured photocatalysts on biochar of different characteristics, with the aim of providing them with higher specific surface areas and increase their effectiveness and stability for their applications as photocatalysts, improving the absorption ability, narrowing the bad-gap where the biochar can act as photosensitizer, improving the electron transport, allowing a better separation of photogenerated carriers and prolonging their lifetime and providing stabilization and photo-stabilization to the systems.

Biochars are carbon-rich materials obtained by thermal treatment of biomass in the absence of oxygen (pyrolysis) and show interesting properties such as high specific surface areas and porosities, and can be tailored by controlling operating conditions, to obtained desired amount and type of functional groups on their surfaces, hydrophobicity or hydrophilicity and surface pH.

The main objectives of the project involve full physico-chemical characterization and optimization of biochar/ heterostructured photocatalysts for the proposed applications under different operation conditions, as solar or visible illumination. The effectiveness of each system in the reduction of emerging contaminants (antibiotic products) and in the inactivation of potentially pathogenic microorganisms usually present in water will be evaluated.

The presence of pathogenic microorganisms in waters is an issue of special concern due to the potential risk of waterborne diseases, and consequently, microbial control is necessary in waters. Likewise, pharmaceuticals and personal care products are commonly used and release to waters. Their potential adverse effects on human health, led to cataloguing them as relevant environmental contaminants belonging to the class of emerging contaminants.

The project is approached from an interdisciplinary point of view and in the context of the circular economy, by revalorizing a waste product (biomass) to develop photocatalysts that provide a solution to a problem (decontamination and disinfection of water) by means of environmentally friendly processes (heterogeneous photocatalysis).

DiSeño de catalizadores Multifuncionales para la conversión de gAs de síntesis Rico en CO_2 en combusTibles líquidos sostenibles, en una única etapa, vía síntesis de FTS y HCR: SMART-FTS

DeSign of Multifunctional cAtalysts foR one poT sustainable fuel synthesis from CO_2-rich syngas via hybrid Fischer-TropSch/Hydrocracking processes · SMART-FTS

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2021-126876OB-I00	01-09-2022 31-08-2025	Ministerio de Ciencia e Innovación	272.250 €

Investigador Principal Research Head	Componentes Research Group
José Antonio Odriozola Gordón Tomás Ramírez Reina	Luis F. Bobadilla Baladrón Anna Dimitrova Penkova Francisco Manuel Baena Moreno José Rubén Blay Roger Nuria García Moncada Miriam González Castaño Ligia Amelia Luque Álvarez

RESUMEN / ABSTRACT

Siguiendo las indicaciones de los Objetivos de Desarrollo Sostenible de las Naciones Unidas (UNSDG), es obligatorio tomar acción al respecto buscando alternativas de energía limpia y asequible (objetivo 7) para favorecer ciudades y comunidades sostenibles (objetivo 11) mientras se mitiga el cambio climático. cambio (objetivo 13). De hecho, Horizon Europe da prioridad a las tecnologías bajas y cero emisiones de carbono como objetivos clave para la próxima generación de Europa. Sobre la base

de estas premisas, la biomasa, y en particular los residuos de biomasa, representan un prometedor sustituto de los combustibles fósiles y una excelente materia prima para la fabricación de combustibles bajos en carbono. Durante su breve ciclo de vida, todo el carbono de la biomasa proviene de la atmósfera y el suelo y se libera al medio ambiente cuando se quema. Por lo tanto, la biomasa se considera un combustible neutro en carbono. Además, los combustibles derivados de biomasa son hidrocarburos de alta densidad energética que son ideales para vehículos de aviación, marítimos y pesados, a diferencia de las baterías y los dispositivos electroquímicos, que son adecuados para aplicaciones más ligeras y, por lo tanto, complementarios de los biocombustibles. En pocas palabras, no podemos hacer volar un avión con baterías durante largas distancias, pero podemos alimentarlo con biocombustibles sostenibles. Por lo tanto, los biocombustibles de biomasa están destinados a desempeñar un papel clave en la descarbonización del sector del transporte. Además, ofrecer una segunda vida a los biorresiduos es crucial para algunas comunidades (es decir, la agricultura y el sector agrícola) cuyos horizontes de mercado pueden expandirse convirtiendo un "residuo" problemático en "precursores de biocombustibles" rentables. En este sentido, SMART-FTS trae conceptos disruptivos sobre la producción de biocombustibles a partir de bio-syngas para impulsar la descarbonización del transporte en armonía con la estrategia de economía circular.

Following the directions of the United Nations Sustainable Development Goals (UNSDG), it is mandatory to take action on this by pursuing affordable and clean energy alternatives (goal 7) to favour sustainable cities and communities (goal 11) while mitigating climate change (goal 13). Indeed, Horizon Europe prioritises low and zero carbon technologies as key objectives for next generation Europe. Based on these premises, biomass, and in particular biomass residues, represent a promising substitute for fossil fuels and an excellent feedstock for low-carbon fuels manufacturing. During its short life cycle, all carbon in biomass comes from the atmosphere and soil and is liberated into the environment when it is burned. Therefore, biomass is considered a carbon-neutral fuel. In addition, biomass-derived fuels are high energy density hydrocarbons which are ideal for aviation, maritime and heavy-duty vehicles in contrast to batteries and electrochemical devices which are suitable for lighter applications and hence complementary to biofuels. In plain words we cannot fly an aircraft on batteries for long distances, but we can power it with sustainable biofuels. Hence biofuels from biomass are meant to play a key role in decarbonising the transport sector. Furthermore, offering a second life to bio-residues is crucial for some communities (i.e. farming and agri-sector) whose market horizons can be expanded by turning a problem “waste” into a profitable “biofuel precursors”. Herein, SMART-FTS is bringing disruptive concepts on biofuel production from bio-syngas to push forward transport decarbonisation in harmony with the circular economy strategy.

Diseño de fotocatalizadores altamente eficientes mediante control de la nanoescala para la producción de H2 · NanoLight2H2

Design of highly efficient photocatalysts by nanoscale control for H2 production · NanoLight2H2

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P20-00156	05-10-2021 30-06-2023	Junta de Andalucía	85.000 €

Investigador Principal Research Head	Componentes Research Group
Gerardo Colón Ibáñez	Alfonso Caballero Martínez Rosa Pereñiguez Rodríguez Juan Pedro Holgado Vázquez

RESUMEN / ABSTRACT

El objetivo principal de este proyecto es el desarrollo de catalizadores heteroestructurados basados en óxidos semiconductores altamente eficientes (Nb_2O_5, WO_3, TiO_2 y Fe_2O_3) y g-C_3N_4, con control a nivel de la nanoescala, y potencial aplicación en la reacción de fotoreformado de alcoholes para la producción de H_2. Así mismo, se pretende estudiar la optimización del proceso catalítico mediante una aproximación multi-catalítica, mediante la combinación de termocatálisis y fotocatálisis. La producción fotocatalítica de H_2 una reacción de gran interés desde el punto de vista energético mediante el uso de una tecnología limpia y sostenible como la fotocatálisis. En este proyecto se pretende el desarrollo de sistemas altamente eficientes para la producción de hidrógeno. Se prestará especial atención al diseño de heteroestructuras que permitan la optimización del proceso fotoinducido. De igual modo se incidirá en el uso de co-catalizadores alternativos a los tradicionales metales nobles; sistemas basados en metales de transición (Cu, Co, Ni), así como estructuras bimetálicas con metales nobles formando aleaciones o core-shell. Junto al proceso fotocatalítico en fase líquida, se estudiará la viabilidad de un proceso de fotoreformado en fase gas, basándonos en recientes estudios que ponen de manifiesto el efecto sinérgico de una aproximación foto-termo catalítica en estos procesos. De esta forma esta propuesta pretende abordar de forma ambiciosa el aumento de la eficiencia del proceso fotocatalítico a fin de poder plantear esta tecnología a mayor escala. En este sentido, además de los estudios de optimización de los catalizadores y del proceso fotocatalítico, se afrontará como algo primordial su escalado a planta solar piloto.

The main objective of this project is the development of heterostructured catalysts based on highly efficient semiconducting oxides (Nb_2O_5, WO_3, TiO_2 and Fe_2O_3) and g-C_3N_4, with control at the nanoscale level, and potential application in the photoreforming reaction of alcohols for the production

of H_2. Furthermore, the aim of this project is to study the optimisation of the catalytic process by means of a multi-catalytic approach, combining thermocatalysis and photocatalysis. The photocatalytic production of H_2 is a reaction of great interest from an energetic point of view through the use of a clean and sustainable technology such as photocatalysis. We will try to develop highly efficient systems for hydrogen production. Special attention will be paid to the design of heterostructures that allow the optimisation of the photoinduced process. Likewise, emphasis will be placed on the use of alternative co-catalysts to the traditional noble metals; systems based on transition metals (Cu, Co, Ni), as well as bimetallic structures with noble metals formed into alloys or core-shell. Together with the liquid phase photocatalytic process, the feasibility of a gas phase photoreforming process will be studied, based on recent studies that show the synergistic effect of a photo-thermo-catalytic approach in these processes. In this way, this proposal aims to ambitiously address the increase in efficiency of the photocatalytic process in order to be able to consider this technology on a larger scale. In this sense, in addition to the optimisation studies of the catalysts and the photocatalytic process, its scaling up to a pilot solar plant will be considered as essential.

Diseño de catalizadores avanzados para procesos de HDO: una apuesta revolucionaria para la conversión de biomasa: CLEVER-BIO

Design of advanced CataLyst for H2-free hydrodeoxygenation - a rEVolutionary approach Enabling pRactical BIOmass upgrading: CLEVER-BIO

Junta de Andalucía

Unión Europea
Fondo Europeo de Desarrollo Regional

Andalucía se mueve con Europa

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P20-00667	05-10-2021 31-01-2022	Junta de Andalucía	49.612 €

Investigador Principal Research Head	Componentes Research Group
Tomás Ramírez Reina	Luis Francisco Bobadilla Baladrón José Antonio Odriozola Gordón Laura Pastor Pérez Anna Dimitrova Penkova

RESUMEN / ABSTRACT

CLEVER-BIO propone un concepto revolucionario para la producción de biocombustibles limitando la emisión de gases de efecto invernadero sembrando las bases de una tecnología verde: conversión de residuos a combustibles y productos de alto valor. La idea central de CLEVER-BIO es el desarrollo de catalizadores avanzados para llevar a cabo la reacción de HDO de bio-aceites derivados de

lignina. El proyecto se llevará a cabo en 24 meses y comprende un programa intenso de investigación multidisciplinar con fuerte participación de instituciones internacionales.

CLEVER-BIO proposes a revolutionary approach to synergise bio-oil upgrading and Green House Gases (GHG) emissions abatement, setting the grounds for a sustainable chemical technology: waste to fuels/chemicals. We aim to develop novel biomass-derived routes to produce deoxygenated aromatic hydrocarbons – highly important chemical compounds in the biofuels and biochemical industries – from lignin-derived bio-oil via designing of advanced catalysts for the H_2-free hydrodeoxygenation (HDO) process. The urgent problem of global warming and the need to decarbonise the transportation and chemical industry in a circular economy context place CLEVER-BIO in a privileged position to become a pioneering approach to contribute towards the development of sustainable societies. CLEVER-BIO will be delivered in 24 months under a comprehensive research program with strong international cooperation and social-scientific impact.

Integración de Energía y Gasificación para procesos sostenibles · GENIUS
Gasification and ENergy Integration for User Sustainability · GENIUS

Junta de Andalucía

Unión Europea
Fondo Europeo de Desarrollo Regional

Andalucía se mueve con Europa

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P20-00594	05-10-2021 31-01-2022	Junta de Andalucía	49.500 €

Investigador Principal Research Head	Componentes Research Group
José Antonio Odriozola Gordón	Luis F. Bobadilla Baladrón Laura Pastor Pérez Anna Dimitrova Penkova Tomás Ramírez Reina

RESUMEN / ABSTRACT

GENIUS representa una propuesta innovadora para la conversión de bio-residuos en vectores energéticos sostenibles. El proyecto propone la combinación de tecnologías maduras como la gasificación y reformado acuoso para aportar soluciones catalíticas al proceso de conversión de bioresiduos. GENIUS desarrollará reactores de microcanales que permiten el diseño de plantas compactas para el procesado de residuos lo que facilita su implementación en aplicaciones deslocalizadas como por ejemplo explotaciones agrícolas donde los residuos pueden convertirse en productos de valor añadido.

GENIUS proposes an innovative approach to transform biogenic residues into a valuable bioenergy carrier. The proposal is based on the combination of modified mature technologies, e.g. gasification, with first-time approached solutions as the continuous aqueous-phase reforming of tars that compromises downstream processes, usually the bottlenecks for upgrading catalytic processes.

The combination of microchannel reactor technologies with state-of-the-art multifunctional catalysts will provide a path to increase the wealth of rural communities on proposing a decentralized approach allowing territory-based solutions for agricultural residues or marginal lands production.

GENIUS focus in the system perspective demanded in HORIZON EUROPE keeping in mind the Objectives for Sustainable Development and industry decarbonisation. GENIUS will be delivered in 24 months under a comprehensive research program with strong international cooperation and social-scientific impact.

OTROS PROYECTOS / OTHER PROJECTS

Aplicaciones de Procesos Avanzados de desinfección de aguas con nanomateriales, para la reducción del impacto procedente de presiones urbanas, en el marco de la economía circular

Código/Code:	TED2021-129267B-I00
Periodo/Period:	01-12-2022 / 30-11-2024
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Investigador responsable/Research head:	Rosa Mosteo Abad (UNIZAR) / Mª Peña Ormad Melero (UNIZAR)
Participantes del ICMS como investigador:	María Carmen Hidalgo López (ICMS), Francisca Romero Sarria (ICMS)

Hacia la transición digital en Química Solar (SolarChem5.0): Fotorreactores

Código/Code:	TED2021-130173B-C43
Periodo/Period:	01-12-2022 / 30-11-2024
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Investigador responsable/Research head:	Sixto Malato Rodríguez (PSA-CIEMAT) / Diego C. Alarcón Padilla (PSA-CIEMAT)
Participante del ICMS como investigador:	Gerardo Colón Ibáñez

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Desarrollo de catalizadores para procesos de metanación

Periodo/Period:	27-07-2022 / 26-07-2023
Organismo Financiador/Financial source:	Asociación de Investigación y Cooperación Industrial de Andalucia
Investigador responsable/Research head:	Tomás Ramírez Reina

Estudio de materiales catalíticos para pilas de combustible SOFC
Periodo/Period: 2-03-2022 / 1-03-2023
Organismo Financiador/Financial source: CERES Power Ltd
Investigador responsable/Research head: Tomás Ramírez Reina

Desarrollo de catalizadores para reformado de biogas
Periodo/Period: 26-01-2023 / 25-01-2024
Organismo Financiador/Financial source: UKICC Accelerator
Investigador responsable/Research head: Tomás Ramírez Reina

Desarrollo de catalizadores avanzados para RWGS
Periodo/Period: 17-07-2023 / 16-07-2024
Organismo Financiador/Financial source: Compañía Española de Petróleos, S.A. (CEPSA)
Investigador responsable/Research head: José Antonio Odriozola Gordón

Evaluación de tecnologías catalíticas para aplicaciones energéticas
Periodo/Period: 1-10-2023 / 30-09-2024
Organismo Financiador/Financial source: UKIIC Acceleratos limited
Investigador responsable/Research head: Tomás Ramírez Reina

Testing and physicochemical characterisation of heterogeneous catalysts for GREENX TECHNOLOGY
Periodo/Period: 4-10-2023 / 3-10-2025
Organismo Financiador/Financial source: GREENX TECHNOLOGY LTD
Investigador responsable/Research head: Tomás Ramírez Reina

Estudio de la composición de una muestra de vidrio
Periodo/Period: 25-05-2021 / 25-05-2025
Organismo Financiador/Financial source: AMC Innova Juice and Drinks, S.L.
Investigador responsable/Research head: Alfonso Caballero Martínez

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Scalable synthesis of 2D Ti_2CT_x MXene and molybdenum disulfide composites with excellent microwave absorbing performance

Miao, BJ; Cao, YE; Zhu, QS; Nawaz, MA; Ordiozola, JA; Reina, TR; Bai, ZM; Ren, JN; Wei, FC
Advanced Composites and Hybrid Materials, **6** (2023) 61
Abril, 2023 · DOI: 10.1007/s42114-023-00643-2

The signal crosstalk and electromagnetic interference (EMI) problems direly need to be resolved in the rapid development of modern microwave communication technology for a better working frequency and transmission power of electronic systems. Where the new absorbing materials such as molybdenum disulfide (MoS_2)/titania (TiO_2)/Ti_2CT_x and MoS_2/Ti_2CT_x composites could meet the requirement of "thin, strong, light weight, and wide band" for excellent absorbing performance. In this work, a lighter Ti_2CT_x material was selected as the matrix, and MoS_2 was in-situ grown on Ti_2CT_x matrix by traditional hydrothermal method and microwave solvothermal method. The fabricated composite exhibited synergic effect of two-dimensional heterostructural interface and double dielectric elements, where a small amount of TiO_2 and a certain proportion of MoS_2 jointly improve the impedance matching of the composite material. In here, the extreme reflection loss (RLmin) can reach - 54.70 dB (with a frequency of 7.59 GHz, 3.39 mm thickness), and the maximum effective absorption bandwidth (EAB(max)) can reach 4 GHz. Polyethylene glycol 200 was used as the solvent instead of water to make Ti_2CT_x less oxidized during the composite process, where the microwave heating would attain fast speed, short time, high efficiency, and uniform product. Since, the MoS_2/Ti_2CT_x composite without oxidizing possessed a wider effective absorption bandwidth (EAB) at a thinner thickness, thus resulting in the excellent microwave absorption performance and confirming the validity and rationality of new microwave absorption materials.

Alkane metathesis over immobilized pincer-ligated iridium complexes: Effect of support nature

Megías-Sayago, C; Centeno-Vega, I; Bobadilla, LF; Ivanova, S; Rendon, N; Suarez, A
Applied Catalysis B-Environmental, **338** (2023) 123002
Diciembre, 2023 · DOI: 10.1016/j.apcatb.2023.123002

In this work, catalytic alkane metathesis has been evaluated as a suitable approach to upcycle hydrocarbons (polyolefins) at moderate temperatures. To this end, a pincer-ligated iridium complex (dehydrogenation catalyst) has been combined with a rhenium-based (metathesis) catalyst, being the effect of immobilizing the Ir complex over different supports deeply investigated. FTIR spectroscopy has been used to confirm the complex grafting and to elucidate the anchoring site to the support. Additionally, the supports have been dehydroxylated at different conditions to evaluate its possible impact in both the complex grafting and the catalytic activity. The influence of the support nature and its participation in the catalytic reaction have been clearly evidenced.

Process design and utilisation strategy for CO_2 capture in flue gases. Technical assessment and preliminary economic approach for steel mills

Navarro, JC; Baena-Moreno, FM; Centeno, MA; Laguna, OH; Almagro, JF; Odriozola, JA
Renewable & Sustainable Energy Reviews, **184** (2023) 113537
Septiembre, 2023 · DOI: 10.1016/j.rser.2023.113537

The steel industry is the most relevant sector in emerging economies due to its application in numerous fields. However, steel manufacturing involves large energy investment and produces significant greenhouse gas emissions. The current world economic and environmental scenario therefore necessitates that improvements in the footprint of the steel industry be made without affecting its viability. Considering the present challenge, we report two possible processes for Carbon Capture and Utilization (CCU). The first process is the competitive capture of CO_2-SO_2, followed by CO_2 valorisation to methane. However, the CO_2 capture capacity and lifetime for the adsorbent after multiple cycles could be improved through preliminary desulphurization of the gas current. The improved system demonstrates net profitability in a typical stainless steel plant. Therefore, it can be implemented in an industrial setting without profitability loss to steelmaking operations, fulfilling bot the goal of reducing CO_2 emissions while protecting the mainstay of the plant.

Hydrogen production by catalytic aqueous-phase reforming of waste biomass: a review

González-Arias, J; Zhang, Z; Reina, TR; Odriozola, JA
Environmental Chemistry Letters, **21** (2023) 3089-3104
Agosto, 2023 · DOI: 10.1007/s10311-023-01643-w

The rising adverse effects of climate change call for a rapid shift to low-carbon energy and reducing our dependence on fossil fuels. For that, biorefineries appear as promising alternatives to produce energy, chemicals, and fuels using biomass and waste as raw materials. Here, we review catalytic aqueous-phase reforming to convert biomass and organic waste carbohydrates into renewable hydrogen, with focus on reforming basics; catalyst design; reforming of model compounds, wastewater and biomass; economics and life cycle assessment. We found that platinum and palladium are technically highly effective, yet their high price may limit upscaling. Alternatively, addition of tin to nickel gives acceptable results and improves hydrogen selectivity from 35 to 90%. We observed that hydrogen production decreases from 14% for crude glycerol to 2% for pure glycerol, thus highlighting the need to do experiments with real wastewater. The rare experiments on real wastewater from brewery, juice, tuna, and cheese industries have given hydrogen production rates of up to 149.7 mg/L. Aqueous-phase reforming could be shortly competitive with prices around 3-6 USD per kg of hydrogen, which are nearing the current market prices of 2-3 USD per kg.

Low CO_2 hydrogen streams production from formic acid through control of the reaction pH

Santos, JL; López, ER; Ivanova, S; Monzon, A; Centeno, MA; Odriozola, JA
Chemical Engineering Journal, **455** (2023) 140645
Febrero, 2023 · DOI: 10.1016/j.cej.2022.140645

There are multiple factors that influence the catalyst performance in the reaction of formic acid dehydrogena-tion: the nature of catalyst and/or support, the used solvent and reaction variables such as temperature, time, formic acid concentration, presence/absence of formates and pH of the solution. This work evaluates a series of important parameters like the influence of the pH by itself, the influence of the nature of used alkali agents and the effect of direct formate addition as reactive on hydrogen production via formic acid dehydrogenation over a commercially available catalyst. The catalytic performance appears to depend on the ionic radius of the cations of the used base which reflects consequently

on the hydrogen selectivity. The best base to be used must have lower hydrated cationic radii and a starting pH around 4 to achieve important hydrogen selectivity for medium term formic acid conversion.

Catalytic conversion of syngas to light hydrocarbons via simulated intermediates $CO/CO_2/DME/N_2/H_2$ over the regulated acidity of SAPO-34

Meng, FH; Wang, LA; Nawaz, MA; Wang, Q; Gong, ZY; Li, Z
Chemical Engineering Journal, **474** (2023) 145895
Octubre, 2023 · DOI: 10.1016/j.cej.2023.145895

Direct conversion of syngas to light hydrocarbons has been intensively studied in recent years; however, the high selectivity of light hydrocarbons is still a challenging task to achieve a high CO conversion. Here, a bifunctional catalyst consisting of a methanol synthesis catalyst (CZA) and a methanol to dimethyl ether (DME) catalyst (Al_2O_3) was employed with a hydrocarbon synthesis catalyst (SAPO-34), for syngas conversion to light hydrocarbons in a dual fixed-bed reactor. The conversion of simulated intermediates $CO/CO_2/DME/N_2/H_2$ with a molar ratio of 9/6/4/5/76, obtained from syngas conversion to DME over CZA and Al_2O_3, was studied over SAPO-34 zeolites. It was found that SP34-0.1 with Si/Al ratio of 0.1, exhibited low amount of strong acid (0.60 mmol/g) and high selectivity to light olefins (74.1%), while SP34-0.4 with Si/Al ratio of 0.4 exhibited high amount of strong acid (1.00 mmol/g) leading to high selectivity of light paraffins (88.4%). The in-situ DRIFTS analysis illustrated that DME can be rapidly adsorbed on the hydroxyl site of SAPO-34 and decomposed into the surface methyl species, where SP34-0.4 could produce more dimethylcyclopentenyl cationic species than SP340.1. It was suggested that the overall reaction route led to a high selectivity to light olefins (84.2%) with a CO conversion of 61.2% on (CZA + Al_2O_3) catalyst combined with SP34-0.1, while a high selectivity to light paraffins (76.3%) could be achieved by combining with SP34-0.4 at 70.3% CO conversion. Since, the current study interprets that the selectivity of hydrocarbons can be adjusted by regulating the acidity of SAPO-34 to achieve a high CO conversion in the dual fixed-bed reactor scheme.

The Need for Flexible Chemical Synthesis and How Dual-Function Materials Can Pave the Way

Merkouri, LP; Paksoy, AI; Reina, TR; Duyar, MS
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Mayo, 2023 · DOI: 10.1021/acscatal.3c00880

Since climate change keeps escalating, it is imperative that the increasing CO_2 emissions be combated. Over recent years,research efforts have been aiming for the design and optimization of materials for CO_2 capture and conversion to enable a circular economy. The uncertainties in the energy sector and the variation sin supply and demand place an additional burden on the commercialization and implementation of these carbon capture and utilization technologies.Therefore, the scientific community needs to think out of the box if it is to find solutions to mitigate the effects of climate change. Flexible chemical synthesis can pave the way for tackling market uncertainties.The materials for flexible chemical synthesis function under a dynamic operation, and thus, they need to be studied as such. Dual-function-materials are an emerging group of dynamic catalytic materials that integrate the CO_2 capture and conversion steps. Hence, they can be used to allow some flexibility in the production of chemicalsas a response to the changing energy sector. This Perspective highlights the necessity of flexible chemical synthesis by focusing on understanding the catalytic characteristics under a dynamic operation and by discussing the requirements for the optimization of materials at the nanoscale.

Enroute to the Carbon-Neutrality Goals via the Targeted Development of Ammonia as a Potential Nitrogen-Based Energy Carrier

Nawaz, MA; Blay-Roger, R; Saif, M; Meng, FH; González-Arias, J; Miao, BJ; Bobadilla, LF; Ramírez-Reina, T; Odriozola, J.A.

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The reliance of a future carbon-free horizon is strongly aligned with the long-term energy storage avenues which are completely derived from renewable energy resources. Ammonia with its high energy content and density can perform as a decent candidate for buffering the short-term storage options. However, the current NH_3 production majorly feeding the current huge desire for ammonia is dominated by the conventional nonrenewable Haber–Bosch (H–B) process route, thus continuously damaging the target of carbon neutrality goals. High-purity hydrogen (H_2) gas is an essential precursor for the H–B process; however, it is a significant energy consumer (about 2% of the global energy supply) and contributes over 420 million tons of CO_2/annum. Therefore, the research on the renewable synthesis of nitrogen-based energy carriers (such as ammonia) from the direct electrochemical, photocatalytic, or plasma catalytic processes; its conversion; and utilization to the potential derivatives has been a hot topic in the past few decades. A prospective analysis of the highly appealing processes has been summarized in this study, which could facilitate the adaption of renewable alternatives as an effective approach for zero carbon emission, paving the excellent pathways along the road to the development of nitrogen-based energy technologies, especially the targeted development of ammonia. Further, this Review covers the current and future impacts of the H–B process, the development of aspiring ammonia synthesis routes (via electro, photo, bio, chemical loop, or plasma catalysis), and its conversion and utilization to the renewable derivatives in terms of fabrication of model catalysts, advanced characterization technology, and efficient device design.

Are Ni/ and Ni_5Fe_1/biochar catalysts suitable for synthetic natural gas production? A comparison with γ-Al_2O_3 supported catalysts

González-Castaño, M; Morales, C; de Miguel, JCN; Boelte, JH; Klepel, O; Flege, JI; Arellano-Garcia, H

Green Energy & Environment, **8** (2023) 744-756
Junio, 2023 · DOI: 10.1016/j.gee.2021.05.007

Among challenges implicit in the transition to the post-fossil fuel energetic model, the finite amount of resources available for the technological implementation of CO_2 revalorizing processes arises as a central issue. The development of fully renewable catalytic systems with easier metal recovery strategies would promote the viability and sustainability of synthetic natural gas production circular routes. Taking Ni and NiFe catalysts supported over γ-Al_2O_3 oxide as reference materials, this work evaluates the potentiality of Ni and NiFe supported biochar catalysts for CO_2 methanation. The development of competitive biochar catalysts was found dependent on the creation of basic sites on the catalyst surface. Displaying lower Turn Over Frequencies than Ni/Al catalyst, the absence of basic sites achieved over Ni/C catalyst was related to the depleted catalyst performances. For NiFe catalysts, analogous Ni_5Fe_1 alloys were constituted over both alumina and biochar supports. The highest specific activity of the catalyst series, exhibited by the NiFe/C catalyst, was related to the development of surface basic sites along with weaker NiFe-C interactions, which resulted in increased Ni^0:NiO surface populations under reaction conditions. In summary, the present work establishes biochar supports as a competitive material to consider within the future low-carbon energetic panorama.

Unravelling the CO_2 capture and conversion mechanism of a NiRu-Na_2O switchable dual-function material in various CO_2 utilisation reactions

Merkouri, LP; Martin-Espejo, JL; Bobadilla, LF; Odriozola, JA; Penkova, A; Reina, T; Duyar, MS
Journal of Materials Chemistry A, **11** (2023) 13209-13216
Mayo, 2023 · DOI: 10.1039/d3ta01892j

Time-resolved operando DRIFTS-MS was performed to elucidate the CO_2 capture and conversion mechanisms of a NiRuNa/CeAl DFM in CO_2 methanation, reverse water-gas shift, and dry reforming of methane. CO_2 was captured mainly in the form of carbonyls and bidentate carbonates, and a spillover mechanism occurred to obtain the desired products.

Engineering morphologies of yttrium oxide supported nickel catalysts for hydrogen production

Zhang, RB; Tu, ZA; Meng, S; Feng, G; Lu, ZH; Yu, YZ; Reina, TR; Hu, FY; Chen, XH; Ye, RP
Rare Metals, **42** (2023) 176-188
Enero, 2023 · DOI: 10.1007/s12598-022-02136-5

The catalytic performance is highly related to the catalyst structure. Herein, a series of Ni nanoparticles supported on Y_2O_3 with different morphologies were successfully synthesized via hydrothermal process screening different pH environments. These Ni/Y_2O_3 catalysts were applied to efficiently produce CO_x-free H-$_2$ through ammonia decomposition. We identify a significant impact of Y_2O_3 supports on nickel nanoclusters sizes and dispersion. The experimental results show that Ni/Y11 catalyst achieves 100% ammonia decomposition conversion under a gas hour space velocity (GHSV) of 12,000 $ml.h^{-1}.g_{cat}^{-1}$ and temperature of 650 °C. Such a high level of activity over Ni/Y11 catalyst was attributed to a large specific surface area, appropriate alkalinity, and small Ni nanoparticles diameter with high dispersion.

Guaiacol hydrotreatment in an integrated APR-HDO process: Exploring the promoting effect of platinum on Ni-Pt catalysts and assessing methanol and glycerol as hydrogen sources

Jin, W; Gandara-Loe, J; Pastor-Pérez, L; Villora-Pico, JJ; Sepulveda-Escribano, A; Rinaldi, R; Reina, TR
Renewable Energy, **215** (2023) 118907
Octubre, 2023 · DOI: 10.1016/j.renene.2023.118907

This study presents an integrated approach combining aqueous phase reforming (APR) and hydrodeoxygenation (HDO) for the hydrotreatment of guaiacol, a model compound representing lignin-derived phenols in pyrolysis bio-oils. The APR process enables in-situ H_2 generation, elimi-nating the need for an external hydrogen source. We examine the interplay between metal spe-cies, the Pt-promoting effect on Ni-Pt catalyst supported on activated carbon (AC), and the choice of hydrogen source (methanol or glycerol). Amongst the monometallic catalysts, a 1% Pt/AC catalyst notably achieved over 96% guaiacol conversion at 300 °C with either hydrogen source. Interestingly, when 0.5-1% of the Ni loading is replaced with Pt, the resulting bimetallic Ni-Pt/AC catalysts demonstrate a significant improvement in guaiacol conversion, reaching 70% when methanol is employed as the hydrogen source. Surprisingly, no comparable enhancement in guaiacol conversion is observed when employing glycerol as the hydrogen source. This observation underlines one of the pivotal effects of the hydrogen source on catalyst performance. X-ray photoemission spectroscopy (XPS) pinpointed strong Ni-Pt interactions in the ca-

talyst. It also revealed distinctive electronic features of Ni-Pt/AC, which are favourable for steering selectivity towards cyclohexanol rather than phenol when Pt loading is increased from 0.5 to 1%. Moreover, Pt enhanced catalyst stability by inhibiting the oxidation of Ni sites and mitigating Ni-Pt phase sintering. Overall, our findings offer important insights into integrating APR and HDO processes, the promotion effect of Pt, and the importance of hydrogen source selection in terms of guaiacol conversion and catalyst stability.

Is the RWGS a viable route for CO_2 conversion to added value products? A techno-economic study to understand the optimal RWGS conditions

Portillo, E; Gandara-Loe, J; Reina, TR; Pastor-Pérez, L
Science of the Total Environment, **857** (2023) 159394
Enero, 2023 · DOI: 10.1016/j.scitotenv.2022.159394

Understanding the viability of the RWGS from a thermodynamic and techno-economic angle opens new horizons within CO_2 conversion technologies. Unfortunately, profitability studies of this technology are scarce in literature and mainly focused on overall conversion and selectivity trends with tangential remarks on energy demands and process costs. To address this research gap, herein we present a comprehensive techno-economic study of the RWGS reaction when coupling with Fischer-Tropsch synthesis is envisaged to produced fuels and chemicals using CO_2 as building block. We showcase a remarkable impact of operating conditions in the final syngas product and both CAPEX and OPEX. From a capital investment perspective, optimal situations involve RWGS unit running at low temperatures and high pressures as evidenced by our results. However, from the running cost angle, operating at 4 bar is the most favorable alternative within the studied scenarios. Our findings showcase that, no matter the selected temperature the RWGS unit should be preferentially run at intermediate pressures. Ultimately, our work maps out multiple operating scenarios in terms of energy demand and process cost serving as guideline to set optimal reaction conditions to un-lock the potential of the RWGS for chemical CO_2 recycling.

H_2-rich syngas production from biogas reforming: Overcoming coking and sintering using bimetallic Ni-based catalysts

Carrasco-Ruiz, S; Zhang, Q; Gándara-Loe, J; Pastor-Pérez, L; Odriozola, JA; Reina, TR; Bobadilla, LF
International Journal of Hydrogen Energy, **48** (2023) 72
Agosto, 2023 · DOI: 10.1016/j.ijhydene.2023.03.301

Dry reforming of methane is a very appealing catalytic route biogas (mainly composed by greenhouse gases: carbon dioxide and methane) conversion into added value syngas, which could be further upgraded to produce liquid fuels and added value chemicals. However, the major culprits of this reaction are coking and active phase sintering that result in catalysts deactivation. Herein we have developed a highly stable bimetallic Ni–Rh catalyst supported on mixed CeO_2–Al_2O_3 oxide using low-noble metal loadings. The addition of small amounts of rhodium to nickel catalysts prevents coke formation and improves sintering resistance, achieving high conversions over extended reaction times hence resulting in promising catalysts for biogas upgrading.

Effect of noble metal addition over active Ru/TiO_2 catalyst for CO selective methanation from H_2 rich-streams

Bobadilla, LF; Muñoz-Murillo, A; Gandara-Loe, J; Pérez, A; Laguna, OH; Martinez, TLM; Penkova, A; Centeno, MA; Odriozola, JA

International Journal of Hydrogen Energy, **48** (2023) 25065-25074
Julio, 2023 · DOI: 10.1016/j.ijhydene.2022.07.072

Selective CO methanation from H_2-rich stream has been regarded as a promising route for deep removal of low CO concentration and catalytic hydrogen purification processes. This work is focused on the development of more efficient catalysts applied in practical conditions. For this purpose, we prepared a series of catalysts based on Ru supported over titania and promoted with small amounts of Rh and Pt. Characterization details revealed that Rh and Pt modify the electronic properties of Ru. The results of catalytic activity showed that Pt has a negative effect since it promotes the reverse water gas shift reaction decreasing the selectivity of methanation but Rh increases remarkably the activity and selectivity of CO methanation. The obtained results suggest that RuRh-based catalyst could become important for the treatment of industrial-volume streams.

Photoreforming of glycerol to produce hydrogen from natural water in a compound parabolic collector solar photoreactor

Villachica-Llamosas, JG; Sowik, J; Ruiz-Aguirre, A; Colón, G; Peral, J; Malato, S

Journal of Environmental Chemical Engineering, **11** (2023) 111216
Diciembre, 2023 · DOI: 10.1016/j.jece.2023.111216

To improve TiO_2 for H_2 generation, one strategy for the separation of photogenerated charges is the formation of heterostructures with other materials. In particular, NiO is a photocatalyst known for its good stability and low cost. However, no studies at pilot scale using solar energy have been described. Consequently, an evaluation of a physical $NiO:TiO_2$ mixture at pilot scale (25 L) with natural irradiation (2.10 m^2 of sun-exposed surface) and with simultaneous glycerol photoreforming was explored. $NiO:TiO_2$ 50 mgL^{-1} resulted in the highest hydrogen production, showing an STH = 1.44%, considering only the UV fraction of the solar irradiation. H_2 and CO_2 production were analysed by on-line GC; Glycerol, dissolved organic carbon, carboxylic acids and nickel leaching were also evaluated. The $NiO:TiO_2$ mixtures rendered a systematically lower H_2 production in natural water than in high-purity water. The increase of ionic strength increased the mean size of particle clusters, promoting rapid sedimentation. All this indicates the importance of testing under real field conditions for attaining reliable solar to hydrogen (STH) efficiency.

Hydrothermal carbonization vs. anaerobic digestion to valorize fruit and vegetable waste: A comparative technical and energy assessment

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Journal of Environmental Chemical Engineering, **11** (2023) 109925
Junio, 2023 · DOI: 10.1016/j.jece.2023.109925

Herein, the valorization of vegetable and fruit waste was assessed via hydrothermal carbonization (HTC) and anaerobic digestion (AD) in terms of product characterization and energy requirements.

HTC was conducted at reaction temperatures between 150 °C and 190 °C, and residence times between 20 min and 40 min. The increase in the process severity resulted in hydrochars with higher carbon contents and higher energy densification ratios. AD was performed in two different ways. i.e., batch and semi-continuous reactions. From the batch experiments a methane yield of 300 L CH4/kg VS was obtained, while for the semi-continuous, the average specific methane production estimated (for HRTs from 75 to 50 days) was 213±32 L CH_4/kg VS. To estimate the energy re-quirements, mass and energy balances were performed considering the basic stages of each process to obtain a suitable biofuel material. In this sense, it was concluded that for this specific waste, AD was a more suitable process with a positive energy net balance. On the contrary, HTC presented a negative energy net balance being required 1.29 MJ/kg of fresh food waste. A combined HTC-AD treatment may be an efficient method to take advantage of both technologies leading to higher energy efficiencies and other valuable products.

Water-assisted HDO of biomass model compounds enabled by Ru-based catalysts

Carrasco-Ruiz, S; Parrilla-Lahoz, S; Santos, JL; Penkova, A; Odriozola, JA; Reina, TR; Pastor-Pérez, L
Fuel Processing Technology, **249** (2023) 107860
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Biofuels upgrading gathering momentum in view of the gradual depletion of fossil fuels and the pursuit of renewable energy sources to mitigate global warming. Hydrodeoxygenation (HDO) is a key reaction in the upgrading of bio-oil to produce hydrocarbon fuels or high-value chemicals. Oxygen removal in bio-oil increases its calorific value, improve thermal and chemical stability, reduce corrosiveness, etc., making the upgraded biooil suitable as a fuel or blending fuel. However, the dependence on high-pressure hydrogen is a serious disadvantage, as it is an expensive resource whose use also poses safety concerns. In this scenario, we propose a pioneering route for model biomass compounds upgrading via H_2-free HDO. Herein we have developed multifunctional catalysts based on Ru and ceria supported on carbon able conduct the hydrodeoxygenation reaction using water as hydrogen source. We found that cerium oxide improves ruthenium metallic dispersion and the overall redox properties of the multicomponent system leading to enhanced catalytic performance. Along with the successful catalytic formulation we identify 300 °C as an optimal temperature validating the H_2-free HDO route for biocompounds upgrading.

Experimental optimization of Ni/P atomic ratio for nickel phosphide catalysts in reverse water-gas shift

Hameed, G; Goksu, A; Merkouri, LP; Penkova, A; Ramirez Reina, T; Carrasco Ruiz, S; Duyar, MS
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Noviembre, 2023 · DOI: 10.1016/j.jcou.2023.102606

Nickel phosphide catalysts show a high level of selectivity for the reverse water-gas shift (RWGS) reaction, inhibiting the competing methanation reaction. This work investigates the extent to which suppression of methanation can be controlled by phosphidation and tests the stability of phosphide phases over 24-hour time on stream. Herein the synthesis of different phosphide crystal structures by varying Ni/P atomic ratios (from 0.5 to 2.4) is shown to affect the selectivity to CO over CH_4 in a significant way. We also show that the activity of these catalysts can be fine-tuned by the synthesis Ni/P ratio and identify suitable catalysts for low temperature RWGS process. $Ni_{12}P_5$-SiO_2 showed 80–100% selectivity over the full temperature range (i.e., 300–800 °C) tested, reaching 73% CO_2 conversion at 800 °C. Ni_2P-SiO_2 exhibited CO selectivity of 93–100% over a full temperature range, and 70% CO_2 conversion

at 800 °C. The highest CO_2 conversions for $Ni_{12}P_5$-SiO_2 at all temperatures among all catalysts showed its promising nature for CO_2 capture and utilisation. The methanation reaction was suppressed in addition to RWGS activity improvement through the formation of nickel phosphide phases, and the crystal structure was found to determine CO selectivity, with the following order $Ni_{12}P5 > Ni_2P > Ni_3P$. Based on the activity of the studied catalysts, the catalysts were ranked in order of suitability for the RWGS reaction as follows: $Ni_{12}P_5$-SiO_2 (Ni/P = 2.4) > Ni_2P-SiO_2 (Ni/P = 2) > NiP-SiO_2 (Ni/P = 1) > NiP_2-SiO_2 (Ni/P = 0.5). Two catalysts with Ni/P atomic ratios; 2.4 and 2, were selected for stability testing. The catalyst with Ni/P ratio = 2.4 (i.e., $Ni_{12}P_5$-SiO_2) was found to be more stable in terms of CO_2 conversion and CO yield over the 24-hour duration at 550 °C. Using the phosphidation strategy to tune both selectivity and activity of Ni catalysts for RWGS, methanation as a competing reaction is shown to be no longer a critical issue in the RWGS process for catalysts with high Ni/P atomic ratios (2.4 and 2) even at lower temperatures (300–500 °C). This opens up potential low temperature RWGS opportunities, especially coupled to downstream or tandem lower temperature processes to produce liquid fuels.

Spinel ferrite catalysts for CO_2 reduction via reverse water gas shift reaction

Navarro, JC; Hurtado, C; González-Castaño, M; Bobadilla, LF; Ivanova, S; Cumbrera, FL; Centeno, MA; Odriozola, JA

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The production of CO via Reverse Water Gas Shift (RWGS) reaction is a suitable route for CO_2 valorization. In this study a series of modified spinels AB_2O_4 (A site symbolscript Ni, Zn and Cu and B symbolscript are investigated as RWGS catalysts and their structure-to-function relationships derived from the changes on the A-site cation are rationalized. For all ferrite systems, the RWGS reaction the process main activity and selectivity is governed by the β-site cation, but the variations on the A-site metals determines catalysts' structural features and stability in the reaction. Among the catalyst series, superior RWGS performance displayed the ferrites modified with Cu and Ni associated to the greater oxygen vacancy population for those spinels enabled by the partial allocation on symbolscript cations into the tetrahedral sites.

Catalytic performance of cobalt supported onto APTES functionalized TiO_2 for Fischer-Tropsch reaction

Platero, F; Caballero, A; Colon, G

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Cobalt supported TiO_2 catalysts have been prepared by wet-impregnation and by immobilization over APTES (3-aminopropyl triethoxysilane) grafted TiO_2. Impregnated system showed better catalytic performance after reduction at 260 °C but significant deactivation is observed. On the contrary, functionalized catalyst showed better catalytic performance after reduction at 400 °C with notable stability. We have stated from CO-DRIFT operando analysis that impregnated system is strongly affected by negative SMSI (strong metal-support inter-action) upon reduction at higher temperature. While immobilization on APTES hinders the loss of metal active sites. The study of spent catalysts denotes that Co is redispersed in the impregnated catalyst while functionalized trends to form agglomerates.

In-situ DRIFTS steady-state study of CO_2 and CO methanation over Ni-promoted catalysts

González-Castaño, M; González-Arias, J; Bobadilla, LF; Ruíz-López, E; Odriozola, JA; Arellano-García, H
Fuel, **338** (2023) 127241
Abril, 2023 · DOI: 10.1016/j.fuel.2022.127241

Promoting the performance of catalytic systems by incorporating small amount of alkali has been proved effective for several reactions whilst controversial outcomes are reported for the synthetic natural gas production. This work studies a series of Ni catalysts for CO_2 and CO methanation reactions. In-situ DRIFTS spectroscopy evidenced similar reaction intermediates for all evaluated systems and it is proposed a reaction mechanism based on: i) formate decomposition and ii) hydrogenation of lineal carbonyl species to methane. Compared to bare Ni, the enhanced CO_2 methanation rates attained by NiFe/Al and NiFeK/Al systems are associated to promoted formates decomposition into lineal carbonyl species. Also for CO methanation, the differences in the catalysts' performances were associated to the relative concentration of lineal carbonyl species. Under CO methanation conditions and opposing the CO_2 methanation results where the incorporation of K delivered promoted catalytic behaviours, worsened CO methanation rates were discerned for the NiFeK/Al system.

High-Performance Photocatalytic H_2 Production Using a Binary $Cu/TiO_2/SrTiO_3$ Heterojunction

González-Tejero, M; Villachica-Llamosas, JG; Ruiz-Aguirre, A; Colon, G
ACS Applied Energy Materials, **6** (2023) 4007-4015
Abril, 2023 · DOI: 10.1021/acsaem.3c00219

$Cu/TiO_2/SrTiO_3$ hybrid structures have been synthesized by the simple impregnation method from Cu/TiO_2 and $SrTiO_3$ systems. The structural and surface characterization stated that $Cu/TiO_2/SrTiO_3$ composites form an effective covering of $SrTiO_3$ by Cu/TiO_2. The heterostructured catalysts lead to an outstanding improved photoactivity for hydrogen production from methanol photoreforming that would be related with the efficient separation of charge pairs favored by the $Cu/TiO_2/SrTiO_3$ heterojunction. The best photoproduction is attained for the 30 wt % $SrTiO_3$ heterojunction showing 81.7 mmol/g H_2 after 6 h (leading to an apparent quantum yield of ca 1%), 1.7 times higher than that of bare Cu/TiO_2.

Cobalt Stabilization through Mesopore Confinement on TiO2 Support for Fischer-Tropsch Reaction

Platero, F; Todorova, S; Aoudjera, L; Michelin, L; Lebeau, B; Blin, JL; Holgado, JP; Caballero, A; Colón, G
ACS Applied Energy Materials, 6 (2023) 9475-9486
Septiembre, 2023 · DOI: 10.1021/acsaem.3c01432

Cobalt supported on mesostructured TiO_2 catalysts has been prepared by a wet-impregnation method. The Co/TiO2 catalytic system showed better catalytic performance after support calcination at 380 °C. Co nanoparticles appeared well distributed along the mesopore channels of TiO_2. After reduction pretreatment and reaction, a drastic structural change leads to mesopore structure collapse and the dispersion of the Co nanoparticles on the external surface. Along this complex process, Co species first form discrete nanoparticles inside the pore and then diffuse out as the pore collapses. Through this

confinement, a strong metal–support interaction effect is hindered, and highly stable metal active sites lead to better performance for Fischer–Tropsch synthesis reaction toward C5+ products.

Coal Chemistry Industry: From Production of Liquid Fuels to Fine Chemicals to Carbon Materials

Zhang, YY; Li, HT; Reina, TR; Liu, J
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Noviembre, 2023 · DOI: 10.1021/acs.energyfuels.3c02661

Coal resources are one of the key energy sources and essential for modern economic development. Despite the traditional coal industries having made considerable contributions to chemical production and energy storage, the accompanying environmental pollution and high energy consumption have also arisen that cause significant influence of the ecological balance. Hence, there is an urgent need to exploit feasible approaches to the sustainable utilization of coal resources. This review begins with a comprehensive summary of the representative coal chemistry technologies with critical discussions. Subsequently, a novel strategy coupled with green hydrogen is discussed for sustainable conversion of coal and highly efficient manufacture of downstream products. Moreover, the unique role of coal in terms of high-value-added carbon material production is highlighted as a low-cost resource for distinct applications. Finally, we propose several future directions for advanced coal chemistry development.

Review and Perspectives of CO_2 Absorption by Water- and Amine-Based Nanofluids

Yuan, CT; Wang, Y; Baena-Moreno, FM; Pan, Z; Zhang, R; Zhou, H; Zhang, Z
Energy & Fuels, **37** (2023) 8883-890
Junio, 2023 · DOI: 10.1021/acs.energyfuels.3c00874

The emission of greenhouse gases, especially CO_2, has become a major cause of environmental degradation, and carbon capture,utilization, and storage (CCUS) is a proposed solution to mitigate its impact. Nanofluids, a relatively new method for CO_2 absorption, have gained attention in recent years. This review focuses on conventional methods for preparing nanofluids along with techniques to improve their stability and enhance the CO_2 absorption and desorption mechanisms. Additionally, the influences of factors,i.e., nanoparticle and base solution types as well as nanoparticleconcentration, on the CO_2 absorption process are summarized. Furthermore, models that can predict the absorption of CO_2 accurately are outlined. It is found that the types of both base liquids and nanoparticles have an important impact on the absorptionby nanofluids. In-depth studies on the predictive capabilities of artificial intelligence (AI) models hold immense potential in this regard. This review also puts forth effective strategies to address prevailing challenges. This will provide a solid theoretical basis for this field and underscore the promising potential of nanofluids as CO_2 solvents. There are still many unexplored aspects to be considered, such as the economic viability and energy consumption of this technology.

Low-temperature reverse water gas-shift reaction over highly efficient Cu-hydrotalcites: Mechanistic insights on the role of malachite phase

Alvarez-Hernandez, D; Marín-Sánchez, M; Lobo-Andrades, L; Azancot, L; Bobadilla, LF; Ivanova, S; Centeno, MA
Catalysis Today, **422** (2023) 114235
Octubre, 2023 · DOI: 10.1016/j.cattod.2023.114235

Carbon dioxide (CO_2) transformation into valuable fuels and chemicals is in most cases a challenge far from readiness nowadays. One possible route for its conversion is the reverse water gas shift reaction (rWGS), crucial for syngas generation and required for the chemical conversion of CO_2 to fuels and platform chemicals. In this paper, well organized Cu/Zn/Al structures were proposed as efficient catalysts for rWGS reaction at low tem-peratures. The results of in situ XRD revealed the formation of layered structures such malachite and hydro-talcite. The operando DRIFTS-MS studies of those structure suggests a participation of Cu^{2+}/Cu^{+} pair in the reaction, promoting the redox mechanism and enhancing the activity at lower temperature. This work also provides a new strategy to design Cu-based rWGS catalysts able to prevent the sintering of active phase.

Glucose dehydration reaction over metal halides supported on activated charcoal catalysts

Delgado Martin, G; Lara, B; Bounoukta, CE; Domínguez, MI; Ammari, F; Ivanova, S; Centeno, MA
Catalysis Today, **423** (2023) 114012
Noviembre, 2023 · DOI: 10.1016/j.cattod.2023.01.019

Different metal halide catalysts supported on a commercial active charcoal have been synthesized, activated, characterized and tested in glucose dehydration to 5-hydroxymethylfurfural using a biphasic water/methyl isobutyl ketone media. The influence of the cation nature (K^{+}, Ca^{2+}, Sr^{2+}, Mg^{2+}) and anion nature (F^{-}, Cl^{-}, Br^{-}) on the catalytic performance of the solid is discussed in terms of glucose conversion, HMF yield and products selectivity. The activation of the impregnated catalysts results in a great diversity of active sites, such as Bronsted sites (carboxylic groups), basic sites (metal oxide), and Lewis acid site (M^{n+}). Their distribution within the samples determinates the resulting products and the final HMF yield.

Multicomponent graphene based catalysts for guaiacol upgrading in hydrothermal conditions: Exploring "H_2-free" alternatives for bio-compounds hydrodeoxygenation

Parrilla-Lahoz, S; Jin, W; Pastor-Pérez, L; Duyar, MS; Martinez-Quintana, L; Dongil, AB; Reina, TR
Catalysis Today, **422** (2023) 114235
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Catalytic hydrodeoxygenation (HDO) is a critical technique for upgrading biomass derivatives to deoxygenated fuels or other high-value compounds. Phenol, guaiacol, anisole, p-cresol, m-cresol and vanillin are all monomeric phenolics produced from lignin. Guaiacol is often utilised as a model lignin compound to deduce mechanistic information about the bio-oil upgrading process. Typically, a source of H_2 is supplied as reactant for the HDO reaction. However, the H_2 supply, due to the high cost of production and additional safety precautions needed for storage and transportation, imposes significant economic infeasibilities on the HDO process's scaling up. We investigated a novel H_2-free hydrodeoxygenation (HDO) reaction of guaiacol at low temperatures and pressures, using water as both a reaction medium and hydrogen source. A variety of Ni catalysts supported on zirconia/ graphene/with/without nitrogen doping were synthesised and evaluated at 250 °C and 300 °C in a batch reactor, with the goal of performing a multi-step tandem reaction including water splitting followed by HDO. The catalysts were characterised using H_2-TPR, XRD, TEM and XPS to better understand the physicochemical properties and their correlation with catalytic performance of the samples in the HDO process. Indeed, our $NiZr_2O$/Gr-n present the best activity/selectivity balance and it is deemed as a promising catalyst to

conduct the H_2-free HDO reaction. The catalyst reached commendable conversion levels and selectivity to mono-oxygenated compounds considering the very challenging reaction conditions. This innovative HDO approach provides a new avenue for cost-effective biomass upgrading.

Selective hydrodeoxygenation of levulinic acid to gamma-valerolactone over Ru supported on functionalized carbon nanofibers

Bounoukta, CE; Megias-Sayago, C; Rendon, N; Ammari, F; Penkova, A; Ivanova, S; Centeno, MA; Odriozola, JA
Sustainable Energy & Fuels, **7** (2023) 857-867
Enero, 2023 · DOI: 10.1039/d2se01503j

In this work, carbon nanofibers (CNFs) have been successfully functionalized by using different approaches and finally used for the preparation of Ru based catalysts. The *organometallic* approach has been demonstrated to be suitable for CNF functionalization, leading to well-defined Ru NPs (by adding organosilane, amino or mercapto functionalities, among others) in comparison with mineral acid treatments conventionally used to activate and/or functionalize carbonaceous solids. All catalysts have been tested in levulinic acid hydrodeoxygenation to γ-valerolactone under mild conditions, with the impact of CNF functionalization on the catalysts' performance fully discussed in comparison with unmodified commercial CNFs.

Effect of zeolite topological structure in bifunctional catalyst on direct conversion of syngas to light olefins

Meng, FH; Gong, ZY; Yang, LL; Wang, Q; Xing, MQ; Nawaz, MA; Li, Z
Microporous and Mesoporous Materials, **362** (2023) 112792
Diciembre, 2023 · DOI: 10.1016/j.micromeso.2023.112792

Bifunctional catalyst composed of metal oxide and zeolite (OX-ZEO) is a promising strategy for the direct conversion of syngas to light olefins (STO), where the structure of zeolite plays a vital role in determining the selectivity of product. Herein, three kinds of silicoaluminophosphate zeolites with different topological structures, i.e., the ERI(SP17), AEI(SP18) and CHA(SP34), were hydrothermally synthesized, after the combination with Mn-Ga oxide, the prepared OX-ZEO was applied for STO reaction. The variation in the crystallization time for SP17 synthesis has a great impact on the generation of impurity phase of SAPO-5, where a crystallization time of 48-96 h is found to be beneficial in synthesizing SP17 zeolite with pure phase. SP17 zeolite with a crystallization time of 96 h, possesses the micropores and columnar morphology, where the small cage-defining 8-ring size of SP17 shows the olefins selectivity of 87.0% at a low CO conversion of 19.4%, significantly deviating towards the major fraction of ethylene (45.6%) than that of butene (8.2%). In a contrast, SP18 and SP34 zeolites with the same and large cage-defining 8-ring size, are richer in propylene and butene fractions than that of ethylene in overall similar olefins selectivity of 87.0% and 87.1% at CO conversion of 28.7% and 28.5%, respectively. Interestingly, it is further interpreted that the SP17 sample generated more carbon species during the reaction due to the small 8-ring size, while those amounts of carbon species were restricted in the hierarchical pore structure and plate-like morphology in SP18 and SP34 samples.

Impact of topology framework of microporous solids on methanol carbonylation: An operando DRIFTS-MS study

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Microporous and Mesoporous Materials, **360** (2023) 112725
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Methanol carbonylation was evaluated over heterogeneous catalysts based on Cu-exchanged zeolitic materials with different topology: Cu@MOR, Cu@FER, and Cu@ZSM-5. Despite the similar Si/Al ratios, it is crucial to acknowledge that the acid strength is influenced by the framework topology, as supported by the NH_3-TPD results. This, along with other characterization techniques allowed us to estimate the impact of pore size and pore distribution in these microporous materials on catalytic performance. The channel structure influenced catalytic parameters such as conversion and selectivity. The higher methanol conversion achieved on Cu@FER shows the importance of Bronsted acid sites and redox centres location regarding the topology of the material. Concerning the selectivity, the production of acetic acid was endorsed by the 12-MR (MOR) channels, methyl acetate's production by the 10-MR (FER) channels. Finally, the presence of 6-MR (ZSM-5) channels led to a complete selectivity towards DME production. The reaction mechanism was elucidated via operando DRIFTS-MS and results revealed a bifunctional mechanism in which methanol adsorbs and dehydrates on acidic Bronsted sites and CO is activated over Cu^+ species.

Highly dispersed Rh single atoms over graphitic carbon nitride as a robust catalyst for the hydroformylation reaction

Jurado, L; Esvan, J; Luque-Alvarez, LA; Bobadilla, LF; Odriozola, JA; Posada-Pérez, S; Poater, A; Comas-Vives, A; Axet, MR
Catalysis Science & Tecnology, **13** (2022) 1425-1436
Enero, 2023 · DOI: 10.1039/d2cy02094g

Rhodium-catalysed hydroformylation, effective tool in bulk and fine-chemical synthesis, predominantly uses soluble metal complexes. For that reason, the metal leaching and the catalyst recycling are still the major drawbacks of this process. Single-atom catalysts have emerged as a powerful tool to combine the advantages of both homogeneous and heterogeneous catalysts. Since using an appropriate support material is key to create stable, finely dispersed, single-atom catalysts, here we show that Rh atoms anchored on graphitic carbon nitride are robust catalysts for the hydroformylation reaction of styrene.

Flexible NiRu Systems for CO_2 Methanation: From Efficient Catalysts to Advanced Dual-Function Materials

Merkouri, LP; Martin-Espejo, JL; Bobadilla, LF; Odriozola, JA; Duyar, MS; Reina, TR
Nanomaterials, **13** (2023) 506
Febrero, 2023 · DOI: 10.3390/nano13030506

CO_2 emissions in the atmosphere have been increasing rapidly in recent years, causing global warming. CO_2 methanation reaction is deemed to be a way to combat these emissions by converting CO_2 into synthetic natural gas, i.e., CH_4. NiRu/CeAl and NiRu/CeZr both demonstrated favourable activity for CO_2 methanation, with NiRu/CeAl approaching equilibrium conversion at 350 °C with 100% CH_4 selectivity. Its stability under high space velocity (400 $L{\cdot}g^{-1}{\cdot}h^{-1}$) was also commendable. By adding an adsorbent, potassium, the CO_2 adsorption capability of NiRu/CeAl was boosted, allowing it to function as

a dual-function material (DFM) for integrated CO_2 capture and utilisation, producing 0.264 mol of CH_4/kg of sample from captured CO_2. Furthermore, time-resolved operando DRIFTS-MS measurements were performed to gain insights into the process mechanism. The obtained results demonstrate that CO_2 was captured on basic sites and was also dissociated on metallic sites in such a way that during the reduction step, methane was produced by two different pathways. This study reveals that by adding an adsorbent to the formulation of an effective NiRu methanation catalyst, advanced dual-function materials can be designed.

Facile Synthesis of Heterogeneous Indium Nanoparticles for Formate Production via CO_2 Electroreduction

Pérez-Sequera, AC; Diaz-Pérez, MA; Angulo, MAL; Holgado, JP; Serrano-Ruiz, JC
Nanomaterials, **13** (2023) 3052
Abril, 2023 · DOI: 10.3390/nano13081304

In this study, a simple and scalable method to obtain heterogeneous indium nanoparticles and carbon-supported indium nanoparticles under mild conditions is described. Physicochemical characterization by X-ray diffraction (XRD), X-ray photoelectron microscopy (XPS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) revealed heterogeneous morphologies for the In nanoparticles in all cases. Apart from In^0, XPS revealed the presence of oxidized In species on the carbon-supported samples, whereas these species were not observed for the unsupported samples. The best-in-class catalyst (In_{50}/C_{50}) exhibited a high formate Faradaic efficiency (FE) near the unit (above 97%) at -1.6 V vs. Ag/AgCl, achieving a stable current density around -10 $mA{\cdot}cm_{geo}^{-2}$, in a common H-cell. While In^0 sites are the main active sites for the reaction, the presence of oxidized In species could play a role in the improved performance of the supported samples.

Functionalized Biochars as Supports for Ru/C Catalysts: Tunable and Efficient Materials for γ-Valerolactone Production

Bounoukta, CE; Megias-Sayago, C; Navarro, JC; Ammari, F; Ivanova, S; Centeno, MA
Nanomaterials, **13** (2023) 1129
Marzo, 2023 · DOI: 10.3390/nano13061129

Cotton stalks-based biochars were prepared and used to synthetize Ru-supported catalysts for selective production of gamma-valerolactone from levulinic acid in aqueous media. Different biochars' pre-treatments (HNO_3, $ZnCl_2$, CO_2 or a combination of them) were carried out to activate the final carbonaceous support. Nitric acid treatment resulted in microporous biochars with high surface area, whereas the chemical activation with $ZnCl_2$ substantially increases the mesoporous surface. The combination of both treatments led to a support with exceptional textural properties allowing the preparation of Ru/C catalyst with 1422 m^2/g surface area, 1210 m^2/g of it being a mesoporous surface. The impact of the biochars' pre-treatments on the catalytic performance of Ru-based catalysts is fully discussed.

Bismuth ferrite as innovative and efficient photocatalyst for the oxidation of As(III) to As(V) under visible light

Chianese, L; Murcia, JJ; Hidalgo, MC; Vaiano, V; Iervolino, G
Materials Science in Semiconductor Processing, **167** (2023) 107801
Noviembre, 2023 · DOI: 10.1016/j.mssp.2023.107801

The presence of As in drinking water is a problem felt all over the world. In particular, arsenic is present in +3 (As(III)) and +5 (As(V)) oxidation states. However, As(III) is the most toxic and difficult to remove with conventional adsorption processes. A pre-oxidation process is therefore necessary. In this work, we report, for the first time, the use of $BiFeO_3$ as a visible-light active photocatalyst for the complete and fast oxidation of As(III) to As(V) in water. In particular, the influence of annealing temperature for $BiFeO_3$ preparation was studied and the prepared photocatalysts were characterized through XRD, N2 adsorption at −196°C, TEM, XPS, Raman and UV–Vis DRS spectroscopy. The best photocatalytic activity was achieved with $BiFeO_3$ calcined at 550°C. The influence of catalyst dosage and the role of the main oxidizing species was evaluated, evidencing the key role of h^+ in the photooxidation reaction of As(III) to As(V). Moreover, the efficiency of the photocatalyst was also evaluated in the case of drinking water contaminated by arsenic. The results demonstrated that, despite the presence of dissolved salts in the drinking water, the photocatalyst maintained its activity. The results obtained in this work prove that $BiFeO_3$ calcined at 550°C evidenced photocatalytic performances better than different photocatalyst formulations studied for the photooxidation of As(III) to As(V) under visible light.

Biochar production from cellulose under reductant atmosphere: influence of the total pyrolysis time

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RSC Advances, **13** (2023) 21071-21079
Julio, 2023 · DOI: 10.1039/d3ra03093h

Today's rising energy costs, coupled with increasing energy demand, make it necessary to search for more efficient energy processes. In recent years, there have been increasing efforts to develop efficient catalysts based on waste-derived char, by a single step where the carbon precursor and the metallic active phase one undergo a single common thermal process under a reductant atmosphere at high temperature. The use of a reductant atmosphere drives the formation of carbonaceous materials with different characteristics than those obtained under the standard nitrogen-inert one. Our work evaluates the influence of the residence time and the heating rate on the physicochemical properties of the biochar obtained. Relatively long residence times and slow heating rates, improve the yield to the resulting biochar, without increasing production cost, making the subsequent char-based metallic catalyst synthesis more efficient. The heating rate was shown to be key in improving the properties of the char in a smoother and more controlled way, unlocking a new working pathway for the efficient design and production of char-based catalysts in a one-pot synthesis.

Formic Acid Dehydrogenation over a Monometallic Pd and Bimetallic Pd:Co Catalyst Supported on Activated Carbon

Pelaez, MR; Ruiz-López, E; Domínguez, MI; Ivanova, S; Centeno, MA
Catalysts, **13** (2023) 977
Junio, 2023 · DOI: 10.3390/catal13060977

In this study, palladium is proposed as an active site for formic acid dehydrogenation reaction. Pd activity was modulated with Co metal with the final aim of finding a synergistic effect that makes possible efficient hydrogen production for a low noble metal content. For the monometallic catalysts, the metal loadings were optimized, and the increase in the reaction temperature and presence of additives were carefully considered. The present study aimed, to a great extent, to enlighten the possible routes for

decreasing noble metal loading in view of the better sustainability of hydrogen production from liquid organic carrier molecules, such as formic acid.

CO_2 Methanation over Nickel Catalysts: Support Effects Investigated through Specific Activity and Operando IR Spectroscopy Measurements

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Catalysts, **13** (2023) 448
Febrero, 2023 · DOI: 10.3390/catal13020448

Renewed interest in CO_2 methanation is due to its role within the framework of the Power-to-Methane processes. While the use of nickel-based catalysts for CO_2 methanation is well stablished, the support is being subjected to thorough research due to its complex effects. The objective of this work was the study of the influence of the support with a series of catalysts supported on alumina, ceria, ceria-zirconia, and titania. Catalysts' performance has been kinetically and spectroscopically evaluated over a wide range of temperatures (150-500 °C). The main results have shown remarkable differences among the catalysts as concerns Ni dispersion, metallic precursor reducibility, basic properties, and catalytic activity. Operando infrared spectroscopy measurements have evidenced the presence of almost the same type of adsorbed species during the course of the reaction, but with different relative intensities. The results indicate that using as support of Ni a reducible metal oxide that is capable of developing the basicity associated with medium-strength basic sites and a suitable balance between metallic sites and centers linked to the support leads to high CO_2 methanation activity. In addition, the results obtained by operando FTIR spectroscopy suggest that CO_2 methanation follows the formate pathway over the catalysts under consideration.

New 3D Printing Strategy for Structured Carbon Devices Fabrication

Delgado-Martin, G; Rodríguez, N; Domínguez, MI; Agamez-Pertuz, YY; Tejada, MM; Ruiz-López, E; Ivanova, S; Centeno, MA
Catalysts, **13** (2023) 1039
Julio, 2023 · DOI: 10.3390/catal13071039

This work shows a new method for the preparation of 100% carbon-structured devices. The method is based on resorcinol-formaldehyde polymerization, using starch as a binder with the addition of a certain amount of external carbon source before polymerization. Molds obtained by 3D printing are used to shape the structured devices in the desired shape, and the ultimate pyrolysis step consolidates and produces the carbonaceous devices. The proposed method allows obtaining supports with different textural and surface properties varying the carbonaceous source, the solvent, or the pyrolysis conditions, among other factors. The as-obtained devices have demonstrated their usefulness as palladium supports for the gas-phase formic acid dehydrogenation reaction. The monolith shows a high conversion of formic acid (81% according to H_2 production) and a high selectivity towards hydrogen production at mild temperatures (80% at 423 K).

Methanation of CO_2 over High Surface Nickel/Aluminates Compounds Prepared by a Self-Generated Carbon Template
Roudane, S; Bettahar, N; Caballero, A; Holgado, JP
Catalysts, **13** (2023) 142
Enero, 2023 · DOI: 10.3390/catal13010142

Catalytic gas-phase hydrogenation of CO_2 into CH_4 was tested under three different nickel/aluminate catalysts obtained from precursors of hexaaluminate composition ($MAl_{16}O_{19}$, M = Mg, Ca, Ba). These catalysts were prepared using a carbon template method, where carbon is self-generated from a sol-gel that contains an excess of citric acid and the Al and M salts (Ba^{2+}, Ca^{2+}, Mg^{2+}) by two-step calcination in an inert/oxidizing atmosphere. This procedure yielded Ni particles decorating the surface of a porous high surface area matrix, which presents a typical XRD pattern of aluminate structure. Ni particles are obtained with a homogeneous distribution over the surface and an average diameter of ca 25-30 nm. Obtained materials exhibit a high conversion of CO_2 below 500 °C, yielding CH_4 as a final product with selectivity >95%. The observed trend with the alkaline earth cation follows the order NiBaAlO-PRx > NiCaAlO-PRx > NiMgAlO-PRx. We propose that the high performance of the NiBaAlO sample is derived from both an appropriate distribution of Ni particle size and the presence of $BaCO_3$, acting as a CO_2 buffer in the process.

Carbon Capture Enhancement by Water-Based Nanofluids in a Hollow Fiber Membrane Contactor
Yuan, CT; Pan, Z; Wang, Y; Baena-Moreno, FM; Constantinou, A; Zhang, Z
Energy Technology, **11** (2023) 2300254
Mayo, 2023 · DOI: 10.1002/ente.202300254

Nanoparticles are being used in the CO_2 solvents to improve the capture performance. Herein, a 2D model is proposed to study the CO_2 capture performance from a gaseous mixture using a hollow fiber membrane contactor (HFMC). Both water-based nanofluids of carbon nanotubes (CNT) and SiO_2 are deployed as the carbon absorbents. It is verified that Brownian motion and grazing effect are the major reasons to enhance the mass transfer of nanofluids. The simulation findings show that the modeling data conform well with the experimental studies. The root-mean-square errors for SiO_2 nanofluid and CNT nanofluid are 2.37% and 2.56%, respectively. When the amounts of nanoparticles increase between 0.02 and 0.06 wt%, CO_2 capture efficiencies of SiO_2 and CNT nanofluids increase by 7.92% and 13.17%, respectively. Also, the CNT nanofluid has a better capture performance than the SiO_2 nanofluid. Furthermore, research is conducted into how membrane characteristics affect HFMC performance. It is indicated that increasing the membrane porosity and decreasing the membrane tortuosity have a positive impact on the capture efficiency. This work demonstrates the potentials in the use of nanoparticles in CO_2 solvents and provides a solid theoretical basis for nanofluids to significantly enhance gas absorption.

MIL-100(Fe)-derived catalysts for CO_2 conversion via low- and high-temperature reverse water-gas shift reaction
Loe, JG; Pena, AP; Espejo, JLM; Bobadilla, LF; Reina, TR; Pastor-Pérez, L
Heliyon, **9** (2023) e16070
Mayo, 2023 · DOI: 10.1016/j.heliyon.2023.e16070

Fe-derived catalysts were synthesized by the pyrolysis of MIL-100 (Fe) metal-organic framework (MOF) and evaluated in the reverse water-gas shift (RWGS) reaction. The addition of Rh as a dopant by in-situ incorporation during the synthesis and wet impregnation was also considered. Our characterization data showed that the main active phase was a mixture of α-Fe, Fe_3C, and Fe_3O_4 in all the catalysts evaluated. Additionally, small Rh loading leads to a decrease in the particle size in the active phase. Despite all three catalysts showing commendable CO selectivity levels, the C@Fe* catalyst showed the most promising performance at a temperature below 500 °C, attributed to the in-situ incorporation of Rh during the synthesis. Overall, this work showcases a strategy for designing novel Fe MOF-derived catalysts for RWGS reaction, opening new research opportunities for CO_2 utilization schemes.

Mechanistic aspects of the reduction of rutile titanium dioxide and its Re-oxidation. Development and destruction of crystallographic shear structures

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Journal of Solid State Chemistry, **326** (2023) 124174
Octubre, 2023 · DOI: 10.1016/j.jssc.2023.124174

A model is presented giving the mean dimensions of acicular octadecahedral microcrystallites of a rutile titanium dioxide powder. Reduction at 823 K, in conjunction with ESR, electrical conductivity and controlled re-oxidation has enabled the model to be applied to reduced microcrystallites. At 300 K they contain <0.1% of paramagnetic [$Ti^{3+\uparrow}$ V_O: $^{\uparrow}Ti^{3+}$] reduced edge sites and >99.9% of reduced spin-paired [$Ti^{3+\uparrow\downarrow}$ Ti^{3+} V_O:] sites. These sites are situated on the external crystal faces and on polygonal bulk crystallographic shear (CS) structures inclined to the microcrystal four-fold symmetry axis. CS structures are quantum-sized [$Ti_4O_7V_O$:] environments which broaden the paramagnetic signals at 78 K. Temperature programmed reduction in H_2(g) reveals atomic hydrogen as a precursor to CS structure formation via a lattice template formed on microcrystallite faces. Shear structures are oxidised on their polygonal perimeters at differing rates on the respective microcrystallite faces by anionic vacancy transfer from sub-surface regions.

Formic Acid Dehydrogenation over Ru- and Pd-Based Catalysts: Gas- vs. Liquid-Phase Reactions

Ruiz-López, E; Pelaez, MR; Ruz, MB; Leal, MID; Tejada, MM; Ivanova, S; Centeno, MA
Materials, **16** (2023) 472
Enero, 2023 · DOI: 10.3390/ma16020472

Formic acid has recently been revealed to be an excellent hydrogen carrier, and interest in the development of efficient and selective catalysts towards its dehydrogenation has grown. This reaction has been widely explored using homogeneous catalysts; however, from a practical and scalable point of view, heterogeneous catalysts are usually preferred in industry. In this work, formic acid dehydrogenation reactions in both liquid- and vapor-phase conditions have been investigated using heterogeneous catalysts based on mono- or bimetallic Pd/Ru. In all of the explored conditions, the catalysts showed good catalytic activity and selectivity towards the dehydrogenation reaction, avoiding the formation of undesired CO.

Boosting the photocatalytic properties of $NaTaO_3$ by coupling with AgBr

Puga, F; Navío, JA; Hidalgo, MC
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Marzo, 2023 · DOI: 10.1007/s43630-022-00334-9

AgBr/$NaTaO_3$ composites, with different molar % of $NaTaO_3$ (Br/NTO(X%)), have been synthesized by simple precipitation methods; bare $NaTaO_3$ was synthesized by hydrothermal procedure, while AgBr was synthesized by a precipitation procedure using cetyl-tri-methyl-ammonium bromide (CTAB) and $AgNO_3$. Samples have been characterized by X-ray diffraction (XRD), N_2 adsorption, UV–vis diffuse reflectance spectroscopy (DRS), Fourier-transform infrared spectroscopy (FT-IR), Transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS). Photocatalytic activity of the as-prepared photo-catalysts was evaluated through photocatalytic degradation of rhodamine B (RhB), methyl orange (MO) and caffeic acid (CAFA) under UV and visible illumination. Single AgBr material and Br/NTO(X%) composites displayed the ability to absorb light in the visible region, while $NaTaO_3$ is only photoactive under UV irradiation. Based on the position of conduction and valence bands of AgBr and $NaTaO_3$, the heterojunction between these two photo-catalysts corresponds to a type II junction. In the case of photocatalytic degradation of RhB and CAFA, Br/NTO(x%) composites have highest photocatalytic activity than that obtained by both parental materials under the same operational conditions. AgBr and Br/NTO(x%) composites achieve a fast degradation of MO, together with a considerable adsorption capacity, attributed to the presence of a remaining amount of residual CTAB on the AgBr surface. In summary, coupling AgBr with $NaTaO_3$ improves the photocatalytic activity under both UV and visible illumination with respect to the parental components, but the performance of the composites is highly dependent on the type of substrate to be degraded and the illumination conditions.

Effect of phenol concentration on the photocatalytic performance of ZnO nanoparticles

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Febrero, 2023 · DOI: 10.1002/jctb.7334

BACKGROUND: Phenol and its derivatives are considered toxic compounds, even at low concentrations. Their accumulation in water effluents has become a serious problem that could be resolved by using zinc oxide (ZnO)-based photocatalysts.
RESULTS: ZnO nanoparticles were synthesized through the precipitation method, using zinc nitrate and sodium carbonate as reagents. The as-synthesized powder was calcined for 4 h at 500 °C (2°C min^{-1}. X-Ray diffraction analysis confirmed a hexag-onal crystalline phase (wurtzite) with an average crystallite size of 38 nm. The Kubelka-Munk method was used to determine a band gap of 3.27 eV through UV-Vis diffuse reflectance spectrum and a Brunauer-Emmett-Teller (BET) specific area of 12 m^2g^{-1} was obtained from N_2 adsorption analysis. The photocatalytic activity of ZnO was evaluated under visible light (300 W) lamp, with 1 mg mL^{-1} of photocatalyst and using phenol solutions at different concentrations of 5,10, 25, and 50 ppm; the obtained degradation percentages were 98%, 97%, 94%, and 71%, respectively. Three cycles were performed with the ZnO used in the reactions with phenol at 5 and 50 ppm, decreasing the degraded percentages to 87% and 65%, respectively. The generation of hydroxyl radicals was estimated for the ZnO and ZnO samples after three cycles by means of fluorescence spectroscopy analy-sis. It was observed that the first-used ZnO material generated a significant amount of hydroxyl radicals.

CONCLUSION: When compared to ZnO after three cycles of reaction, the amount of generated hydroxyl radicals decreased. It was observed that the higher the amount of phenol, the lower the generation of hydroxyl radicals after reuse; this was probably due to the presence of some adsorbed by-products of the photocatalytic reaction on the surface of ZnO, as the FTIR spectrum of the post-reaction sample showed.

Engineering exsolved catalysts for CO_2 conversion

Ali, SA; Safi, M; Merkouri, LP; Soodi, S; Iakovidis, A; Duyar, MS; Neagu, D; Reina, TR; Kousi, K
Frontiers in Energy Research, **11** (2023) 1150000
Marzo, 2023 · DOI: 10.3389/fenrg.2023.1150000

Introduction: Innovating technologies to efficiently reduce carbon dioxide (CO_2) emission or covert it into useful products has never been more crucial in light of the urgent need to transition to a net-zero economy by 2050. The design of efficient catalysts that can make the above a viable solution is of essence. Many noble metal catalysts already display high activity, but are usually expensive. Thus, alternative methods for their production are necessary to ensure more efficient use of noble metals.
Methods: Exsolution has been shown to be an approach to produce strained nanoparticles, stable against agglomeration while displaying enhanced activity. Here we explore the effect of a low level of substitution of Ni into a Rh based A-site deficienttitanate aiming to investigate the formation of more efficient, low loading noblemetal catalysts.Results: We find that with the addition of Ni in a Rh based titanate exsolution is increased by up to similar to 4 times in terms of particle population which in turn results in up to 50% increase in its catalytic activity for CO_2 conversion.
Discussion: We show that this design principle not only fulfills a major research need in the conversion of CO_2 but also provides a step-change advancement in the design and synthesis of tandem catalysts by the formation of distinct catalytically active sites.

Toluene combustion on MnO_x, CeO_2, and Mn-Ce-O solids prepared via citrate complexation, and citrate and urea combustion methods

Rahou, S; Benadda-Kordjani, A; Ivanova, S; Odriozola, JA; Chebout, R; Mahzoul, H; Zouaoui, N
Journal of Nanoparticle Research, **25** (2023) 114
Junio, 2023 · DOI: 10.1007/s11051-023-05759-6

MnO_x, CeO_2, and MnCe-O (Mn/Ce = 1) solids have been prepared via the citrate complexation and combustion method using citrate and urea precursors. The solids have been characterized by XRD, SEM-EDX, N_2-adsorption-desorption, UV-Vis spectroscopy, TPR, O_2-TPD, and XPS techniques. The catalytic reactivity of the manganese oxides was not affected by the preparation protocol. In the case of ceria and mixed oxides, the synthesis method greatly affected the structural and chemical properties, ultimately altering their reactivity. The citrate complexation method produced the most homogeneous and active mixed oxide, whereas the urea combustion method resulted in less active solids. The mixed oxide prepared via urea combustion was less active than the manganese single oxide; the decrease in activity was attributed to phase separation and the formation of Mn_3O_4 domains on the surface of ceria. In contrast, citrate complexation resulted in solids with the lowest particle size (similar to 3 nm), the highest oxidation state for manganese, and the highest proportion of oxygen vacancies, which promote the oxidation reaction.

ZnO/TiO_2 and ZnO/Nb_2O_5 as effective systems for the treatment of enteric bacteria and commercial dyes

Hernandez, JS; Murcia, JJ; Rojas, H; Hidalgo, MC; Navio, JA
Revista Facultad de Ingeniería-Universidad de Antioquia, **108** (2023) 9-17
Julio, 2023 · DOI: 10.17533/udea.redin.20220785

In this study, ZnO/TiO_2 and ZnO/Nb_2O_5 photocatalysts were evaluated in the river pollution remediation and wastewater treatment from textile factories, thus, the target pollutants selected for this study were enteropathogenic bacteria and commercial dyes. The mixed oxide systems were extensively analyzed in order to explore their physicochemical properties. From this analysis, it was found that the coupling of two oxides did not modify the crystallinity of the pristine semiconductors. As a result, XRD Wurtzite phase, hexagonal phase, and anatase phases were identified for ZnO, Nb_2O_5, and TiO_2 photocatalyst, respectively. Using UV-Vis DRS, a higher absorption for mixed oxides in the visible region of the electromagnetic spectrum was observed, along with a decrease in the band gap value in these materials. The results of the photocatalytic activity evaluation showed that the coupling of ZnO with Nb_2O_5 and TiO_2 increased the effectiveness of the total organic carbon (TOC) and E. Coli elimination. 83% of TOC and elimination of 64% of E. coli were achieved using ZnO/Nb_2O_5 photocatalyst for the treatment of water samples from the polluted river.

Photocatalytic treatment based on TiO_2 for a coal mining drainage

Murcia-Mesa, JJ; Patino-Castillo, CG; Rojas-Sarmiento, HA; Navio-Santos, A; Hidalgo-López, MD; Angel-Botero, A
Revista Facultad de Ingeniería-Universidad de Antioquia, **107** (2023) 88-101
Abril, 2023 · DOI: 10.17533/udea.redin.20211063

The aim of the present work was to evaluate the effectiveness of a heterogeneous photocatalyst based on TiO_2 in the treatment of coal mining drainage which contains a variety of heavy metals and high concentration sulfates and sulfides. The photocatalytic behavior of the commercial reference Sigma Aldrich and the different materials synthesized using the Sol-gel methodology with surface modifications using sulfation and fluorination processes were analyzed. To find a possible correlation between the physicochemical properties of photocatalysts and their behavior, a characterization was carried out using X-Ray Diffraction (XRD), X-Ray Fluorescence spectrometry (XRF), Fourier transform infrared spectroscopy (FT-IR), UV-Vis diffuse reflectance Spectra (UV-Vis DRS), N_2 physisorption, X-ray photoelectron spectroscopy (XPS), and particle size analysis. Results indicated that the modification of the TiO_2 prepared in the laboratory using sulfation and fluorination allowed the successful control of the physicochemical properties of this oxide. However, commercial TiO_2 showed the greatest effectiveness in removing metals such as: Fe, Cu, Cr, and As after a photocatalytic reaction for a maximum of 1 hour under continuous nitrogen flow and a light intensity of 120 W/m^2.

Charting a path to catalytic upcycling of plastic micro/nano fiber pollution from textiles to produce carbon nanomaterials and turquoise hydrogen

Parrilla-Lahoz, S; Zambrano, MC; Stolojan, V; Bance-Soualhi, R; Pawlak, JJ; Venditti, RA; Ramirez Reina, T; Duyar, MS
RSC Sustainability, **1** (2023) 1177-1183
Agosto, 2023 · DOI: 10.1039/D3SU00095H

Washing synthetic textile fibers releases micro/nano plastics, endangering the environment. As new filters and associated regulations are developed to prevent fiber release from washing machines, there emerges a need to manage the collected waste, for which the only current options are combustion or landfill. Herein we show for the first time the application of a catalytic pyrolysis approach to upcycle textile derived fibrous micro/nano plastics waste, with the aim of keeping carbon in the solid phase and preventing its release as a greenhouse gas. Herein, we demonstrate the co-production of hydrogen and carbon nanomaterials from the two most prevalent global textile microfiber wastes: cotton and polyester. Our results pave a way forward to a realistic process design for upcycling mixed micro/nano fiber waste collected from laundering, drying, vacuuming, and environmental cleanup.

Effect of Alkaline Salts on Pyrolyzed Solid Wastes in Used Edible Oils: An Attenuated Total Reflectance Analysis of Surface Compounds as a Function of the Temperature
Romero-Sarria, F; Real, C; Córdoba, JM; Hidalgo, C; Alcalá, MD
Spectroscopy Journal, **1** (2023) 98-110
Septiembre, 2023 · DOI: 10.3390/spectroscj1020009

Biochars obtained via the pyrolysis of biomass are very attractive materials from the point of view of their applications and play key roles in the current energy context. The characterization of these carbonaceous materials is crucial to determine their field of application. In this work, the pyrolysis of a non-conventional biomass (solid wastes in used edible oils) was investigated. The obtained biochars were characterized using conventional techniques (TG, XRD, and SEM-EDX), and a deep analysis via ATR-FTIR was performed. This spectroscopic technique, which is a rapid and powerful tool that is well adapted to study carbon-based materials, was employed to determine the effect of temperature on the nature of functional groups on the surface. Moreover, the water washing of the raw sample (containing important quantities of inorganic salts) before pyrolysis evidenced that the inorganic salts act as catalysts in the biomass degradation and influence the degree of condensation (DOC) of PAH. Moreover, it was observed that these salts contribute to the retention of oxygenated compounds on the surface of the solid.

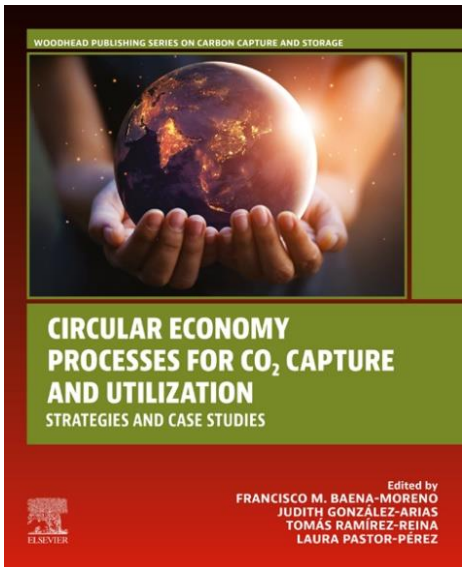
ARTICULOS PUBLICADOS EN REVISTAS (NO SCI) / PAPERS IN NON-SCI JOURNALS

Formic Acid as Renewable Reagent and Product in Biomass Upgrading
Achour, M; Álvarez-Hernández, D; Ruiz-López, E; Megías-Sayago, C; Ammari, F; Ivanova, S; Centeno, MA
Tetrahedron Green Chemistry, 2 (2023) 10020
Diciembre, 2023 · DOI: 10.1016/j.tgchem.2023.100020

Thermodynamic Equilibrium Modelling for the Optimal Performance of a Wood Biomass Downdraft Gasifier for Hydrogen Production
Kushwah, A; Ramírez-Reina, T; Short, M
Computer Aided Chemical Engineering, 52 (2023) 203-208
DOI: 10.1016/B978-0-443-15274-0.50033-0

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Circular Economy Processes for CO_2 Capture and Utilization · Strategies and Case Studies



Editors: Francisco M. Baena-Moreno, Judith González-Arias, Tomás Ramírez-Reina, Laura Pastor-Pérez
Language: English
Paperback ISBN: 9780323956680
eBook ISBN: 9780323956697
N. Páginas: 386

Description: Circular Economy Processes for CO_2 Capture and Utilization: Strategies and Case-Studies presents an innovative resource or integrating carbon capture, storage and utilization into the sustainable circular economy of the future. Split into two parts, the book offers readers a grounding in the fundamentals of the circular economy and the potential contribution of CCS. Strategies for implementing CCS into a circular economy are explained, with benefits and limitations analyzed. The book then offers a gallery of case studies from the newest research in the area, allowing readers to access lessons learned and critical considerations for integrating CCS into the circular economy.
Marrying theory and practice for a holistic perspective, this book offers readers an essential guide to theorizing and implementing a sustainable future economy that utilizes the full potential of carbon capture.

Capítulo 01 - Páginas 001-004
Introduction to strategies for implementing CO_2 utilization in circular economy processes
J. González-Arias, F.M. Baena. L. Pastor-Pérez, T.R. Reina

Capítulo 05 - Páginas 093-118
Catalytic processes for fuels production from CO_2-rich streams: Opportunities for industrial flue gases upgrading
L.P. Merkouri, Q. Zhang, T.R. Reina, M.S. Duyar

Capítulo 10 - Páginas 233-251
Profitability analysis of biomethane and calcium carbonate co-production from biogas and FGD gypsum
J. González-Arias, F.M. Baena. L. Pastor-Pérez, T.R. Reina

Capítulo 12 - Páginas 271-286
Methanation of unconventional flue gases
J.C. Navarro, E. Ruiz-López, S. Ivanova, M.A. Centeno

Capítulo 14 - Páginas 307-323
Valorization of unconventional CO_2-rich feedstock via reverse water gas shift reaction
M. González-Castaño, P. Tarifa, A. Monzón, H. Arellano-García

Capítulo 16 - Páginas 347-367
$MgCO_3$ production from $MgCl_2$ waste and CO_2: A process design and economic approach
J. González-Arias, F.M. Baena-Moreno, L. Pastor-Pérez, T. Ramírez-Reina

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

26th World Congress & Exhibition Ozone and Advanced Oxidation
02-07 julio · Milán, Italia

Peroxydisulphate Activation by Ag/TiO_2 Under Sunlight: elucidation of routes for a fluoroquinolone degradation, evolution of the antimicrobial activity, and potentialities for water disinfection. *S.D. Jojoa-Sierra, C. Jaramillo-Páez, M.C. Hidalgo, J.A. Navío, M.P. Ormad, E.A. Serna-Galvis, R.A. Torres-Palma, R. Mosteo.* PÓSTER

15th European Congress on Catalysis · EUROPACAT2023
27 agosto - 01 septiembre · Praga, República Checa

CO_2 upgrading via low-temperature RWGS reaction: operando mechanistic insights to guide an optimal catalysts design. *G. Torres-Sempere, L.A. Luque-Álvarez, L.F. Bobadilla, T.R. Reina, L. Pastor-Pérez, J.A. Odriozola.* COMUNICACIÓN ORAL

Dual function material design for circular methanol economy. *A.I. Paksoy, A. Goksu, T.R. Reina, M.S. Duyar.* COMUNICACIÓN ORAL

Hydrogen charge/discharge cycles via formic acid on Pd/activated carbon catalyst. *M. Ribota, M.I. Domínguez, M.A. Centeno, S. Ivanova.* COMUNICACIÓN ORAL

Vanadium-based catalysts for the sustainable production of formic acid from glucose. *D. Álvarez-Hernández, M.I. Domínguez, M. Martínez Tejada, S. Ivanova, M.A. Centeno.* COMUNICACIÓN ORAL

Engineering exsolved catalysts for CO_2 utillisation. *S.A. Ali, M. Safi, L.P. Merkouri, S. Soodi, A. Iakovidis, M.S. Duyar, D. Neagu, T.R. Reina, K. Kousi.* PÓSTER

Catalytic pyrolysis can offer a means to upcycle micro/nano plastics released from synthetic fibres during laundering. *S. Parrilla-Lahoz, M.C. Zambrano, V. Stolojan. R. Bance-Soualhi, J.J. Pawlak, R.A. Venditti, T.R. Reina, M.S. Duyar.* PÓSTER

8th International Conference on Semiconductor Photochemistry · SP8
11-15 septiembre · Estrasburgo, Francia

Evaluation of the disinfection capacity on bacteria and protozoa of the photo-assisted advanced technologies based on faceted F-TiO_2. *M.C. Hidalgo, L. Pérez-Luna, P. Goñi, N. Larumbe, R. Mosteo.* PÓSTER

Heterostructured $NaTaO_3$-WO_3 systems with improved photocatalytic properties for water decontamnination under UV and visible illumination. *M.C. Hidalgo, M. Hernández-Laverde, M. Patiño-Quintero, J.A. Navío, J.J. Murcia.* PÓSTER

Peroxydisulphate activation by Ag/ZnO under sunlight: Elucidation of routes during water disinfection. *S.D. Jojoa-Sierra, C. Jaramillo-Páez, M.C. Hidalgo, J.A. Navío, I. García Rubio, M.P. Ormad, E.A. Serna-Galvis, R.A. Torres-Palma, R. Mosteo.* PÓSTER

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

I Congreso de Química Aplicada a la Energía y al Medio Ambiente · QUIEMA-23
12 – 23 junio · Córdoba, España

Hacia un modelo energético sostenible: La economía del hidrógeno. *M.A. Centeno.* CONFERENCIA PLENARIA

Reunión de la Sociedad Española de Catálisis · SECAT'23
20-23 junio · Torremolinos, Málaga, España

Catalizadores basados en óxido de vanadio para la producción de ácido fórmico a partir de glucosa. *D. Álvarez, M.I. Domínguez, M. Martínez, S. Ivanova, M.A. Centeno.* COMUNICACIÓN ORAL

Estudio de micro-monolitos catalíticos Ni-Mg-Ce/CDC para la metanación de CO_2. *F. Cazaña, P. Tarifa, E. Romero, N. Latorre, M.A. Centeno, L.M. Martínez, M.I. Domínguez, S. Ivanova, A. Monzón.* COMUNICACIÓN ORAL

Ni stabilised on inorganic complex structures based on cerium and zirconium for dry reforming of methane. *J.L. Martín-Espejo, L.P. Merkouri, J. Gándara-Loe, J.A. Odriozola, T.R. Reina, L. Pastor-Pérez.* COMUNICACIÓN ORAL

Operando study of the Fischer-Tropsch reaction for the production of hydrocarbons on iron-potassium catalysts. *R. Blay-Roger, L.F. Bobadilla, M.A. Nawaz, T. Ramírez-Reina, J.A. Odriozola.* COMUNICACIÓN ORAL

Cobalt/APTES Functionalized TiO_2 for Fischer-Tropsch Reaction. *F.J. Platero, A. Caballero, G. Colón.* PÓSTER

Cobalt-based Mesoporous TiO_2 Catalyst for Fischer-Tropsch Reaction. *F.J. Platero, L. Aoudjera, L. Michelin, B. Lebeau, J.L. Blin, S.Z. Todorova, G. Colón, A. Caballero.* PÓSTER

Efecto de Ru como Promotor en Catalizadores Co/TiO_2 para la Síntesis de Fischer-Tropsch. *F.J. Platero, J.P. Holgado, A. Caballero, G. Colón*. PÓSTER

Improving the H_2 Photoproduction by Using Binary Cu/TiO_2-$SrTiO_3$ Heterojunction. *G. Colón, M. González-Tejero, J.G. Villachica-Llamosas, A. Ruiz-Aguirre*. PÓSTER

Is water assisted HDO a viable route for biofuel production? Using ru-based catalysts and model compounds as case of study. *S. Carrasco-Ruiz, S. Parrilla-Lahoz, A. Penkova, J.A Odriozola, J.L. Santos, T.R. Reina, L. Pastor-Pérez*. PÓSTER

Efecto de la estructura cristalina de materiales basados en MnO_2 para la producción de ácido fórmico. *D. Álvarez, M.I. Domínguez, M. Martínez, S. Ivanova, M.A. Centeno*. PÓSTER

Dynamic study of the influence of morphology on Pd/CeO_2 catalysts for methanol decomposition. *L.A. Luque-Álvarez, A. Núñez-Carballo, B. Lacroix, L.F. Bobadilla, L. Pastor-Pérez, M.A. Centeno, J.A. Odriozola*. PÓSTER

Ciclos de carga y descarga de hidrógeno en catalizadores basados en Pd/C. *M. Ribota Peláez, M.I. Domínguez Leal, M.A. Centeno, S. Ivanova*. PÓSTER

Catalysts design for CO_2 methanation beyond ideal conditions: upgrading of biomass gasification streams. *G. Torres-Sempere, L.F. Bobadilla, L. Pastor-Pérez, J.A. Odriozola, T.R. Reina*. PÓSTER

Influencia de la temperature de descomposición de metano con catalizadores de Fe-Mg-Al. *F.D. Martín, F. Cazaña, E. Romeo, R. Mallada, P. Tarifa, M.A. Centeno, A. Monzón*. FLASH PÓSTER

Seminario Técnico: Contaminantes Emergentes en Aguas y Lodos

20-21 julio · Oviedo, España

Biochar procedente de residuos agrícolas: en busca de materiales alternativos de bajo coste para la eliminación de antibióticos en agua. *S. Moles, N. Miguel, M.P. Ormad, M.C. Hidalgo, F. Romero, R. Mosteo*. COMUNICACIÓN ORAL

XXXVII Jornadas Nacionales de Ingeniería Química
13-15 septiembre · Castellón, España

Evaluación de la capacidad desinfectante de procesos fotoasistidos mediante TiO_2 facetado. *N. Larumbe, S. Moles, P. Goñi, M.C. Hidalgo, M.P. Ormad, R. Mosteo*. PÓSTER

XIII Simposio Colombiano de Catálisis · XIII-SiCCat
11-13 octubre · Bucaramanga, Colombia

Procesos de washcoating de hidrotalcitas (HT) de NiCo para la fabricación de monolitos de FeCralloy. *C.A. Rodríguez Monroy, M. Martínez T., M.A. Centeno, S. Moreno, R. Molina*. PÓSTER

Modificaciones Superficiales de TiO_2 con actividad fotocatalítica mejorada en la degradación de Cafeína. *M. Hernández-Laverde, J.J. Murcia, M.C. Hidalgo, J.A. Navío*. PÓSTER

XVI Reunión del GEC
22-25 octubre · Gijón, España

Influencia de la concentración de Fe en la descomposición de metano con catalizadores de Fe-Mg-Al. *D. Martín, F. Cazaña, E. Romeo, R. Mallada, P. Tarifa, M.A. Centeno, A. Monzón*. COMUNICACIÓN ORAL

Catalizadores Ni-Ce-Mg soportados sobre carbón derivado de celulosa (CDC) estructurados sobre micromonolitos metálicos para la metanación de CO_2. *F. Cazaña, P. Tarifa, E. Romeo, N. Latorre, M.A. Centeno, L.M. Martínez, M.I. Domínguez, S. Ivanova, A. Monzón*. COMUNICACIÓN ORAL

Estructuración de un catalizador Pd/C_3N_4 para la producción de hidrógeno por descomposición de ácido fórmico. *V. Ramírez, M.I. Domínguez, L.M. Martínez, S. Ivanova, A. Monzón, F. Cazaña, M.A. Centeno*. PÓSTER

Carbones nitrogenados como soportes de catalizadores para la producción de ácido fórmico vía hidrogenación de CO_2. *M. Puente Dorado, M. Ribota Peláez, E. Ruiz López, M.I. Domínguez, L.M. Martínez, S. Ivanova, M.A. Centeno*. PÓSTER

V Congreso de Procesos Avanzados de Oxidación. II Simposio de Química Básica y Aplicada
01-03 noviembre · Santiago de Cali, Colombia

Fotocatalizadores heteroestructurados soportados en biocarbones para procesos de descontaminación de agua y desinfección. M.C. Hidalgo. CONFERENCIA INVITADA

Inmovilización de fotocatalizadores basados en TiO_2 facetado y estudio de su desempeño fotocatalítico en fase gas. *M. Hernández, J. Murcia, M.C. Hidalgo, J.A. Navío, N. Morante, D. Sannino*. COMUNICACIÓN ORAL

Explorando las actividades fotocatalíticas de un TiO_2 con alta exposición de la cara {001} sensibilizado por acoplamiento con AgBr o Ag_3PO_4. *F. Puga, M.A. Paulete-Romero, J.M. Córdoba, M.C. Hidalgo, J.A. Navío*. COMUNICACIÓN ORAL

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Optimización de Sistemas Catalíticos de Co Activos para la Síntesis de Fischer-Tropsch: Efecto de la Adición de un Segundo Metal, la Estructuración del Soporte y el Anclaje del Metal a la Superficie**
Autor:	Francisco Jesús Platero Moreno
Directores:	Alfonso Caballero Martínez, Gerardo Colón Ibáñez
Centro:	Universidad de Sevilla
Fecha Defensa:	30 de junio de 2023

Título:	**Préparation et caractérisation des catalyseurs type hexa-aluminates pour des applications environmentales basées sur des reactions de méthanation**
Autor:	Sarra Roudane
Directores:	Noureddin Bettahar, Juan Pedro Holgado Vázquez
Centro:	Universidad de Sevilla
Fecha Defensa:	01 de septiembre de 2023

FORMACIÓN DE POSTGRADO / MASTER DEGREE THESIS

Título:	**Characterization of thermoplastic composite-composite welded joints and metal (TITANIUM64)-composite adhesive joints**
Autor:	Marina León Lago
Tutores:	Sergio González López, (CATEC), Marcela Martínez Tejada
Grado:	Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro:	Universidad de Sevilla
Fecha Defensa:	05 de julio de 2023

Título:	**Estructuración de catalizadores para la producción de hidrógeno libre de CO por descomposición de ácido fórmico**
Autor:	Víctor Ramírez Cerezo
Tutores:	Miguel Angel Centeno Gallego, María Isabel Domínguez Leal, Marcela Martínez Tejada
Grado:	Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro:	Universidad de Sevilla
Fecha Defensa:	05 de julio de 2023

Título:	**Silicalita de titanio (TS-1) para la biorrefinería: Intensificación de reacciones de (epo)oxidación**
Autor:	Ignacio Centeno Vega
Tutores:	Svetlana Ivanova, Cristina Megías Sayago (IIQ)
Grado:	Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro:	Universidad de Sevilla
Fecha Defensa:	05 de julio de 2023

Título:	**Cracking de metano para la producción de H_2 con catalizadores de Fe**
Autor:	Juan Rodríguez Casado
Tutores:	Marcela Martínez Tejada, Miguel Angel Centeno Gallego, María Isabel Domínguez Leal
Grado:	Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro:	Universidad de Sevilla
Fecha Defensa:	05 de julio de 2023

Título:	**Obtención de productos de alto valor añadido a partir de azúcares: deshidratación de fructosa a HMF**
Autor:	Carmen Cabello Illanes
Tutores:	Marcela Martínez Tejada, Miguel Angel Centeno Gallego
Grado:	Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro:	Universidad de Sevilla
Fecha Defensa:	05 de septiembre de 2023

Título:	**Optimización de catalizadores basados en tungsteno para la valorización de biomasa: aplicación de reacciones de oxidación**
Autor:	Adrián Montilla Pérez
Tutores:	Svetlana Ivanova, Cristina Megías Sayago (IIQ)

Grado: Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro: Universidad de Sevilla
Fecha Defensa: 05 de septiembre de 2023

Título: **Processability of aluminium alloys by PDF-L/M additive manufacturing**
Autor: Ignacio González-Barba Gómez
Tutores: Marcela Martínez Tejada
Grado: Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro: Universidad de Sevilla
Fecha Defensa: 05 de septiembre de 2023

Título: **Uso de biocarbones para la adsorción de metales pesados en aguas residuales industriales**
Autor: Ana Moreno Parejo
Tutores: Nuria Ofelia Núñez Álvarez, Francisca Romero Sarriá, María del Carmen Hidalgo López
Grado: Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro: Universidad de Sevilla
Fecha Defensa: 15 de septiembre de 2023

FORMACIÓN DE GRADUADOS / BACHELOR DEGREE THESIS

Título: **Catalizadores heterogéneos para la producción de ácido fórmico por procesos de biorrefinería**
Autor: Leonardo Canales Quesada
Tutores: Miguel Angel Centeno Gallego, María Isabel Domínguez Leal
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 25 de abril de 2023

Título: **Catalizadores de Co para la reacción de Reverse Water-Gas Shift**
Autor: María Jordano Cruz
Tutores: Anna Penkova, Miriam González Castaño
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 26 de junio de 2023

Título:	**Efectos de tratamientos en biocarbones producidos desde biomasa vegetal para su uso como soportes de fotocatalizadores**
Autor:	Alejandro Duque Ponce
Tutores:	José Manuel Córdoba Gallego, María del Carmen Hidalgo López
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	25 de julio de 2023

Título:	**Hidrogenación de CO_2 para la producción de ácido fórmico con catalizadores heterogéneos**
Autor:	Mario Puente Dorado
Tutores:	Marcela Martínez Tejada, María Isabel Domínguez Leal
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	21 de julio de 2023

Título:	**Síntesis y caracterización de materiales con aplicaciones fotocatalíticas**
Autor:	Mauricio Patiño Quintero
Tutores:	Francisca Romero Sarria, María del Carmen Hidalgo López
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	24 de julio de 2023

DOCENCIA / TEACHING

MÁSTER EN CIENCIA Y TECNOLOGÍA DE NUEVOS MATERIALES

Catalizadores para la Energía y el Medio Ambiente Dr. José Antonio Odriozola Gordón, Dr. Tomás Ramírez Reina
Corrosión y Recubrimientos Protectores Dra. Marcela Martínez Tejada
Materiales con Funcionalidad Superficial Dra. Marcela Martínez Tejada
Química del Estado Sólido Dr. Luis Bobadilla Baladrón
Recuperación y Transformación de Materiales Dra. Marcela Martínez Tejada, Dra. M. Isabel Domínguez Leal, Svetlana Ivanova
Técnicas de Caracterización de Materiales Anna Dimitrova Penkova

El personal del ICMS imparte docencia en titulaciones de Grado y Doble Grado de la Universidad de Sevilla. La docencia se desarrolla en diversos centros: Facultad de Física, Facultad de Biología, Facultad de Química, Facultad de Farmacia y Escuela Técnica Superior de Ingeniería Informática.

ESTANCIAS DE INVESTIGADORES EN EL ICMS
PERSONNEL OF THE OTHER LABORATORIES IN THE ICMS

Università degli Studi di Trieste		
Trieste, Italia	**Letizia Liccardo**	14/11/22 - 15/03/23
Universidad Nacional de Colombia		
Bogotá, Colombia	**Cesar Andrés Rodríguez Monroy**	12/09/22 - 17/03/23

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European Federation of Catalysis Societies EFCATS
Dr. Tomás Ramírez Reina
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XI Premio Losada Villasante
Dra. Laura Pastor Pérez
Premio a la Investigación en Economía Circular por su trabajo "Conversión avanzada de biogás a precursores de bioplásticos y textiles renovables: soluciones catalíticas para una economía circular'"

Premio Real Academia Sevillana de Ciencias 2023
Dra. Laura Pastor Pérez
Premio a Investigadores Jóvenes por su trayectoria científica

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Accesorio DRIFTS, celdas de alta y baja temperatura
- Analizador de Carbón Orgánico (TOC-V CHP Shimadzu 5000ª)
- Baño de ultrasonidos: P-Selecta Ultrasons Medi-II
- Cromatógrafos de Gases
- Cromatografos de líquidos HPLC
- Dip-Coater con cámara de temperatura
- Equipo de ultra-alto vacío para espectroscopía XPS y Auger equipado con cañón de argón para realizar devastado iónico.
- Espectrofotómetro FTIR con celdas DRIFTS y ATR.
- Espectrómetro de masas: Balzers Thermostar
- Espectrómetro UV-Vis, con esfera integradora para muestras sólidas)
- Espectrómetros de masas
- Estufas
- Horno de soldadura: Microtest Máquina de ensayos EM2/200/FR

- Horno Energon
- Horno para tratamiento de aceros a alta temperatura equipado con medidores de flujo e inyector de agua.
- Micro-cromatógrafos, microGC
- Microscopio metalográfico
- Molino de bolas de movimiento planetario PM100 de RETSCH
- pH-metros
- Planta Piloto de Integración de reacciones catalíticas Reference PID Eng&Tech
- Reactores catalíticos de gases con detección por cromatografía de gases y espectrometría de masas.
- Reactores catalíticos de líquidos de alta presión y temperatura con agitación interna y control de flujo de gases.
- Reactores fotocatalíticos con lámparas de Xe y Hg.
- Reactores fotocatalíticos con lámparas Led, UV y Visible.
- Rotavapor
- Sistema de análisis TPR/TPO con detector TCD y espectrómetro de masas.
- Sistema de vacío cuarzo/vidrio para adsorción de moléculas sonda seguido por FT-IR

INGENIERÍA DE CERÁMICOS PARA AMBIENTES EXTREMOS

ENGINEERED CERAMICS FOR EXTREME ENVIRONMENTS

GRUPO DE INVESTIGACIÓN

Materiales de Diseño para la Energía y Medioambiente | 642007

Designed Materials for the Energy and Environment

http://mem.icms.us-csic.es/

PERSONAL / PERSONNEL

Catedráticos de Universidad	Miguel Ángel Castro Arroyo Manuel Jiménez Melendo Pilar Malet Maenner Julián Martínez Fernández Antonio Ramírez de Arellano-López Joaquín Ramírez Rico
Investigadores Científicos	María Dolores Alba Carranza
Científicos Titulares	José Jesús Benítez Jiménez
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Doctores Contratados	Joâo Carlos Mesquita Coelho Esperanza Pavón González

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Cerámicas Conductoras de Protones para Electrolizadores Reversibles de Alta Eficiencia y Aplicaciones Power to X

Proton conducting ceramics for high efficiency reversible electrolyzers and power to X applications

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2019-107019RB-I00	01-06-2020 31-05-2023	Ministerio de Ciencia e Innovación	72.600 €

Investigador Principal Research Head	Componentes Research Group
Joaquín Ramírez Rico Ricardo Chacartegui Ramírez	Alfonso Bravo León Manuel Jiménez Melendo Julián Martínez Fernández Miguel Torres García

RESUMEN / ABSTRACT

PROCEX aborda el Reto social 3 "Energía limpia, eficiente y segura" y pretende abrir camino a una nueva generación de electrolizadores reversibles de alta eficiencia que operan a temperaturas intermedias (sobre 500°C). Su éxito abriría una vía muy prometedora para nuevos sistemas de almacenamiento de energía fotovoltaica y eólica con características sobresalientes, tales como eficiencias de ida y vuelta (superiores al 75%) o tasas de retorno energético (>10). Estos valores son muy superiores a los que se pueden alcanzar con los mejores sistemas de almacenamiento térmico. Además, el uso de electrolizadores de alta eficiencia encontraría un enorme campo de aplicación en la producción de H_2 y en la industria química. Para desarrollar estos sistemas, es necesario superar numerosos retos en el ámbito de los materiales cerámicos: en particular, es necesario desarrollar nuevos electrolitos conductores de protones con baja conductividad electrónica.

El objetivo principal del proyecto es identificar, sintetizar y demostrar nuevos materiales cerámicos conductores de protones con bajas pérdidas electrónicas en electrólisis, usando estrategias de dopado en compuestos de circonatos y ceratos de bario. Ponemos énfasis no sólo en mejorar la eficiencia sino también en la durabilidad de estos materiales. El proyecto demostrará el procesado de los electrolitos y su integración en pilas tipo botón a escala laboratorio, y estudiará los principales mecanismos de reacción, desarrollando modelos que permitan predecir su comportamiento a gran escala. Este proyecto parte de resultados publicados muy recientemente en la literatura y pretende superarlos apoyándose en las capacidades y experiencia previa del equipo investigador. En el proyecto ampliaremos el rango de composiciones y dopantes a estudiar y realizaremos un estudio sistemático que nos permita

relacionar la composición y procesado con las propiedades y el rendimiento en condiciones de servicio (i.e. la degradación y el envejecimiento). A partir de la información obtenida pretendemos desarrollar y validar nuevos modelos que permitan evaluar la integración de estos sistemas en distintas aplicaciones. La ambición del este proyecto requiere un tratamiento multidisciplinar fruto de la combinación de dos grupos de investigación, uno de Ciencia de Materiales y otro de Ingeniería Energética, que poseen las capacidades e instalaciones necesarias para llevar a buen término el proyecto: síntesis y procesado de materiales, caracterización física, modelado numérico e integración de sistemas de almacenamiento de energía.

PROCEX is aimed at the Social Challenge 3 "Secure, Clean and Efficient Energy". It aims to open a new pathway for high-efficiency reversible electrolyzers for intermediate temperatures (around 500ºC). Its successful development would open a very promising pathway for energy storage systems in PV and Wind facilities with outstanding characteristics, round-trip efficiencies (75% or higher), and Energy Returned On Investment (>10). These values are much higher than those that can be reached with state of art of thermal energy storage systems. Besides, such a high efficiency concept electrolyzer would have a huge field of application for H_2 production and application in the chemical industry. To develop such systems, several materials challenges need to be solved. In particular, novel electrolytes formulations with reduced electronic conductivities are needed.

The project is aimed at the identification and demonstration of new proton conducting ceramic materials that will have reduced electronic leakages in electrolysis operation, based on doping and co-doping strategies in barium cerate and zirconate systems. Emphasis will be placed not only in improving the efficiency but also the durability of such materials. The project will demonstrate the manufacturing of material and electrolyte at laboratory level and it will study the main reaction mechanisms developing models for their understanding and to support the pathways for concept application and scaling up. The project departs from results presented in literature this year that are fully aligned with capacities and previous experience of the participating R&D teams. The project will go further from these results extending the material compositions to develop, tailoring them to specific applications, widening the understanding of the reactions mechanisms and the effects of materials as well to the operation in the materials (i.e. degradation and aging effects). From this approach, within the project new models are expected to be developed and validated and the integration of the concept in different applications will be assessed. The ambition of the project requires a multidisciplinary approach that is developed by two R&D teams, from Material Science and Energy Engineering areas with all the capacities required for the successful development of the project: manufacturing, testing modelling and develop the new concepts and with expertise in materials processing and characterization, electrochemical models, and energy storage systems.

Revalorización de los subproductos de la piel de patata en lacas multifuncionales sostenibles para envases metálicos de alimentos

Upcycling of potato peel by-products into sustainable, multifunctional lacquers for food metal packaging (POP-UP)

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
TED2021-129656B-I00	01-12-2022 30-11-2024	Ministerio de Ciencia e Innovación	108.100 €

Investigador Principal Research Head	Componentes Research Group
José Jesús Benítez Jiménez José Alejandro Heredia Guerrero (IHSM)	Eva María Domínguez Carmona (IHSM) Mª de la Montaña Durán Barrantes (IHSM) Antonio Heredia Bayona (IHSM) Jorge Rencoret Pazo (IRNAS) José Carlos del Río Andrade (IRNAS) Diego Francisco Romero Hinojosa (IHSM)

RESUMEN / ABSTRACT

El proyecto POP-UP tiene como objetivo proporcionar, en términos de bioeconomía circular, soluciones sostenibles, seguras y económicamente viables al uso masivo de resinas a base de petróleo de bisfenol A (BPA) en el envasado de alimentos a través de la fabricación de recubrimientos multifuncionales de alto rendimiento para sustratos metálicos de bajo costo a partir de subproductos agroalimentarios infrautilizados. En particular, las pieles resultantes del procesamiento industrial de patatas se utilizarán como un recurso bio-renovable de monómeros de suberina para fabricar lacas biodegradables de base biológica mediante tecnologías verdes y escalables (por ejemplo, pulverización de soluciones acuosas y policondensación en estado fundido no catalizada) para envases alimentarios sostenibles e inocuos. Este recubrimiento a base de suberina ofrecerá los mismos beneficios y propiedades con respecto a las resinas de BPA, pero estará diseñado para ser completamente atóxico y con propiedades antimicrobianas. Por lo tanto, los principales objetivos están relacionados con mejorar la seguridad alimentaria, contribuir a la transición ecológica de una economía lineal basada en los fósiles a una bioeconomía circular y aumentar la productividad agrícola mediante la revalorización de residuos vegetales.

POP-UP project aims to provide, in terms of circular bioeconomy, sustainable, safe, and economically viable solutions to the massive use of petroleum-based BPA resins in food packaging through the fabrication of multifunctional, high-performance coatings for metal substrates from inexpensive, underutilized agro-food by-products. In particular, peels resulting from the industrial food processing of potatoes will be used as a bio-renewable resource of suberin monomers to fabricate biodegradable,

bio-based lacquers by green and large-scalable technologies (i.e. spray from aqueous solutions and free-solvent, non-catalyzed melting polycondensation) for sustainable and innocuous food packaging. This suberin-based coating will offer same benefits and properties with respect to BPA resins, but it will be designed to be fully non-toxic and with antimicrobial properties. Hence, main objectives are related to improve food security, to contribute to an ecological transition from a linear fossil-based economy to a circular bioeconomy, and to increase agricultural productivity by upcycling plant residues.

Materiales biomórficos para almacenamiento de energía
Biomorphic materials for energy storage (BioMatStor)

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P20_011860	05-10-2021 31-03-2023	Junta de Andalucía	106.505 €

Investigador Principal Research Head	Componentes Research Group
Joaquín Ramírez Rico	María Dolores Alba Carranza Alfonso Bravo León Manuel Jiménez Melendo Esperanza Pavón González

RESUMEN / ABSTRACT

El objetivo principal de esta propuesta es desarrollar materiales de carbono a medida para aplicaciones relacionadas con tecnologías energéticas y medioambientales, con un enfoque en tres aplicaciones principales: almacenamiento de energía, soportes de catalizador en pilas de combustible y electrolizadores y el almacenamiento y captura de gas, especialmente hidrógeno y dióxido de carbono. Proponemos producir estos materiales mediante pirólisis de desecho de biomasa y otros residuos orgánicos. El uso de biomasa como precursor en la síntesis de materiales tiene interés dada su abundancia y bajo costo, y presenta una oportunidad para convertir los residuos de la industria agroalimentaria local en un producto de alto valor añadido.

BioMatStor desarrolla I+D en diferentes niveles de aplicación: fundamental para la caracterización y fabricación de la ciencia de los materiales, y ciencia aplicada para el modelado y caracterización de sistemas de almacenamiento de energía. Este proyecto combina ciencia de materiales e ingeniería energética con el objetivo de obtener materiales de alto rendimiento para una amplia gama de aplicaciones en la producción y almacenamiento de energía. Proponemos un enfoque multidisciplinar que tiene su base en la excelencia científica, responde a los desafíos sociales y puede resultar en una trans-

ferencia de tecnología significativa a la industria. Este proyecto también aborda los objetivos socio-estratégicos de Horizonte 2020, ya que tiene como objetivo contribuir a la mejora de nuestro entorno a través de la ciencia avanzada y la investigación multidisciplinar, y está totalmente alineado con los objetivos y políticas de la Unión Europea, Horizon2020, SET Plan y los objetivos RIS3 de la región de Andalucía.

Biomass derived carbon materials will play a key role in several energy conversion and storage technologies in the future, with application in supercapacitors and batteries, power-to-X systems (fuel cells and electrolyzers), CO_2 and H_2 storage. Large amounts of biomass waste are generated in local agrofood industries. Among these wastes, the overall estimated production of olive stones in Spain is approximately 1,050,000–1,400,000 tons per year (campaign of 2017). The main use of this byproduct has been as solid biofuel for domestic applications, but given its abundance and low cost, this project presents an opportunity to convert what is considered waste into an added value product.

This proposal's main objective is to develop tailored carbon materials for applications related to energy and environmental technologies, with a focus on three main applications: i) electrochemical energy storage; ii) catalyst supports in fuel cells and electrolyzers; iii) and gas storage and capture, with a focus on both hydrogen and carbon dioxide storage and separation processes. The main proposed synthesis approach for these materials will be the pyrolysis of biomass precursors, with a focus on biomass waste products such as grain husks, peels, pits and stones and other organic waste. A first objective will be to perform a survey of readily available biomass waste materials from regional agrofood industries. A second objective will be the investigation and optimization of pyrolysis and activation routes to obtain carbon materials with tailored properties for each of the applications targeted in this project. Lastly, a third objective is to assess the applicability and the potential for the application of these materials at commercial scale.

Extensive physical and chemical characterization of the obtained carbon materials will be performed and testing of the resulting materials for the targeted applications will allow us to tailor the processing parameters. A scale-up analysis, with definition of materials integration and systems configurations will be performed by means of simulations, as well as technological and industrial applicability evaluation and assessment of the feasibility of the proposed approach in the large scale. BioMatStor develops R&D at different levels of application: fundamental for materials science characterization and manufacturing, and applied science for energy storage systems modeling and characterization. This Project combines Materials Science and Energy Engineering with the goal of obtaining highly performing materials for a wide range of applications in energy production and storage. Such a proposal requires a multidisciplinary approach, as evidenced in the research team and collaborators. We propose a multidisciplinary approach which has its foundation in scientific excellence, responds to societal challenges and may result in a significant technology transfer to the industry. This project also addresses the socio-strategic goals of Horizon 2020 as it aims to contribute to the improvement of our environment through advanced science and multidisciplinary research. It is fully aligned with the objectives and policies of European Union, the Energy Union Energy, H2020, SET Plan and Andalucía region RIS3 objectives.

OTROS PROYECTOS / OTHER PROJECTS

Genética y Biofísica de la Cutícula del Fruto del Tomate

Código/Code:	PID2021-126604OB-C21
Periodo/Period:	01-09-2022 / 31-08-2025
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovacion
Importe total/Total amount:	121.000 €
Investigador responsable/Research head:	Eva María Domínguez Carmona (IHSM) y Rafael Fernández Muñoz (IHSM)
Participante del ICMS como investigador:	José Jesús Benítez

Análisis de la cutícula del fruto del olivo y su relación con daños mecánicos

Código/Code:	PROYEXCEL_01000
Periodo/Period:	02-12-2022 / 31-12-2025
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	121.000 €
Investigador responsable/Research head:	Eva María Domínguez Carmona (IHSM)
Participante del ICMS como investigador:	José Jesús Benítez

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Elaboración de productos biodegradables generados en la cadena de valor del cacao

Periodo/Period:	31-08-2022 / 31-03-2023
Organismo Financiador/Financial source:	Fundación Ayuda en Acción
Importe total/Total amount:	31.476 €
Investigador responsable/Research head:	Susana Guzmán Puyol (IHSM)
Participante del ICMS como investigador:	José Jesús Benítez

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Plasticized, greaseproof chitin bioplastics with high transparency and biodegradability

Heredia-Guerrero, JA; Benitez, JJ; Porras-Vazquez, JM; Tedeschi, G; Morales, Y; Fernandez-Ortuno, D; Athanassiou, A; Guzman-Puyol, S

Food Hydrocolloids, **145** (2023) 109072

Diciembre, 2023 · DOI: 10.1016/j.foodhyd.2023.109072

A mixture of trifluoroacetic acid:trifluoroacetic anhydride (TFA:TFAA) was used to dissolve chitin from shrimp shells. Free-standing films were prepared by blending the chitin solution and glycerol at different percentages, followed by drop-casting, and the complete evaporation of the solvents. After this process,

the chitin matrix showed an amorphous molecular structure, as determined by X-ray diffraction. Optical, mechanical, thermal, and antioxidant properties were also thoroughly investigated. The incorporation of glycerol induced a plasticizing effect on the mechanical response of films and improved their transparency. In addition, hydrodynamic and barrier properties were determined by contact angle and water vapor/oxygen transmission rates, respectively, and revealed typical values of other polysaccharides. These bioplastics also presented an excellent greaseproof behavior with the highest degree of oil repellency as determined by the Kit test. Moreover, the overall migration was evaluated by using Tenax & REG; as a dry food simulant and levels were compliant with European regulations. Their antifungal properties were tested using Botrytis cinerea as a model. Biodegradability was also determined by measuring the biological oxygen demand in seawater. Degradation rates were high and similar to those of other fully-degradable materials.

Bio-based lacquers from industrially processed tomato pomace for sustainable metal food packaging

Benitez, JJ; Ramirez-Pozo, MC; Duran-Barrantes, MM; Heredia, A; Tedeschi, G; Ceseracciu, L; Guzman-Puyol, S; Marrero-López, D; Becci, A; Amato, A; Heredia-Guerrero, JA
Journal of Cleaner Production, **386** (2023) 1356836
Febrero, 2023 · DOI: 10.1016/j.jclepro.2022.135836

Bio-based lacquers prepared from an underutilized tomato processing residue such as pomace have been investigated as sustainable alternatives to bisphenol A (BPA)-based coatings for metal food packaging. The fabrication methodology consisted of a two-step process: spray-coating of a paste of the lipid fraction of tomato pomace with a mixture ethanol:H_2O (3:1, v:v) on common metal substrates, used for food canning, such as aluminum (Al), chromium-coated tin-free steel (TFS), and electrochemically tin-plated steel (ETP), followed by the self melt-polycondensation of such lipid fraction. The polymerization reaction was conducted at 200 °C for different times (10, 20, 30, 40, 50, and 60 min) and was monitored by specular infrared spectroscopy, resulting in maximum degrees of esterification of-92% for Al and-85% for TFS and ETP substrates. The anticorrosion performance of the coatings was studied by electrochemical impedance spectroscopy at different immersion times (time intervals of 2-5 h during an overall stability test up to 170 h) in an aqueous solution of 1 wt% NaCl. The degree of polymerization and the physical properties of the coatings showed a strong dependence on the metal substrate used. In general, the best results were found for tomato pomace-based lacquers applied on aluminum, achieving higher mechanical strength (critical load of 1739±198mN for Al, 1078±31mN for ETP, and 852± 206mN for TFS), hydrophobicity (water contact angle ~95° for Al, ~91° for ETP, and ~88° for TFS), and improved anticorrosion performance (coating resistance of 0.7 MΩcm^2 after 170 h of immersion for Al, 0.7 MΩcm^2 after 70 h of immersion for TFS, and negligible coating resistance for ETP). In view of the technical innovation proposed in the present paper, the estimation of the environmental sustainability of the process has been considered relevant to fit the circular economy target. For this purpose, a life cycle analysis (LCA) was applied to the overall process, revealing multiple advantages for both the environment and human health.

Incorporation of bioactive compounds from avocado by-products to ethyl cellulose-reinforced paper for food packaging applications

Acquavia, MA; Benitez, JJ; Bianco, G; Crescenzi, MA; Hierrezuelo, J; Grife-Ruiz, M; Romero, D; Guzman-Puyol, S; Heredia-Guerrero, JA
Food Chemistry, **429** (2023) 136906

Diciembre, 2023 · DOI: 10.1016/j.foodchem.2023.136906

Reinforced films were fabricated by impregnating paper in ethyl cellulose solutions. After solvent evaporation, the infused ethyl cellulose acted as binder of the paper microfibres and occupied the pores and cavities, thus improving the mechanical and barrier properties. To prepare active films, avocado by-products from guacamole industrial production were extracted in ethyl acetate. Then, the extract (optimized to be rich in phenolic compounds and flavonoids and mainly composed by lipids) was incorporated to the paper reinforced with the highest content of ethyl cellulose. In general, the addition of the avocado by-products extract decreased the water uptake and permeability, improved the wettability, and increased the biodegradability in seawater and the antioxidant capacity. In addition, these films acted as barriers and retainers for Escherichia coli and Bacillus cereus. The potentiality of these materials for food packaging was demonstrated by low overall migrations and a similar food preservation to common low-density polyethylene.

A technological approach based on engineered nanoclay composites for cesium and iodine retention

Osuna, FJ; Pavon, E; Alba, MD
Chemosphere, **341** (2023) 140128
Noviembre, 2023 · DOI: 10.1016/j.chemosphere.2023.140128

The development of effective and environmentally friendly methods for separating hazardous radionuclides from waste poses a significant technological challenge. ^{137}Cs and ^{131}I are among the most important radionuclides discharged into the environment by nuclear power plants. One of the best ways to eliminate them involves adsorption on clay minerals. In this regard, studies have demonstrated that organofunctionalized clay minerals are effective adsorbents. Thus, this study investigates the capability of organofunctionalized synthetic design clay minerals to jointly eliminate cesium and iodine. The adsorbents studied are a range of organofunctionalized clay minerals with alkylammonium cations of different alkyl chain lengths (2, 3 and 18) and some physical mixtures of raw clay minerals and octadecylammonium compounds. Organofunctionalized synthetic swelling highly charged micas are effective adsorbents for the simultaneous adsorption of cesium and iodine. In addition, the optimal system is a mixture of Na-M4 with octadecylammonium (50% w/w).

Improved stability of design clay minerals at high temperature: A comparison study with natural ones

Osuna, FJ; Chaparro, JR; Pavon, E; Alba, MD
Ceramics International, **49** (2023) 5279-5291
Febrero, 2023 · DOI: 10.1016/j.ceramint.2022.10.046

Clay minerals are ceramics materials that are involved in a wide range of economic uses. But, their structure and composition are modified by heating and, consequently, compromise their final applications. The actual temperatures at which changes occur vary greatly from one group to another group and even for different specimens within a given group. The aim of this research has been to evaluate the thermal behaviour of a set of design swelling micas, Na-Mica-*n* (Mn) and compare them with a set of natural smectites. All samples were heated in the range 200 °C to 1000 °C; afterwards, they were rehydrated thorough water suspension (0.4% wt). The results have shown that swelling micas have

better property of hydration/dehydration than natural clay minerals and those with higher layer charge exhibited higher rehydration ability and dehydration temperature.

Biodegradability Assessment of Prickly Pear Waste-Polymer Fibers under Soil Composting

Correa-Pacheco, ZN; Bautista-Baños, S; Benítez-Jiménez, JJ; Ortega-Gudiño, P; Cisneros-López, EO; Hernández-López, M
Polymers, **15** (2023) 4164
Octubre, 2023 · DOI: 10.3390/polym15204164

Nowadays, solving the problems associated with environmental pollution is of special interest. Therefore, in this work, the morphology and thermal and mechanical properties of extruded fibers based on polylactic acid (PLA) and poly(butylene adipate-co-terephthalate) (PBAT) added to prickly pear flour (PPF) under composting for 3 and 6 months were evaluated. The highest weight loss percentage (92 ± 7%) was obtained after 6-month degradation of the PLA/PBAT/PPF/CO/AA blend, in which PPF, canola oil (CO), and adipic acid (AA) were added. Optical and scanning electron microscopy (SEM) revealed structural changes in the fibers as composting time increased. The main changes in the absorption bands observed by Fourier transform infrared spectroscopy (FTIR) were related to the decrease in -C=O (1740 cm^{-1}) and -C-O (1100 cm^{-1}) groups and at 1269 cm^{-1}, associated with hemicellulose in the blends with PPF. Differential scanning calorimetry (DSC) showed an increase in the cold crystallization and melting point with degradation time, being more evident in the fibers with PPF, as well as a decrease in the mechanical properties, especially Young's modulus. The obtained results suggest that PPF residues could promote the biodegradability of PLA/PBAT-based fiber composites.

The Role of Protective Surface Coatings on the Thermal Stability of Delithiated Ni-Rich Layered Oxide Cathode Materials

Reissig, F; Ramirez-Rico, J; Placke, TJ; Winter, M; Schmuch, R; Gómez-Martin, A
Batteries, **9** (2023) 245
Abril, 2023 · DOI: 10.3390/batteries9050245

To achieve a broader public acceptance for electric vehicles based on lithium-ion battery (LIB) technology, long driving ranges, low cost, and high safety are needed. A promising pathway to address these key parameters lies in the further improvement of Ni-rich cathode materials for LIB cells. Despite the higher achieved capacities and thus energy densities, there are major drawbacks in terms of capacity retention and thermal stability (of the charged cathode) which are crucial for customer acceptance and can be mitigated by protecting cathode particles. We studied the impact of surface modifications on cycle life and thermal stability of $LiNi_{0.90}Co_{0.05}Mn_{0.05}O_2$ layered oxide cathodes with WO_3 by a simple sol-gel coating process. Several advanced analytical techniques such as low-energy ion scattering, differential scanning calorimetry, and high-temperature synchrotron X-ray powder diffraction of delithiated cathode materials, as well as charge/discharge cycling give significant insights into the impact of surface coverage of the coatings on mitigating degradation mechanisms. The results show that successful surface modifications of WO_3 with a surface coverage of only 20% can prolong the cycle life of an LIB cell and play a crucial role in improving the thermal stability and, hence, the safety of LIBs.

Mechanical treatments on design powder ceramic materials: Insight into the textural and structural changes
Osuna, FJ; Fernández, M; Pavón, E; Sánchez, RMT; Alba, MD
Advanced Powder Technology, **34** (2023) 104189
Octubre, 2023 · DOI: 10.1016/j.apt.2023.104189

Mechanical treatment of porous ceramics, such as porous clay minerals, is a crucial step in ceramic processing. Among clay minerals, design swelling brittle micas have shown exceptional properties for further applications, although they exhibit low surface area and porosity. But, their mechanical activation could improve their textural properties and deserves to be investigated. Thus, the aim of this work was to evaluate the effects of gradual grinding in their surface and framework. At short grinding times, the surface area increases and mesoporous and microporous are generated. Long grinding time provokes particle agglomeration with the consequent change in their colloidal stability. At bulk level, framework defects are observed in both tetrahedral and octahedral sheets and increase with the total layer charge.

Revealing the Impact of Different Iron-Based Precursors on the 'Catalytic' Graphitization for Synthesis of Anode Materials for Lithium Ion Batteries
Frankenstein, L; Glomb, P; Ramirez-Rico, J; Winter, M; Placke, T; Gómez-Martin, A
ChemElectroChem, **10** (2023) e202201073
Marzo, 2023 · DOI: 10.1002/celc.202201073

Low cost and environmentally friendly production of graphite anodes from naturally available biomass resources is of great importance to satisfy the increasing material demand for lithium ion batteries. Herein, graphitization of coffee ground was performed using four different iron-based activating additives, including iron (III) chloride, iron (III) nitrate, iron (III) oxide and pure iron, following either a wet or a dry mixing approach. The structural development regarding the type of activator used and the impact on the corresponding electrochemical performance are systematically investigated. A maximum degree of graphitization between 55 and 74 % (as determined by Raman spectroscopy) is attained using iron (III) chloride and iron powder, respectively. The graphitic anode material synthesized using iron powder reached a maximum reversible capacity of ≈320 mAh g^{-1} at a rate of 0.1 C. This study provides significant insights into the impact of activators on the design of synthetic graphite from renewable sources.

Sustainable Integration of Zinc Oxide Nanoparticles: Enhancing Properties of Poly(ε-Caprolactone) Electrospun Nanofibers and Cast Films
Abdullah, JAA; Benítez, JJ; Guerrero, A; Romero, A
Coatings, **13** (2023) 1665
Octubre, 2023 · DOI: 10.3390/coatings13101665

This study investigated the impact of adding zinc oxide nanoparticles (ZnO-NPs) to electrospun membranes and cast films made of poly(epsilon-caprolactone) (PCL). The physicochemical, mechanical, and morphological properties of the samples were analyzed. Physicochemical parameters included water contact angle (WCA), water vapor transmission rate (WVTR), permeance, water vapor permeability (WVP), light transmission (T-600), and transparency (T). Mechanical properties, such as maximum

stress (6(max)), elongation (epsilon(max)), and Young's modulus (MPa), were also evaluated. Morphological properties were analyzed in terms of thickness, dispersion, and surface roughness (measured by the arithmetic (Ra) and quadratic (Rq) averages). The crystallinity and melting point, as well as the functional DPPH center dot scavenging percentage (SP%), were also studied. The results showed that adding 1 wt% ZnO-NPs improved the water barrier properties of PCL membranes and films, increasing WCA by 1%-6% and decreasing WVTR by 11%-19%, permeance by 34%-20%, and WVP by 4%-11%, respectively. The T-600 values of PCL/ZnO-NPs membranes and films were 2-3 times lower than those of neat PCL samples, indicating improved optical properties. The mechanical properties of the composite membranes and films also improved, with 6(max) increasing by 56%-32% and Young's modulus increasing by 91%-95%, while epsilon(max) decreased by 79%-57%. The incorporation of ZnO-NPs also increased the thickness and surface roughness of the samples. The SP% of PCL/ZnO-NPs increased by almost 69%, demonstrating the beneficial effects of ZnO-NPs on the system. These findings suggest that incorporating ZnO-NPs into PCL membranes and films can enhance their properties, making them well suited for various applications, such as those within the realm of materials science and nanotechnology.

Effect of Mo and W interlayers on microstructure and mechanical properties of Si_3N_4-nickel-base superalloy joints

Singh, M; Fernandez, JM; Asthana, R; Ramirez-Rico, J; Valera-Feria, FM
International Journal of Applied Ceramic Technology, **20** (2023) 987-994
Marzo, 2023 · DOI: 10.1111/ijac.14266

Si_3N_4/nickel-base superalloy (Inconel-625) and Si_3N_4/Si_3N_4 joints with refractory metal (W and Mo) interlayers were vacuum brazed using a Ti-active braze Cu-ABA (92.75Cu-3Si-2Al-2.25Ti) at 1317 K for 30 min with the following interlayered arrangements: Si_3N_4/Mo/W/Inconel and Si_3N_4/Mo/W/Si_3N_4. The joints exhibited Ti segregation at the Si_3N_4/Cu-ABA interface, elemental interdiffusion across the joint interfaces, and sound metallurgical bonding. Knoop microhardness profiles revealed hardness gradients across the joints that mimicked the interlayered arrangement. The compressive shear strength of Si_3N_4/Si_3N_4 joints both with and without W and Mo layers was ~142 MPa but the strength of Si_3N_4/Inconel joints increased from ~9 MPa for directly bonded joints without interlayers to 53.5 MPa for joints with Mo and W interlayers.

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

Jornada ACerS Materiales vítreos y cerámicos para aplicaciones de alta tecnología

26 octubre [Sevilla, España]

Residual stresses in anode supported $BaZr_{1-x}Y_xO_{2-\delta}$ electrolytes for protonic conductive fuel cells. *S. Fernández Muñoz, R. Chacartegui Ramírez, M.D. Alba, J. Ramírez Rico*. COMUNICACIÓN ORAL

FORMACION / TRAINING

FORMACIÓN DE POSTGRADO / MASTER DEGREE THESIS

Título:	**Materiales de carbono para aplicaciones en energía y medioambiente**
Autor:	Ana Castro Chincho
Tutores:	Joaquín Ramírez Rico, Mª Dolores Alba Carranza
Grado:	Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro:	Universidad de Sevilla
Fecha Defensa:	05 de julio de 2023

FORMACIÓN DE GRADUADOS / BACHELOR DEGREE THESIS

Título:	**Depuración de aguas de salmuera mediante materiales arcillosos**
Autor:	Ezequiel Mora
Tutores:	Esperanza Pavón González, Mª Dolores Alba Carranza
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	18 de julio de 2023

DOCENCIA / TEACHING

El personal del ICMS imparte docencia en titulaciones de Grado y doble Grado de la Universidad de Sevilla. La docencia se desarrolla en diversos centros: Facultad de Física, Facultad de Biología, Facultad de Química, Facultad de Farmacia y Escuela Técnica Superior de Ingeniería Informática.

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Horno tubular hasta 1200 °C
- Horno tubular en atmósfera controlada hasta 1700 °C
- Horno de Cámara hasta 1650 °C
- Horno de Cámara hasta 1200 °C
- Estufa hasta 400 °C
- Estufa hasta 200 °C
- Caja de guantes

- Reactores hidrotermales
- Línea de vacío
- 3 microscopios AFM
- Microscopio STM en aire
- Calorímetro diferencial de barrido (DSC)
- Analizador mecánico dinámico (DMA)
- Máquina de ensayos mecánicos por tracción
- Analizador de ángulo de contacto
- Balanza Langmuir-Blodgett (LB)
- Spin coater

MECANOQUÍMICA Y REACTIVIDAD DE MATERIALES
MECHANOCHEMISTRY AND REACTIVITY OF MATERIALS

GRUPOS DE INVESTIGACIÓN

Materiales Avanzados | 642010
Advanced Materials

Propiedades Mecánicas, Modelización y Caracterización de Cerámicos Avanzados |642016
Mechanical properties, Modelling and Characterization of Advanced Ceramics

Reactividad de Sólidos | 642008
Reactivity of Solids

PERSONAL / PERSONNEL

Profesores de Investigación	Luis Allan Pérez Maqueda
Catedráticos de Universidad	Diego Gómez García
Investigadores Científicos	Francisco José Gotor Martínez Concepción Real Pérez Pedro José Sánchez Soto
Científicos Titulares	Rosalía Poyato Galán María Jesús Sayagués de Vega
Profesores Titulares de Universidad	María Dolores Alcalá González María Regla Ayala Espinar Antonio Perejón Pazo
Talentia Senior CCAA	Pedro E. Sánchez Jiménez
Doctores Contratados	Eva Gil González Diego Sebastián Lascano Aimacana Alejandro F. Manchón Gordón
Investigadores en Formación	Ana Castro Chincho Sandra Molina Molina Esther Robles Solano
JAE Intro	Francisco Javier Coto Ruíz Clara Delgado Álvarez María Teresa Linares Serrano Lucía Santiago Andrades

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Materiales termoquímicos para almacenamiento de energía mejorados mediante control microestructural
Thermochemical energy storage materials enhanced by microstructural control

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
TED2021-131839B-C22	01-09-2022 30-11-2024	Ministerio de Ciencia e Innovación	161.000 €

Investigador Principal Research Head	Componentes Research Group
Luis Allan Pérez Maqueda Pedro Enrique Sánchez Jiménez	Joaquín Ramírez Rico José Manuel Valverde Millán Antonio Perejón Pazo

RESUMEN / ABSTRACT

El objetivo principal del proyecto MOTHERESE es el desarrollo de un nuevo concepto de almacenamiento termoquímico de energía basado en el proceso de "Calcium-Looping". La novedad del concepto radica en disminuir la escala del componente de almacenamiento y dotarlo de un carácter modular, fácilmente integrable en plantas de generación de energía de diversa naturaleza, almacenable y móvil. El subproyecto 2 se centra en los aspectos relacionados con el desarrollo de materiales adecuados a estas nuevas condiciones de operación, así como a la optimización de las mismas a esta nueva escala.

Se pretende abordar el desarrollo de estos materiales haciendo hincapié en técnicas de preparación que favorezcan morfologías y microestructuras que optimicen (i) la cinética de las reacciones sólido-gas, con el objeto de reducir los tiempos de residencia, (ii) estabilidad multicíclica, minimizando la desactivación por sinterizado y bloqueo de poros, y (iii) superficie activa, maximizando la cantidad de reactivo disponible para conversión en cada ciclo. Esto se conseguirá utilizando las técnicas de freeze casting y freeze granulation, especialmente adecuadas para la fabricación de estructuras cerámicas con porosidad abierta y morfología dirigida. También se plantea el uso de aditivos que mejoren el rendimiento del material. Finalmente, se contempla la integración del material activo y aditivos de alta conductividad térmica en estructuras tridimensionales estables, que no solo mejoren la ciclabilidad y eficiencia del material activo sino también asegure transferencias de calor rápidas y eficientes, necesarias para el sistema modular. Finalmente, se van a explorar nuevas condiciones de operación compatibles con la nueva escala, desde presiones reducidas hasta altas presiones de hasta 5 bares, manteniendo siempre un ciclo cerrado que evite la necesidad de separación de gases.

MOTHERESE apuesta por la economía circular, por lo que apunta al uso, como fuente de los aditivos e incluso del propio material activo, CaO, de subproductos y residuos procedentes de otras industrias, favoreciendo el aprovechamiento de residuos. Entre los planteados, escoria de acería, carbonatos biogénicos (moluscos), materiales celulósicos y cascarilla de arroz (fuente de SiO_2).

Para abordar estos objetivos, el subproyecto cuenta con un equipo multidisciplinar de químicos, ingenieros, físicos y especialistas en materiales con experiencia en la gestión y participación en proyectos de investigación nacionales e internacionales, incluyendo proyectos relevantes centrados en almacenamiento termoquímico de energía. Además, el equipo tiene una red internacional de colaboradores tanto académicos como industriales que permitiría en la explotación de los resultados obtenidos y la propuesta de nuevos proyectos internacionales en esta misma línea.

The main objective of the MOTHERESE project is the development of a new concept of thermochemical energy storage based on the "Calcium-Looping" process. The novelty of the concept lies in scaling down the storage component and making it modular, easily integrated in power generation plants of different nature, storable and mobile. Subproject 2 focuses on aspects related to the development of materials suitable for these new operating conditions, as well as their optimization at this new scale.

The aim is to address the development of these materials with emphasis on preparation techniques that favor morphologies and microstructures that optimize (i) the kinetics of solid-gas reactions, in order to reduce residence times, (ii) multicyclic stability, minimizing deactivation by sintering and pore blocking, and (iii) active surface area, maximizing the amount of reagent available for conversion in each cycle. This will be achieved by using freeze casting and freeze granulation techniques, particularly suitable for the fabrication of ceramic structures with open porosity and directed morphology. The use of additives to improve the performance of the material is also considered. Finally, the integration of the active material and additives of high thermal conductivity in stable three-dimensional structures is contemplated, which not only improve the cyclability and efficiency of the active material but also ensure fast and efficient heat transfer, necessary for the modular system. Finally, new operating conditions compatible with the new scale will be explored, from low pressures to high pressures of up to 5 bar, always maintaining a closed cycle that avoids the need for gas separation.

MOTHERESE is committed to the circular economy, and therefore aims to use by-products and waste from other industries as a source of additives and even of the active material itself, CaO, favoring the use of waste. These include steel mill slag, biogenic carbonates (mollusks), cellulosic materials and rice husks (source of SiO_2).

To address these objectives, the subproject has a multidisciplinary team of chemists, engineers, physicists and materials specialists with experience in the management and participation in national and international research projects, including relevant projects focused on thermochemical energy storage. In addition, the team has an international network of academic and industrial collaborators that would allow in the exploitation of the results obtained and the proposal of new international projects in this same line.

Demostración en entorno relevante del uso de reacciones de calcinación-solar/carbonatación para el almacenamiento de energía térmica

Validation in a relevant environment of solar-calcination/carbonation reactions for termal energy storage

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PDC2021-121552-C21	01-12-2021 30-11-2023	Ministerio de Ciencia e Innovación	68.770 €

Investigador Principal Research Head	Componentes Research Group
Pedro Enrique Sánchez Jiménez	Luis Allan Pérez Maqueda Antonio Perejón Pazo Juan Jesús Arcenegui Troya

RESUMEN / ABSTRACT

España es uno de los países europeos con mayor irradiación solar media y líder mundial en implantación de Energía Solar Concentrada (CSP). Una ventaja de la tecnología CSP es su capacidad de almacenar energía térmica y usarla cuando no hay irradiación. Las plantas CSP de última generación incluyen sistemas de almacenamiento en sales fundidas (calor sensible) que presentan limitaciones: temperatura máxima limitada por degradación térmica, almacenaje a alta temperatura para evitar solidificación, corrosión y coste. En nuestro proyecto CTQ2017 se investigó el almacenamiento termoquímico mediante reacciones de calcinación/carbonatación, proceso calcium-lopping (CaL), usando caliza natural, que es abundante, barata, no corrosiva y permite operar a alta temperatura aumentando la eficiencia de conversión termoeléctrica. Su densidad energética (~1 MWhr/m^3) es superior al de las sales (0.25-0.40 MWhr/m^3). Un problema del CaL para almacenamiento termoquímico es la desactivación del CaO con el número de ciclos. En nuestro proyecto CTQ2017 se propusieron diversas estrategias de mejora con las que se consiguieron rendimientos muy altos incluso después de muchos ciclos: (i) cambio de condiciones de calcinación-carbonatación (reducción de la temperatura de calcinación e incrementar la de carbonatación para mejorar el rendimiento tanto del proceso como de la planta) y (ii) propuesta de otros carbonatos diferentes de la caliza, uso de aditivos, uso de residuos (escorias) y materiales sintéticos de bajo coste. Estos resultados de laboratorio son de extraordinario interés para su aplicación a plantas de CSP, pero para su transferencia se requiere de validación en entorno relevante. En este proyecto se propone escalar los resultados de laboratorio mediante ensayos en planta piloto, el desarrollo y ensayo de un nuevo calcinador solar, así como la evaluación de la viabilidad técnico-económica de la tecnología a escala industrial. En este proyecto se desarrollará una prueba de concepto de un novedoso reactor/intercambiador de calor de tipo ciclón basado en energía solar. La radiación solar concentrada alcanzará el calcinador solar tipo ciclón mediante un sistema beam-down (concentrador

solar secundario) desde el campo solar, formado por 14 heliostatos con una superficie total de 30 m^2 de la planta piloto construida en el marco del proyecto H2020 SOCRATCES, en el que han participado la mayor parte de los miembros del equipo de investigación del proyecto coordinado. El estudio y desarrollo de esta prueba de concepto permitirá establecer la viabilidad del diseño y demostrar su interés a empresas del sector energético y del cemento de cara a una futura integración de energía solar, en busca de una reducción de costes y emisiones de CO_2. Se parte de estudios a nivel de concepto desarrollados en el proyecto CTQ2017 con nivel de madurez tecnológica TRL 4, y se estima que se avanzará hasta niveles TRL 5-6. Se realizará un análisis de la viabilidad económica de la implantación de los nuevos conceptos propuestos en el marco del proyecto CTQ2017 y se elaborará un plan de transferencia. Este plan recogerá las acciones a llevar a cabo para favorecer una transferencia efectiva al sector industrial. Además, dado el potencial de patentabilidad de la tecnología objeto del proyecto, una vez probada en escala relevante (prueba de concepto), se desarrollará un plan de explotación y protección de derechos intelectuales.

Spain is one the European countries with the largest solar irradiation and world leader in concentrated solar power (CSP). A significant advantage of CSP technology is its ability to store thermal energy to be used when there is no irradiation. Last generation CSP plants include a storage system based on molten salts (Sensible Heat Storage) that show certain limitations: maximum temperature limited by thermal degradation, storage at high temperature to prevent solidification, corrosion, costs. In our CTQ2017 project we investigated on thermochemical energy storage by calcination (carbonation reactions, calcium looping (CaL) process, using limestone, which is abundant, cheap, non-corrosive, and allows high temperature operation, increasing the thermoelectric efficiency of the plant. Its energy density (~1 MWhr/m^3) is larger than that of salts (0.25-0.40 MWhr/m^3). A limitation of CaLfor energy storage is the deactivation of CaO with the increasing number of cycles. In our project CTQ20, we proposed several improvement strategies for achieving high performance: (i) change of calcination/carbonation conditions (calcination temperature decrease and carbonation temperature increase) and (ii) proposal of other carbonates different from limestone, use of additives, use of wastematerials (slags) and low-cost synthetic materials. These lab results are of great interest for its application in CSP, but it requires of validation in a relevant environment. In this project we propose the scale up of the lab results by tests in a pilot plant, the test of a new solar calcinator and the evaluation of the technical-economic feasibility of the technology on an industrial scale. Furthermore, a proof of concept of a novel solar power based cyclone type heat exchanger/reactor will be achieved within the project. The concentrated solar radiation will reach the cyclone-type solar calciner through a beam-down system (secondary solar concentrator) from the solar field, made up of 14 heliostats with a total area of 30 m^2 from the pilot plant built within the framework of the H2020 SOCRATCES project, in which most of the members of the research team of the coordinated project have participated. The study and development of this proof of concept will make it possible to establish the viability of the design and demonstrate their interest to companies in the energy and cement sectors with a view to a future integration of solar energy in search of a reduction in costs and CO_2 emissions. It is based on studies at the concept level developed in the CTQ2017 project with a level of technological maturity TRL 4, and it is estimated that it will advance to levels TRL 5-6. An analysis of the economic viability of the implementation of the new concepts proposed in the framework of the CTQ2017 project will be carried out and a transfer plan will be drawn up. This plan will include the actions to be carried out to favor an effective transfer to the industrial sector. In addition, given the potential for patentability of the technology object of the project, once tested on a relevant scale (proof of concept), a plan for the exploitation and protection of intellectual rights will be developed.

Materiales para sistema híbrido de almacenamiento de energía térmica de alto rendimiento basado en sales fundidas y carbonatos Materials for High performance thermal energy storage system based on hybrid molten salts and carbonates

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2022-140815OB-C22	01-09-2023 31-08-2026	Ministerio de Ciencia e Innovación	181.250 €

Investigador Principal Research Head	Componentes Research Group
Luis A. Pérez Maqueda Antonio Perejón Pazo	Pedro Enrique Sánchez Jiménez José Manuel Valverde Millán (US)

RESUMEN / ABSTRACT

El objetivo principal del proyecto HIPERTES es el desarrollo de un nuevo concepto de almacenamiento termoquímico de energía de alta temperatura basado en un sistema híbrido de carbonatos y sales fundidas en un único reactor. El subproyecto 2 se centra principalmente en los aspectos relacionados con el desarrollo de materiales adecuados a estas nuevas condiciones de operación, así como a la optimización de las mismas y el estudio del comportamiento de los materiales durante los ciclos termoquímicos.

Si bien existen soluciones basadas en el uso de aditivos sólidos para intentar mejorar la ciclabilidad y el rendimiento de procesos termoquímicos basados en reacciones de carbonatación/calcinación, estas soluciones tienen un límite, pues siempre se observa un decaimiento de la actividad con el número de ciclos que se hace más evidente a manera que aumenta el número de éstos. En este proyecto se propone una solución novedosa basada en sistemas híbridos de carbonatos con sales fundidas. Las sales aportaran un incremento de la reactividad tanto de calcinación como de carbonatación, mejorando sobre todo las cinéticas de los procesos difusivos.

Así, se espera que las sales aporten (i) cinéticas rápidas de calcinación y carbonatación para que los procesos de carga y descarga sean lo más rápidos posibles y (ii) alta estabilidad multicíclica evitando los procesos de desactivación por sinterizado y bloqueo de poros. Se proponen dos tipos de sistemas, uno basado en pellets porosos que se impregnarían con las sales y otro basado en baños de sales fundidas donde se dispersarían las partículas de carbonato. Para la primera solución se usarán técnicas de peletizado que permitan obtener pellets porosos a partir de suspensiones acuosas de partículas de carbonatos tanto minerales como sintéticas. Los pellets obtenidos se impregnarán con sales de alta temperatura. En la segunda solución, se seleccionarán mezclas de sales de alta estabilidad térmica en las que se dispersarán partículas o pellets de carbonatos. Para la preparación de los pellets porosos se usarán técnicas de "freeze granulation" que permiten obtener pellets porosos y estables a partir de suspensiones de partículas. Todos los materiales preparados se caracterizarán en cuanto a sus propiedades termofísicas

y a su comportamiento multicíclico. Se establecerán las condiciones óptimas de funcionamiento, así como los rangos máximos de trabajo. Estos resultados se usarán como parámetros para el subproyecto 1.

El subproyecto 2 cuenta con la participación de un equipo multidisciplinar con experiencia en química, reactividad de sólidos, cinética heterogénea, física y ciencia de materiales para completar los objetivos propuestos. Tienen experiencia y solvencia avalada en la ejecución de proyectos nacionales e internacionales, además de proyectos industriales, en el campo del diseño y caracterización de materiales para el almacenamiento de energía térmica.

The main objective of the HIPERTES project is the development of a new concept of high-temperature thermochemical energy storage based on a hybrid system of carbonates and molten salts in a single reactor. Subproject 2 focuses mainly on aspects related to the development of materials suitable for these new operating conditions, as well as their optimization and the study of the behavior of the materials during thermochemical cycles.

Although there are proposals based on the use of solid additives to try to improve the cyclability and performance of thermochemical processes based on carbonation/calcination reactions, these solutions have a limit, since a decay of the activity is always observed with the number of cycles, which becomes more evident as the number of cycles increases. In this project, a novel solution based on hybrid systems of carbonates with molten salts is proposed. The salts will provide an increase in the reactivity of both calcination and carbonation, especially improving the kinetics of the diffusive processes.

Thus, the salts are expected to provide (i) fast calcination and carbonation kinetics to make the loading and unloading processes as fast as possible and (ii) high multicyclic stability avoiding deactivation processes by sintering and pore blocking. Two types of systems are proposed, one based on porous pellets that would be impregnated with the salts and the other based on molten salt baths where the carbonate particles would be dispersed. For the first solution, pelletizing techniques will be used to obtain porous pellets from aqueous suspensions of both mineral and synthetic carbonate particles. The pellets obtained will be impregnated with high-temperature salts. In the second solution, mixtures of salts of high thermal stability will be selected in which carbonate particles or pellets will be dispersed. For the preparation of the porous pellets, freeze granulation techniques will be used to obtain porous and stable pellets from particle suspensions. All prepared materials will be characterized in terms of thermophysical properties and multicyclic behavior. Optimal operating conditions as well as maximum working ranges will be established. These results will be used as parameters for subproject 1.

Subproject 2 has the participation of a multidisciplinary team with expertise in chemistry, solid reactivity, heterogeneous kinetics, physics, and materials science to complete the proposed objectives. They have experience and solvency guaranteed in the execution of national and international projects, in addition to industrial projects, in the field of design and characterization of materials for thermal energy storage.

Diseño de cerámicas avanzadas con nanomateriales 2D para dispositivos electroquímicos de alta temperatura Design of advanced ceramics with 2D nanomaterials for high-temperature electrochemical devices

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2022-140191NB-100	01-09-2023 31-08-2027	Ministerio de Ciencia e Innovación	156.250 €

Investigador Principal Research Head	Componentes Research Group
Ana Morales Rodríguez Rosalía Poyato Galán	Ángela Gallardo López Felipe Gutiérrez Mora Rocío del Carmen Moriche Tirado

RESUMEN / ABSTRACT

El avance en el conocimiento en el campo de los materiales compuestos de matriz cerámica con segunda fase de nanomateriales bidimensionales es fundamental de cara a su uso futuro en aplicaciones tecnológicas, como son los dispositivos electroquímicos de alta temperatura. Así, es muy necesaria una comprensión profunda de las bases de sus nuevas funcionalidades y su desempeño optimizado.

La presente propuesta presenta un estudio sistemático de composites con matriz de circona estabilizada con 8 %mol de itria y una segunda fase de nanomateriales laminares bidimensionales -grafeno o nanoláminas de nitruro de boro- pensados para su utilización en celdas de combustible de óxido sólido, con el objetivo de profundizar en la comprensión de los mecanismos que controlan su comportamiento térmico, mecánico y eléctrico.

Se llevará a cabo un estudio de procesado con el objetivo de obtener composites con una microestructura optimizada, siempre persiguiendo una distribución homogénea del nanomaterial 2D en toda la matriz cerámica y una alta densidad. En un primer paso, se optimizará la rutina de procesado del polvo para mejorar la dispersión de la nanoestructura 2D en el polvo compuesto. En un segundo paso, se realizará un estudio de sinterización a diferentes temperaturas y presiones con el objetivo de obtener composites totalmente densos. Se analizará el efecto de la incorporación de la nanoestructura 2D sobre la microestructura del composite cerámico, para lo cual se evaluarán las fases cristalinas y la distribución, tamaño e integridad estructural de los nanomateriales 2D.

Se realizarán medidas de difusividad y conductividad térmica en función de la temperatura bajo diferentes atmósferas con el fin de analizar el efecto de la incorporación de la segunda fase, así como la posible orientación preferencial. Se realizarán ensayos de deformación a alta temperatura controlando las condiciones de tensión, temperatura y ambiente de trabajo, persiguiendo la identificación de los mecanismos microscópicos responsables del comportamiento de fluencia así como la comprensión de los mecanismos de fractura y plasticidad de los composites.

Se realizarán medidas de conductividad eléctrica en función de la temperatura para evaluar el efecto de la incorporación de las diferentes nanoestructuras 2D sobre el comportamiento eléctrico de los composites. Se identificará el tipo de conducción -iónica, mixta o electrónica- para los composites con diferentes contenidos de nanoláminas de grafeno.

The advance in knowledge in ceramic matrix composites with 2D nanomaterial fillers is essential to address their future use in technological applications such as high-temperature electrochemical devices. Thus, a deep understanding of the basis of their new functionalities and optimized performance is needed.

This proposal outlines a systematic study of composites with 8 mol% yttria-stabilized zirconia matrix, a well-known ionic conductor, incorporating two different 2D laminar nanomaterials -graphene or boron nitride nanosheets- as fillers, intended for use in solid oxide fuel cells, with the aim to deepen in the understanding of the mechanisms that control their thermal, mechanical and electrical behavior. To begin with, a processing study will be carried out in order to obtain composites with an optimized microstructure, always pursuing a homogeneous distribution of the 2D nanomaterial throughout the ceramic matrix and a high density. In a first step, the powder processing routine will be optimized in order to enhance the dispersion of the 2D nanostructure in the composite powder. In a second step, a sintering study with different temperatures and pressures will be carried out with the aim of obtaining fully- dense composites. The effect of the 2D nanostructure incorporation on the ceramic composite microstructure will be analyzed in terms of the crystalline phases and distribution, size and structural integrity of the 2D nanomaterials.

Thermal diffusivity and conductivity measurements will be conducted on the sintered composites, as a function of temperature and under different atmospheres to analyze heat dissipation and the effect of the filler dispersion and orientation in the thermal response. These thermal properties are essential since operation of the solid oxide fuel cell takes place at high temperature.

To ensure structural stability of the composites during operation, high-temperature deformation tests will be performed controlling stress, temperature, and working atmosphere conditions. The identification of the microscopic mechanisms responsible of the creep behavior as well as the comprehension of the fracture mechanisms and plasticity of the composites will be pursued to allow for prediction and control of their structural response in service.

The electrical conductivity measurements fundamental for this application will be carried out on the composites as a function of temperature in order to assess the effect of the incorporation of the different 2D nanostructures. The conduction type -ionic, mixed or electronic- for the composites with different graphene nanosheets contents will be identified.

Técnicas innovadoras basadas en campos eléctricos para la preparación de baterías de estado sólido Innovative techniques based on electric fields for the preparation of all solid state batteries

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2022-141199OA-100	01-09-2023 31-08-2026	Ministerio de Ciencia e Innovación	75.000 €

Investigador Principal Research Head	Componentes Research Group
Eva Gil González	Xin Li Sandra Molina Molina Ahmed Taibi

RESUMEN / ABSTRACT

El desarrollo de las tecnologías de almacenamiento energético es fundamental para la transición hacia una economía climáticamente neutra. Las Baterías de Estado Sólido (BES) se presentan como candidatas prometedoras para solventar los graves problemas que presentan las baterías de ion litio que dominan el mercado tecnológico actual. Las BES reemplazan el electrolito líquido, orgánico e inflamable, de estos dispositivos por un sólido no inflamable, lo que aumenta la seguridad de estos dispositivos, entre muchas otras ventajas. Así, en las últimas décadas los electrolitos sólidos han experimentado un gran avance, donde un grupo muy importante lo conforman los electrolitos cerámicos tipo óxidos y fosfatos, por sus altas conductividades iónica, amplia venta de potencial electroquímico y compatibilidad con litio metálico. Sin embargo, las altas temperaturas (por tiempo prolongado) que se requieren para su síntesis y procesado conllevan un gran consumo energético, lo que limita su competitividad económica y, además, favorece la volatilización de los iones litios, deteriorando de manera inevitable sus propiedades. También, el proceso de co-sinterizado con los demás elementos activos de la celda (ánodo y cátodo) es bastante complicado por la aparición de fases secundarias y grandes resistencias interfaciales que merman la vida útil de las BES. Precisamente esta problemática es uno de los grandes retos a abordar para impulsar el desarrollo de estos dispositivos. INNOBEC propone un enfoque innovador para abordar este desafío mediante el empleo de las técnicas de sinterizado Flash (FS) a las BES. El FS consiste en aplicar simultáneamente un campo eléctrico y calor a una muestra cerámica, de tal forma que la densificación del material se consigue de manera casi instantánea y a temperaturas muchos menores que las empleadas en métodos convencionales. Con ello, no solo se reduce el gasto energético, sino que también se facilita el procesado de materiales cuya estabilidad térmica es limitada, como son los electrolitos sólidos. Además, las técnicas de FS son consideradas de “no equilibrio”, lo posibilita la obtención de materiales con propiedades mejoradas, tales como superplasticidad en cerámicas o conductividades iónicas superiores, por la generación de una gran cantidad de defectos. Asimismo, las técnicas

de FS son altamente versátiles ya que también se ha demostrado que mediante la sinterización reactiva Flash (RFS) se puede inducir la reacción química y densificación de materiales cerámicos en un solo paso, lo que mejora aún más la eficiencia del proceso y aumenta las posibilidades brindadas por la técnica.

INNOBEC pretende usar las ventajas competitivas ofrecidas por las técnicas de FS y RFS de menores tiempos y temperaturas de procesado para obtener materiales con propiedades optimizadas para BES, específicamente electrolitos sólidos cerámicos, tipo óxidos y fosfatos, y composites cerámicos con conducción mixta iónica-electrónica para cátodos o ánodos. El objetivo final de INNOBEC es el co-sinterizado en un solo paso de estructuras multicapas tipo BES y la evaluación de su rendimiento electroquímico. INNOBEC es un proyecto novedoso, que fusiona la experiencia previa de la IP tanto en el ámbito de las BES como FS, donde se apuesta por una nueva metodología altamente eficiente que facilite la preparación y procesado de los electrolitos sólidos y, además, palíe los graves problemas derivados del co-sinterizado que frenan el desarrollo de las BES.

The development of energy storage technologies is essential for the transition to a climate-neutral economy. All-Solid-State Batteries (ASSBs) are promising candidates to solve the functional problems of convectional lithium-ion batteries that are currently dominating the technological market. ASSBs replace the flammable organic liquid electrolyte of traditional devices with a non-flammable solid, which improves the safety of this devices, among many other advantages. Thus, solid electrolytes have experienced great development in the last decades, where oxide and phosphate-types solid electrolytes are emerging as a very important group due to their high ionic conductivities, wide electrochemical window, and good compatibility with lithium metal. However, the high temperatures (for long periods of time) required for their synthesis and processing consume a large amount of energy, which considerably limit their economic competitiveness and also deteriorate their physical properties due to lithium volatilization. Furthermore, the co-sintering process with the other active materials of the cells (anode and cathode) is extremely complicated, as the high temperatures promote the appearance of secondary phases and high interfacial resistances that, unfortunately, limit the lifespan of ASSBs. This is precisely one of the major challenges facing the development of these devices. INNOBEC proposes an innovative approach to address the aforementioned problem by implementing the Flash Sintering (FS) to ASSBs. FS consists in simultaneously applying an electric field and heat to a ceramic sample, so that the densification of the material is achieved almost instantaneously and at much lower temperatures than those used in conventional methodologies. FS not only reduces the energy cost, but also enables the processing of materials with limited thermal stability, such as solid electrolytes. Additionally, since FS are considered as "non-equilibrium" techniques, some materials have been granted with exceptional properties, such as suplerplasticity in ceramics and improved ionic conductivities, which has been attributed to the generation of a large number of defects. Furthermore, FS is a highly versatile technique and, very recently, it has been demonstrated the Reaction Flash Sintering (RFS), where not only the sintering but also the chemical reaction are merged in a single step, boosting the efficiency of the process and amplifying the possibilities offered by FS.

INNOBEC aims to take advantages of the competitiveness offered by FS and RFS of reduced processing times and temperatures to prepare materials with optimized properties for ASSBs, specifically, oxide-types and phosphate-type ceramic solid electrolytes as well as ceramic composites with mixed ionic-electronic conduction to be used as cathodes or anodes. The ultimate goal of INNOBEC is the co-sintering in a single step of ASSB-type multilayer structures and the evaluation of their electrochemical performance. INNOBEC is an innovative project, which merges the previous experience of the PI in both fields ASSBs and FS, proposing a new energy efficient methodology to facilitate the preparation and processing of solid electrolytes so that the serious interfacial problems, arising from the co-sintering and that are slowing down the development of ASSBs, can be alleviated.

Técnicas Flash para la obtención de Óxidos de alta entropía con propiedades MAGnéticas (FOMAG)

Flash Techniques for the Production of High-Entropy Oxides with MAGnetic Properties

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
ProyExcel_00360	01-02-2023 31-08-2025	Junta de Andalucía	138.979 €

Investigador Principal Research Head
Alejandro F. Manchón Gordón

RESUMEN / ABSTRACT

El proyecto FOMAG se centra en la aplicación de novedosas técnicas de sinterizado rápido, como el Sinterizado Flash (FS), el Sinterizado Flash Reactivo (SFR) y el Sinterizado Flash Multifásico (MPFS), para la síntesis de óxidos de alta entropía (HEOs) con propiedades magnéticas de interés tecnológico. A pesar de que la técnica FS se propuso por primera vez en 2010, la SFR en 2018 y la MPFS en 2022, el interés por este proceso ha experimentado un notable crecimiento en diversas áreas científicas debido a su gran potencial científico y tecnológico.

Estas técnicas permiten la fabricación de materiales cerámicos a temperaturas y tiempos considerablemente inferiores a los requeridos por los métodos de sinterización convencionales, mediante la aplicación de una pequeña corriente eléctrica a través de la muestra. Además, las condiciones experimentales particulares de las técnicas Flash hacen posible la obtención de materiales cerámicos densos y nanoestructurados, lo cual resulta desafiante mediante métodos convencionales. De manera significativa, el sinterizado Flash no solo reduce de forma drástica el consumo energético necesario para el procesamiento de materiales cerámicos, sino que también amplía sus aplicaciones a nuevos materiales con fines tecnológicos. En este contexto, los HEOs son una clase emergente de materiales cerámicos que contienen cinco o más cationes en composiciones equimolares. La singularidad de estos sistemas, propuestos por primera vez en 2015, radica en su extrema complejidad química, combinada con su simplicidad cristalográfica, ya que los átomos se ordenan en una única estructura cristalina relativamente sencilla, superando las separaciones de fases típicas de sistemas altamente dopados. En términos de la estructura local, estos materiales constan de un número excepcionalmente alto de combinaciones diferentes de enlaces metal-oxígeno-metal, lo que afecta de manera inherente las interacciones magnéticas en función de factores como la geometría de coordinación, la valencia y el tipo de cationes metálicos circundantes. Esto da lugar a una diversidad de respuestas magnéticas muy interesantes.

FOMAG propone la aplicación de las técnicas FS, RFS y MPFS en la producción de HEOs con propiedades magnéticas, aprovechando las ventajas intrínsecas de estas técnicas, especialmente en la obtención de una alta densidad en sistemas donde esto resulta especialmente desafiante.

The FOMAG project focuses on the application of innovative fast sintering techniques, such as Flash Sintering (FS), Reactive Flash Sintering (RFS), and Multifaceted Flash Sintering (MPFS), for the synthesis of high-entropy oxides (HEOs) with technologically relevant magnetic properties. Despite FS being first proposed in 2010, SFR in 2018, and MPFS in 2022, interest in this process has grown significantly in various scientific fields due to its considerable scientific and technological potential

These techniques enable the fabrication of ceramic materials at significantly lower temperatures and times compared to conventional sintering methods, achieved by applying a small electric current through the sample. Furthermore, the specific experimental conditions of Flash techniques allow the production of dense and nanostructured ceramic materials, which can be challenging using conventional methods. Importantly, Flash sintering not only drastically reduces the energy consumption required for ceramic material processing but also extends its applications to new materials for technological purposes. In this context, HEOs represent an emerging class of ceramic materials with equimolar compositions containing five or more cations. The uniqueness of these systems, first proposed in 2015, lies in their extreme chemical complexity coupled with simple crystallography, where atoms arrange in a relatively straightforward crystal structure, overcoming phase separations typical in heavily doped systems. In terms of the local structure, these materials consist of an unusually high number of distinct combinations of metal-oxygen-metal bonds, inherently affecting magnetic interactions based on factors such as coordination geometry, valence, and the types of surrounding metal cations. This results in a wide range of intriguing magnetic responses.

FOMAG proposes the utilization of FS, RFS, and MPFS techniques in producing HEOs with magnetic properties, capitalizing on the inherent advantages of these techniques, particularly in achieving high density in systems where this is particularly challenging.

OTROS PROYECTOS / OTHER PROJECTS

A la Búsqueda de Nuevos Cerámicos Ultraduros a Base de Boro para Aplicaciones Estructurales en la Nueva Generación de Aviones y uso Seguro y Eficiente de la Energía

Código/Code:	PID2019-103847RJ-I00
Periodo/Period:	01-10-2020 / 30-09-2023
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Investigador responsable/Research head:	Bibi Malmal Moshtaghion Entezari
Participante del ICMS como investigador:	Diego Gómez García

Diseño e impresión 3D de implantes bifásicos porosos personalizados para el tratamiento de defectos osteocondrales

Código/Code:	PID2022-137911OB-I00
Periodo/Period:	01-09-2023 / 31-08-2026
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	175.000 €
Investigador responsable/Research head:	Yadir Torres Hernández (US)/Ana Alcudia Crus (US)
Participante del ICMS como investigador:	Francisco José Gotor Martínez

Desarrollo de Nanogeneradores piezoeléctricos flexibles y de alta eficiencia basados en nanocompuestos perovskita/PVDF (NANOGEN)

Código/Code:	TED2021-132021-131458a-100
Periodo/Period:	01-12-2022 / 30-11-2024
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	149.500 €
Investigador responsable/Research head:	Rocío Moriche Tirado (US)
Participantes del ICMS como investigador:	Francisco J. Gotor Martínez, María Jesús Sayagués de Vega, Rosalía Poyato Galán, Ana Morales Rodríguez (US), Felipe Gutiérrez Mora (US), Ángela Gallardo López (US)

Nuevos scaffolds piezoeléctricos de compuestos nanoestructurados para la regeneración ósea mediante fabricación aditiva (PIZAM)

Código/Code:	PID2020-117648RB-I00. Plan Estatal 2017-2020 Retos Proyectos I+D+i.
Periodo/Period:	01-09-2021 / 31-08-2024
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	175.450 €
Investigador responsable/Research head:	Mario Monzón (ULPGC)/ Rubén Paz (ULPGC)
Participante del ICMS como investigador:	Maria Jesús Sayagués, Rocío Moriche Tirado (US)

Diseño y selección de materiales novedosos para fabricar pilas de combustible de óxido sólido reversibles de alto rendimiento (Layered rSSOCs)

Código/Code:	TED2021-132021-132057B-100
Periodo/Period:	01-12-2022 / 30-11-2024
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	149.500 €
Investigador responsable/Research head:	Francisco J. García García (US)
Participantes del ICMS como investigador:	Francisco J. Gotor Martínez, María Jesús Sayagués

Fabricación de materiales porosos de base hierro con características refractarias para sistemas de purificación, uso y almacenaje de hidrógeno

Código/Code:	PID2021-123010OB-100
Periodo/Period:	01-09-2022 / 31-08-2026
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	72.800 €
Investigador responsable/Research head:	Ernesto Chicardi Augusto (US)/Ranier Enrique Sepúlveda Ferrer (US)
Participante del ICMS como investigador:	Francisco J. Gotor Martínez

Aplicando la economía circular en el desarrollo de nuevos conglomerantes hidráulicos activados alcalinamente de baja huella de carbono para soluciones constructivas (CongActiva)

Código/Code:	PID2020-11516RB-I00
Periodo/Period:	01-09-2021 / 31-08-2024
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovación
Importe total/Total amount:	108.900 €
Investigador responsable/Research head:	D. Eliche-Quesada (Universidad de Jaén)
Participante del ICMS como investigador:	Pedro José Sánchez Soto

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Negative emissions power plant based on flexible calcium-looping process integrated with renewables and methane production

Ortiz, C; García-Luna, S; Carro, A; Chacartegui, R; Pérez-Maqueda, L
Renewable & Sustainable Energy Reviews, **185** (2023) 113614
Octubre, 2023 · DOI: 10.1016/j.rser.2023.113614

This paper provides a review of negative carbon capture technologies. Based on these technologies, here it is proposed an innovative negative emissions power plant combining the generation and storage of energy from biomass, photovoltaic, and concentrated solar power, capturing and recovering CO_2 by producing H_2 or CH_4 as green energy carriers. The main features of the system are i) large-scale energy production system with negative CO_2 emissions; ii) 100% renewable system based on biomass and solar energy with the possibility of integrating other renewables; iii) synergistic integration of processes and systems; iv) recovery of O_2 generated by photovoltaic-driven electrolysis within the process of partial biomass oxycombustion and v) solar-driven limestone calcination. A detailed model of the entire plant is developed to evaluate the integration of the process. The model performance is assessed on an hourly basis throughout the whole year. The base case results show an energy consumption from 1 to 2.1 MJ/kg CO_2 to capture 60–77% of CO_2 emitted from the biomass plant and green methane production of more than 7500 tons/year. The negative emissions associated with the process are -612 kg CO_2/MWh. It justifies the interest in the proposed negative emissions power plant.

Partial oxycombustion-calcium looping hybridisation for CO_2 capture in waste-to-energy power plants

Ortiz, C; García-Luna, S; Chacartegui, R; Valverde, JM; Pérez-Maqueda, L
Journal of Cleaner Production, **403** (2023) 136776
Junio, 2023 · DOI: 10.1016/j.jclepro.2023.136776

Integrating bioenergy and carbon capture and storage (BECCS) presents a great opportunity for power produc-tion with negative global CO_2 emissions. This work explores a novel synergetic system that integrates mem-branes, partial biomass oxycombustion and the calcium looping (CaL) process. Polymeric membranes generate oxygen-enriched air (OEA) with an O_2 concentration of 39%v/v, which is used for partial oxycombustion of biomass waste. The CO_2-enriched flue gas evolves from the waste-to-energy plant to the CaL unit, where CO_2 concentration is increased up to 90-95%v/v, ready for

purification and sequestration. Compared to only oxy-combustion systems, the proposed concept presents fewer technological challenges in retrofitting boilers to waste-to-energy plants. Moreover, this new approach is highly efficient as integrating membranes to produce OEA instead of cryogenic distillation systems significantly reduces energy consumption. A novel integration concept is modelled to evaluate the whole process efficiency and the effect of key parameters on the system performance, such as the temperature of the reactors, the membrane surface area, and the partial oxy-combustion degree. The results show that the so-called mOxy-CaL system has an energy consumption associ-ated with CO_2 capture below 4 MJ/kg CO_2 (a 31% lower than that for a conventional CaL process), with a higher CO_2 capture efficiency than oxycombustion and the CaL process separately. On the other hand, the economic analysis shows a higher CO_2 capture cost for the novel configuration than for the typical CaL configuration due to the additional investment cost of the membrane system. Improvements in membrane performance by increasing its permeance and diminishing the required surface area would significantly reduce the economic cost of this novel integration. Using membranes with permeance over 400 GPU would boost the system's competitiveness.

Integration of calcium looping and calcium hydroxide thermochemical systems for energy storage and power production in concentrating solar power plants

Carro, A; Chacartegui, R; Ortiz, C; Arcenegui-Troya, J; Pérez-Maqueda, LA; Becerra, JA
Energy, **283** (2023) 128388
Noviembre, 2023 · DOI: 10.1016/j.energy.2023.128388

Energy storage is a key factor in the development of renewables-based electrical power systems. In recent years, the thermochemical energy storage system based on calcium-looping has emerged as an alternative to molten salts for energy storage in high-temperature concentrated solar power plants. This technology still presents some challenges that could be solved by integrating the thermochemical energy storage system based on calcium hydroxide. This work studies a novel concentrated solar power system integrating calcium-looping and calcium hydroxide thermochemical energy storage systems. The results show that the combined use of hydration -dehydration cycles in the calcination-carbonation processes of the calcium looping for energy storage could partially solve the issue related to the multicyclic deactivation of calcium oxide. The improvement in the con-version of calcium oxide during carbonation is demonstrated experimentally when hydration-dehydration cycles are combined. Numerical simulations demonstrate the technical feasibility of the integrated process, with efficiencies ranging between 38-46%, improved with the increase in calcium oxide conversion in the carbonator, showing the potential of the proposed integration.

Large-scale oxygen-enriched air (OEA) production from polymeric membranes for partial oxycombustion processes

Garcia-Luna, S; Ortiz, C; Chacartegui, R; Pérez-Maqueda, LA
Energy, **268** (2023) 126697
Abril, 2023 · DOI: 10.1016/j.energy.2023.126697

Partial oxycombustion using Oxygen-Enriched Air (OEA), produced by air-gas separation with polymeric membranes, combined synergistically with CO_2 capture technologies, can reduce the overall energy cost of CO_2 capture, and it is a potential alternative to conventional CO_2 capture technologies. An exhaustive review of polymeric membranes for this application is presented. The best membranes showed permeability values in the 450-25,100 barrer and selectivities higher than 3.6 for large-scale

operations. These membranes can produce OEA with oxygen molar concentrations of up to 40% for retrofitting large-scale power plants (~500 MWe) with partial oxycombustion. For OEA production, the polymeric membrane system is more efficient than cryogenic distillation since the specific power consumption of the former is 35.17 kWh/ton OEA. In comparison, that of the latter is 49.57 kWh/ton OEA. This work proposes that the OEA produced by the membranes feed a partial oxycombustion process integrated with calcium looping within a hybrid CO_2 capture system. The power con-sumption of the hybrid CO_2 capture system proposed here is 29.05% lower than in the case OEA is produced from cryogenic distillation, which justifies the potential interest in using polymeric membranes for OEA production.

A national data-based energy modelling to identify optimal heat storage capacity to support heating electrification

Lizana, J; Halloran, CE; Wheeler, S; Amghar, N; Renaldi, R; Killendahl, M; Pérez-Maqueda, LA; McCulloch, M; Chacartegui, R
Energy, **262** (2023) 125298
Enero, 2023 · DOI: 10.1016/j.energy.2022.125298

Heating decarbonisation through electrification is a difficult challenge due to the considerable increase in peak power demand. This research proposes a novel modelling approach that utilises easily accessible national-level data to identify the required heat storage volume in buildings to decrease peak power demand and maximises carbon reductions associated with electrified heating technologies through smart demand-side response. The approach assesses the optimal shifting of heat pump operation to meet thermal heating demand according to different heat storage capacities in buildings, which are defined in relation to the time (in hours) in which the heating demand can be provided directly from the heat battery, without heat pump operation. Ten scenarios (S) are analysed: two baselines (S1-S2) and eight load shifting strategies (S3-S10) based on hourly and daily demand-side responses. Moreover, they are compared with a reference scenario (S0), with heating currently based on fossil fuels. The approach was demonstrated in two different regions, Spain and the United Kingdom. The optimal heat storage capacity was found on the order of 12 and 24 h of heating demand in both countries, reducing additional power capacity by 30-37% and 40-46%, respectively. However, the environmental benefits of heat storage alternatives were similar to the baseline scenario due to higher energy consumption and marginal power generation based on fossil fuels. It was also found that load shifting capability below 4 h presents limited benefits, reducing additional power capacity by 10% at the national scale. The results highlight the importance of integrated heat storage technologies with the electrification of heat in highly gas-dependent regions. They can mitigate the need for an additional fossil-based dispatchable generation to meet high peak demand. The modelling approach provides a high-level strategy with regional specificity that, due to common datasets, can be easily replicated globally. For reproducibility, the code base and datasets are found on GitHub.

Thermochemical energy storage using calcium magnesium acetates under low CO_2 pressure conditions

Amghar, N; Jiménez, PES; Maqueda, LAP; Perejón, A
Journal of Energy Storage, **63** (2023) 106958
Julio, 2023 · DOI: 10.1016/j.est.2023.106958

The calcium looping multicycle performance of CaO-based materials, derived from calcium magnesium acetates with different Mg content were tested under experimental conditions compatible with thermochemical energy storage. In order to reduce the sintering-induced decay in performance, calcination at an absolute CO_2 pressure of 0.1 bar and 0.01 bar is implemented. CaO carbonation is performed at standard 1 bar CO_2 conditions. The samples can be fully calcined in short residence times. Samples with MgO present high cycling stability, even when the MgO content is as low as 5 mol%. The effective conversion values lie within the range 0.88-0.84 over ten calcination/carbonation cycles, which provides an accumulated energy storage density of 90.9 GJ/m^3. This outstanding reactivity is related with the microstructure of the sample after calcination composed of CaO nanoparticles that are highly reactive for carbonation.

A novel, green, cost-effective and fluidizable SiO_2-decorated calcium-based adsorbent recovered from eggshell waste for the CO_2 capture process

Imani, M; Tahmasebpoor, M; Sánchez-Jiménez, PE; Valverde, J; Garcia, VM
Separation and Purification Technology, **305** (2023) 122523
Enero, 2023 · DOI: 10.1016/j.seppur.2022.122523

The reduction, storage, and reuse of greenhouse gas carbon dioxide (CO_2) is a crucial concern in modern society. Bio-waste adsorbents have recently aroused the investigator's attention as auspicious materials for CO_2 capture. However, the adsorption capacity decaying and poor fluidizability during carbonation/calcination cycles of all natural adsorbents used in the calcium-looping process (CaL) are important challenges. The current study ex-plores the performance of a novel SiO_2-decorated calcium-based adsorbent recovered from eggshell waste in terms of both CO_2 capture capacity and fluidity. Two preparation methods of hydration and sol-gel were used to obtain Ca-based adsorbents with different pore configurations and volumes. Modification of the adsorbents was applied by dry physically mixing with different weight percentages of hydrophobic SiO_2 nanoparticles (NPs), in order to maintain stability and fluidity. The adsorbent prepared by the sol-gel method exhibited a fluffier structure with smaller grain sizes and higher porosity than that of prepared by the hydration method, leading to a 6.9 % increase in conversion at the end of the 20th cycle. Also, with the optimal amount of SiO_2 nanoparticles, i. e. 7.5 wt%, the amount of CaO conversion obtained by sol-gel derived adsorbent was 27.59 % higher than that by pristine eggshell at the end of the 20th carbonation/calcination cycles. The fluidizability tests showed that the highest bed expansion ratio (2.29) was achieved for sol-gel derived adsorbent in the presence of 7.5 wt% silica nanoparticles which was considerably higher than the amount of 1.8 and 1.6 belonged to sol-gel derived adsorbent and pristine eggshell without silica at the gas velocity of approximate to 6.5 cm/s, respectively. The high adsorption capacity and proper fluidity of this novel and green calcium-based adsorbent promise its wide application.

An overview of polymeric composite scaffolds with piezoelectric properties for improved bone regeneration

Donate, R; Paz, R; Moriche, R; Sayagués, MJ; Alemán-Domínguez, ME; Monzón, M
Materials & Design, **231** (2023) 112085
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Despite the dramatic change that Tissue Engineering or stem cell therapies have brought to current therapeutic strategies, there is a lack of functionalities in the available biomaterials for manufacturing scaffolds to treat several highly prevalent osseous diseases (osteochondral defects, osteoporosis, etc.). One promising approach to fill this gap involves the development of innovative piezoelectric scaffolds for improved bone regeneration. Scaffolds with the appropriate piezoelectricity can positively influence the proliferation and differentiation of mesenchymal stem cells to regenerate bone tissue, since surface electrical charges play a key role in the mechanotransduction process. In this work, polymeric-based composite scaffolds with piezoelectric properties intended for bone tissue engineering are reviewed. Special attention is paid to biocompatible, piezoelectric polymers that show suitable properties to be pro-cessed by additive manufacturing techniques. Previous works on composite scaffolds based of these poly-meric matrices and containing piezoceramic additives are summarized. The use of piezoelectric nanostructured composite formulations containing lead-free ceramic oxide nanoparticles with per-ovskite structure is highlighted. Also, different commonly applied mechanical stimuli to activate the piezoelectric effect of the developed materials are presented. Finally, other applications of such scaffolds are mentioned, including their capabilities for real-time monitoring

Metal- based eggshell particles prepared via successive incipient wetness impregnation method as a promoted sorbent for CO_2 capturing in the calcium looping process

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Cyclic adsorption by using of bio-waste eggshell particles as a cheap, accessible and environmentally friendly $CaCO_3$ source has been considered as one of the important methods to decrease or remove CO2 from the flue gas. However, deactivation of eggshell particles and CO_2 capture capacity decaying with increasing the cycle's number remained as an important challenge. Using metal nitrates as one of the modification methods has been proposed by the researchers to overcome this problem. Current study investigates the influence of three metal nitrates of Al, La and Mg added to the eggshell particles via successive incipient wetness impregnation (SIWI) method to improve their adsorption performance. The TGA results at the end of the 20th carbonation/calcination cycle revealed a meaningful relationship between CaO molar conversion of eggshell modified with metal nitrates and their crystallite size as well as the surface area of the sorbents, so that the smaller the crystal size and the larger the surface area, the higher the molar conversion of CaO could be achieved. Due to the highest conversion obtained for Mg-containing sample, the effect of different weight percentages of this additive was also investigated. Results showed that 5 wt% MgO contained eggshell particles could be reported as the most outstanding sample for its improved molar conversion, capture capacity at the end of 20th carbonation/calcination cycle and BET surface area, which were 30.18%, 0.23 gr CO_2/gr adsorbent and 3.5 m^2/g while the corresponding amounts for raw eggshell were 17.26%, 0.11 gr CO_2/gr adsorbent and 1.63 m^2/g, respectively.

Limits of powder metallurgy to fabricate porous Ti35Nb7Zr5Ta samples for cortical bone replacements

Rodríguez-Albelo, LM; Navarro, P; Gotor, FJ; de la Rosa, JE; Mena, D; Garcia-Garcia, FJ; Beltran, AM; Alcudia, A; Torres, Y

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Mayo, 2023 · DOI: 10.1016/j.jmrt.2023.04.212

The use of β-Titanium alloys to fabricate metal implants with Young's modulus that re-sembles bone tissues is presented as an alternative to commercially pure titanium or α-Titanium alloys, although it is still necessary to introduce proper implant porosity to reach the Young's modulus of cortical bones. In this work, porous samples were fabricated by loose sintering (0 MPa) and compared to samples manufactured at 1000 MPa, both sintered under the same conditions. Raw powders and sintered samples of the β-Titanium alloy, Ti35Nb7Zr5Ta, were characterized in detail in terms of both physicochemical and micro-structural properties. Moreover, the tribo-mechanical behavior of sintered samples was evaluated by performing ultrasound technique, instrumented micro-indentation (*P-h* curves), and scratch tests. The bio-functional behavior was studied by impedance spec-troscopy and contact angle measurements. The results allowed the evaluation of the limits of conventional powder metallurgy (percentage of porosity, size, and morphology of pores), as well as the influence of the porosity and chemical composition to achieve a better biomechanical and bio-functional behavior that would guarantee bone requirements. The Ti35Nb7Zr5Ta alloy showed relatively high electrical impedance values compared to commercially pure titanium, indicating an improved bio-corrosion behavior. Furthermore, wettability measurements indicated that porous disks fabricated by loose sintering exhibit higher hydrophilicity, often associated with a better antibacterial response

Efficient SrO-based thermochemical energy storage using a closed-loop pressure swing

Amghar, N; Sánchez-Jiménez, PE; Ortiz, C; Pérez-Maqueda, LA; Perejón, A
Applied Thermal Engineering, **235** (2023) 121411
Noviembre, 2023 · DOI: 10.1016/j.applthermaleng.2023.121411

The $SrCO_3$/SrO system has recently attracted interest for thermochemical energy storage due to the high energy densities potentially attainable. However, the high temperatures needed to promote calcination involve a sintering-induced deactivation of SrO to carbonation. In this work, SrO-based samples have been tested using a closed-loop pressure swing approach involving calcinations and carbonations at absolute pressures of 0.01 bar and 1 bar CO_2, respectively. Using low CO_2 absolute pressure for calcination decreases the reaction temperature to 900 C, thus reducing the deactivation of SrO. Moreover, the use of additives further improves the reactivity of the samples. The addition of ZrO_2 and MgO by mechanical mixing and acetic acid treatment, respectively, results in samples with very high multicycle performance, yielding material energy storage densities after twenty cycles above 5.0 GJ/m^3. These results significantly improve those obtained for similar samples in which calcinations and carbonations were carried out at an absolute pressure of 1 bar CO_2. Regarding the integration of the thermochemical energy storage into concentrating solar power plants, calcining SrO-based materials at low pressure increases the net thermal-to-electric efficiencies by up to 6 % points compared to CaO-based materials calcined at the same conditions. The importance of experimental conditions and precursors in the multicycle behaviour of SrO-based materials for thermochemical energy storage is emphasized.

Electrical performance of orthotropic and isotropic 3YTZP composites with graphene fillers

López-Pernia, C; Muñoz-Ferreiro, C; Moriche, R; Morales-Rodríguez, A; Gallardo-López, A; Poyato, R
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3 mol% yttria tetragonal zirconia polycrystal (3YTZP) composites with orthotropic or isotropic microstructures were obtained incorporating few layer graphene (FLG) or exfoliated graphene nanoplatelets (e-GNP) as fillers. Electrical conductivity was studied in a wide range of contents in two configurations: perpendicular ($\sigma_{\perp}$) and parallel ($\sigma_{//}$) to the pressing axis during spark plasma sintering (SPS). Isotropic e-GNP composites presented excellent electrical conductivity for high e-GNP contents ($\sigma_{\perp} \sim$ 3200 S/m and $\sigma// \sim$ 1900 S/m for 20 vol% e-GNP), consequence of their misoriented distribution throughout the matrix. Optimum electrical performance was achieved in the highly anisotropic FLG composites, with high electrical conductivity for low contents ($\sigma_{\perp} \sim$ 680 S/m for 5 vol%), percolation threshold below 2.5 vol% FLG and outstanding electrical conductivity for high contents ($\sigma_{\perp} \sim$ 4000S/m for 20 vol%), result of the high aspect ratio and low thickness of FLG.

Reversibility and thermal dependence of the martensitic transformation in a melt-spun $Ni_{55}Fe_{17}Ga_{26}Co_2$ Heusler alloy

Manchón-Gordón, AF; Vidal-Crespo, A; Blázquez, JS; Kowalczyk, M; Ipus, JJ; Kulik, T; Conde, CF
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An almost single phase 14 M modulated martensite is obtained in melt spun ribbon of $Ni_{55}Fe_{17}Ga_{26}Co_2$ Heusler alloy. The effect of thermal treatments on the stability of the reverse martensitic transformation from 14 M modulated martensite to austenite phase in this system has been investigated by both non-isothermal and isothermal treatments. Heating above martensitic transformation promotes a continuous reduction of the martensitic transformation temperature, which stabilizes the austenite phase at room temperature and induces the precipitation of the gamma phase. However, thermal treatments at temperatures between the austenite start and finish temperatures induce the decoupling of the austenite formation in a subsequent heating. The two successive reverse martensitic transformations could be ascribed to the untransformed martensite in the previous interrupted heating and to the new martensite formed during cooling.

R-curve evaluation of 3YTZP/graphene composites by indirect compliance method

López-Pernia, C; Muñoz-Ferreiro, C; Prada-Rodrigo, J; Moreno, P; Reveron, H; Chevalier, J; Morales-Rodríguez, A; Poyato, R; Gallardo-López, A
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This work addresses the crack growth resistance of 3 mol% Yttria-doped Tetragonal Zirconia Polycrystalline (3YTZP) spark-plasma sintered (SPS) composites containing two types of graphene-based nanomaterials (GBN): exfoliated graphene nanoplatelets (e-GNP) and reduced graphene oxide (rGO). The crack growth resistance of the composites is assessed by means of their R-Curve behavior determined by three-point bending tests on single edge "V" notched beams (SEVNB), in two different orientations of the samples: with the crack path perpendicular or parallel to the pressure axis during the SPS sintering. The sharp edge notches were machined by ultrashort laser pulsed ablation (UPLA). The compliance and optical-based methods for evaluating the crack length are compared on the basis of the experimental R-Curve results in composites with 2.5 vol% rGO tested in the perpendicular orientation. Moreover, the activation of reinforcement mechanisms is evaluated by both the fracture surface inspection by Scanning Electron Microscopy and a compliance analysis. It is shown that the indirect compliance

method is relevant and reliable for calculating the R-Curve of 3YTZP/GBN composites. The effect of the type and content of GBN on the crack growth resistance of the composites is also discussed.

Influence of Long-Term CaO Storage Conditions on the Calcium Looping Thermochemical Reactivity

Amghar, N; Perejón, A; Ortiz, C; Pérez-Maqueda, LA; Sánchez-Jiménez, PE
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Long-term storage capability is often claimed as one of the distinct advantages of the calcium looping process as a potential thermochemical energy storage system for integration into solar power plants. However, the influence of storage conditions on the looping performance has seldom been evaluated experimentally. The storage conditions must be carefully considered as any potential carbonation at the CaO storage tank would reduce the energy released during the subsequent carbonation, thereby penalizing the round-trip efficiency. From lab-scale to conceptual process engineering, this work considers the effects of storing solids at low temperatures (50–200 °C) in a CO_2 atmosphere or at high temperatures (800 °C) in N_2. Experimental results show that carbonation at temperatures below 200 °C is limited; thus, the solids could be stored during long times even in CO_2. It is also demonstrated at the lab scale that the multicycle performance is not substantially altered by storing the solids at low temperatures (under CO_2) or high temperatures (N_2 atmosphere). From an overall process perspective, keeping solids at high temperatures leads to easier heat integration, a better plant efficiency (+2–4%), and a significantly higher energy density (+40–62%) than considering low-temperature storage. The smooth difference in the overall plant efficiency with the temperature suggests a proper long-term energy storage performance if adequate energy integration is carried out.

Influence of firing temperature on the ceramic properties of illite-chlorite-calcitic clays

Martinez-Martinez, S; Pérez-Villarejo, L; Garzon, E; Sánchez-Soto, PJ
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The influence of firing temperature on the ceramic properties of illite-chlorite-calcitic clays has been investigated. Three samples of the same clay deposit have been selected. Weight loss, dimensional changes, water absorption, bulk density, open porosity, flexural and compressive strengths, initial capillary water absorption rate and thermal conductivity have been determined as a function of firing temperature in the range 900-1200 °C with 1 h of soaking time. The microstructures of the fired samples have been examined by SEM and the phase evolution studied by XRD. The water absorption capacity decreased from similar to 22% at 900 °C/1 h to a maximum of 12% at 1200 °C/1 h with a maximum linear shrinkage of similar to 2.7%. The open porosities decreased from similar to 22% at 900 °C/1 h up to similar to 20% at 1200 °C/1 h as an effect of progressive sintering with higher densification degree of the ceramic bodies. The flexural strength reached a maximum value of similar to 34 MPa at 1200 °C/1 h. In contrast, the compressive strengths increased by firing up to a maximum of similar to 114 MPa at 1200 °C/1 h. The thermal conductivity increased slightly as increasing firing temperature with a maximum value of 0.582 W/m.K in samples fired at 1200 ° C/1 h. The Ryshkevitch-Duckworth equation was applied and the results indicated that compressive strength is related linearly with open porosity. A

linear correlation was found between thermal conductivity and open porosity. The microstructural evolution by SEM indicated that there is a change of the fired samples at 1100 °C as compared to SEM observations at 900 and 1000 °C. There is an increase of contacts between particles and layered structures associated to dehydroxylated clay minerals (illite and chlorite), quartz particles and pores developed by firing. At 1200 °C/1 h, the microstructures have changed associated to the higher degree of vitrification in the fired sample, with consolidation of the material, interparticle and neck contacts with formation of vitrified bridges. The formation of closed and large open pores of several sizes has been achieved by firing. Small particles were observed as a fine precipitation of crystals in the vitrified structures associated to anorthite, hematite and quartz relicts. This change in microstructure allowed deduce that the compressive strength increased upon firing, with maximum values of this ceramic property at 1200 °C. The ceramic bodies were more sintered by firing and the open porosity decreased progressively. Brickmaking is the main application of these fired illite-chlorite calcitic clays. These clays fired at 900-1100 °C, with 1 h of soaking time, could be applied in the fabrication of clay roofing tiles, tiles and even porous ceramic supports with small variations on shrinkage and porosity, good flexural strengths and high compressive strengths. Samples fired at higher temperatures, 1100 °C/1 h, could be applied as ceramic bricks showing a medium porosity (similar to 20%). They show almost the same bulk density when they are fired at lower temperatures (900 °C). Samples fired at higher temperatures (1150-1200 °C/1 h) could be applied as dark ceramic products. This investigation was interesting because a better knowledge of illite-chlorite-calcitic clays applied as ceramic raw materials has been achieved.

Characterization, thermal and ceramic properties of clays from Alhabia (Almeria, Spain)

Rat, E; Martinez-Martinez, S; Sánchez-Garrido, JA; Pérez-Villarejo, L; Garzon, E; Sánchez-Soto, PJ
Ceramics International, **49** (2023) 14814-14825
Mayo, 2023 · DOI: 10.1016/j.ceramint.2022.05.328

Clays from Alhabia (Almeria, Spain) have been investigated in this work using several analytical techniques: X-Ray Diffraction (XRD), X-Ray Fluorescence (XRF), thermal analysis (Thermogravimetry, TG, and its first deriv-ative, DTG), Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray Spectroscopy (EDS). Texture characteristics (granulometry) and plasticity have been examined. The main ceramic properties (firing shrinkage, water absorption, bulk density, open porosity, flexural strength and thermal conductivity) have been determined using pressed and fired clay samples. Thus, the mineralogical, chemical, textural and ceramic features of these clays have been evidenced for the first time. The mineralogical analysis by XRD indicated that the clay samples are constituted by a mixture of chlorite and illite, as main clay minerals, being quartz and other minerals in lower relative proportion (calcite, gypsum and hematite). This finding is important because the investigations on chlorite-illite-calcitic clays are very scarce. The chemical analysis by XRF showed that silica and alumina are predominant, as expected by the mineralogy, with medium contents of calcium oxide, from calcite, and alkalis, from illite, being ~8 and ~5%, respectively, besides iron and titanium oxides (~8%). The particle size analysis showed 71.76% of "clay fraction" (<2μm) and 21.66% of silt fraction (2-50μm). The plasticity index (Atterberg) was 14.3%, with acceptable moulding and extrusion properties. Thermal analysis by TG/DTG indicated a weight loss associated to dehydroxylation of structural water of the clay minerals and decarbonation of calcite by progressive heating. After the characterization of raw clays, the next step was the determination of ceramic properties of mixed and ground clays after firing using pressed bodies. For this purpose, two firing temperatures were selected (900 and 1100 °C) for 1 h. The examination of the resultant fired bodies indicated that porous ceramic materials (~36% open porosity and-

22% of water absorption capacity) can be obtained by firing at 900 °C, with small variations in dimensions (<0.8% at 1100 °C). The porosity changed at relatively lower values by firing at 1100 °C (~34-35%), being associated to the presence of decomposed calcite. Bulk density was found almost constant from 900 to 1100 °C, with a maximum value of ~1.67 g/cm^3 at 1100 °C. Flexural strength reached a maximum value of 34.47 MPa at 1100 °C for the ground sample. Finally, thermal conductivity after firing the clay bodies was found almost constant at 900 and 1100 °C (0.457 and 0.479 W/mK, respectively). Taking into account these results, the main applications of the Alhabia clays have been evaluated. These clays can be used for the fabrication of porous ceramic supports and tiles by firing at 900 °C. Firing the clays at higher temperature (1100 °C) is of great interest for the fabrication of ceramic tiles and ceramic bricks of higher flexural strength with variable porosity and practically constant in dimensions. It is economically important although at higher processing costs. Finally, it can be emphasized that this work is a contribution of a better scientific knowledge of chlorite-illite-calcitic clays as ceramic raw materials.

Influence of AC fields and electrical conduction mechanisms on the flash-onset temperature: Electronic ($BiFeO_3$) vs. ionic conductors (8YSZ)

Molina-Molina, S; Perejón, A; Pérez-Maqueda, LA; Sánchez-Jiménez, PE
Ceramics International, **49** (2023) 14834-14843
Mayo, 2023 · DOI: 10.1016/j.ceramint.2022.06.242

This work aims to clarify the influence of AC (up to 50 kHz) vs DC fields on the flash-onset temperature, emphasizing the role of the electrical conduction mechanism. $BiFeO_3$ (BFO) is used as an example of electronic conductor while 8-mol % Yttria-stabilized zirconia (8YSZ) is used as an example of ionic conductor. For 8YSZ, a frequency dependence of the flash-onset temperature and flash-induced heating is observed. This is consistent with the different contributions found in the total electrical response of 8YSZ as characterized by impedance spectroscopy measurements. Estimations based on the blackbody radiation model suggest that 8YSZ samples attain higher temperatures under AC fields due to a more efficient heating. Moreover, a noticeable decrease in the activation energy for the electrical conduction after the flash is triggered is attributed to electronic conduction. Meanwhile, the lack of frequency response and insensitiveness to the type of electrical field found in the case of BFO can be attributed to its mainly electronic bulk conduction.

Nanocrystalline Skinnerite (Cu_3SbS_3) Prepared by High-Energy Milling in a Laboratory and an Industrial Mill and Its Optical and Optoelectrical Properties

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Molecules, **28** (2023) 1
Enero, 2023 · DOI: 10.3390/molecules28010326

Copper, antimony and sulfur in elemental form were applied for one-pot solid-state mechanochemical synthesis of skinnerite (Cu_3SbS_3) in a laboratory mill and an industrial mill. This synthesis was completed after 30 min of milling in the laboratory mill and 120 min in the industrial mill, as corroborated by X-ray diffraction. XRD analysis confirmed the presence of pure monoclinic skinnerite prepared in the laboratory mill and around 76% monoclinic skinnerite, with the secondary phases famatinite (Cu_3SbS_4; 15%), and tetrahedrite ($Cu_{11.4}Sb_4S_{13}$; 8%), synthesized in the industrial mill. The nanocrystals were agglomerated into micrometer-sized grains in both cases. Both samples were nanocrystalline, as was confirmed with HRTEM. The optical band gap of the Cu_3SbS_3 prepared in the laboratory mill was determined to

be 1.7 eV with UV-Vis spectroscopy. Photocurrent responses verified with I-V measurements under dark and light illumination and Cu_3SbS_3 nanocrystals showed similar to 45% enhancement of the photoresponsive current at a forward voltage of 0.6 V. The optical and optoelectrical properties of the skinnerite (Cu_3SbS_3) prepared via laboratory milling are interesting for photovoltaic applications.

Direct comparison of surface crystal growth kinetics in chalcogenide glass measured by microscopy and DSC

Shanelova, J; Honcova, P; Malek, J; Perejón, A; Pérez-Maqueda, LA
Journal of the American Ceramic Society, **106** (2023) 6051-6061
Mayo, 2023 · DOI: 10.1111/jace.19204

Surface crystallization in fine powder $Se_{70}Te_{30}$ chalcogenide glass was studied by differential scanning calorimetry (DSC) and optical microscopy. A complex kinetic analysis of these experimental data reveals that the contracting sphere mechanism (R3 model) is the rate determining step of crystal growth, and the conventional Johnson-Mehl-Avrami-Kolmogorov model cannot be used in this case. Moreover, it is clearly shown that the particle size distribution should be considered in crystallization studies. Actually, when the particle size effect is taken into account, the simulated DSC curves for the R3 model agree very well with the experimental data over the entire temperature range. The crystallization kinetics determined from the nonisothermal DSC data are consistent with previously reported isothermal crystallization data for the same powder fraction. The crystal growth rate calculated from isothermal and nonisothermal DSC data agrees very well with the microscopically measured surface and bulk crystal growth rate.

Touch-free reactive flash sintering of dense strontium hexaferrite permanent magnet

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Agosto, 2023 · DOI: 10.1111/jace.19389

This work presents an extension of the touch-free flash sintering technique. In the proposed technique, chemical reaction and sintering occur in a single step, without the use of electrodes, in the presence of electric and magnetic fields. We show that a dense, single-phase strontium hexaferrite magnet can be produced from a mixture of commercial carbonate and oxide powders in a single step in a little more than a minute. This new technique implies significant reduction in energy and time consumption (primarily because of ultrafast processing) relative to conventional sintering.

Effect of thermal treatments below devitrification temperature on the magnetic and magnetocaloric properties in mechanically alloyed $Fe_{70}Zr_{30}$ powders

Manchón-Gordón, AF; Blázquez, JS; Kowalczyk, M; Ipus, JJ; Kulik, T; Conde, CF
Journal of Non-Crystalline Solids, **609** (2023) 122267
Junio, 2023 · DOI: 10.1016/j.jnoncrysol.2023.122267

In this work, the relaxation of the amorphous structure of mechanically alloyed $Fe_{70}Zr_{30}$ powders has been analyzed through interrupted heating ramps below the devitrification temperature. As a result of

such thermal treatment, Curie temperature and temperature at maximum magnetic entropy change curves shift to higher temperatures as the temperature of heating treatment increases. This effect can be attributed to both the release of the stress accumulated in the amorphous powder during the milling process and to the initiation of nucleation of α-Fe crystallites, as it has been shown by Mo center dot ssbauer spectroscopy.

A practical analysis for decelerated growth processes to get physically meaningful kinetic parameters from classical nucleation and growth theory despite of over-growth

Blázquez, JS; Caballero-Flores, R; Manchón-Gordón, AF; Borrego, JM; Conde, CF
Journal of Non-Crystalline Solids, **610** (2023) 122305
Junio, 2023 · DOI: 10.1016/j.jnoncrysol.2023.122305

We have analyzed the overgrowth problem arising in decelerated growth processes of spherical crystals in the frame of classical nucleation and growth theory developed by Kolmogorov, Johnson and Mehl, and Avrami (KJMA). To do that, simulations of decelerated growth transformations with a constant nucleation rate have been performed, changing the linear growth rate of spherically shaped nuclei from null (instantaneous growth rate) to constant (characteristic of interface controlled growth processes). We propose the determination of the actual kinetic parameters through the analysis of the inflection point of time evolution of transformed fraction. The correlations found between the effective kinetic parameters from direct KJMA analysis and the actual ones make it possible obtaining physically meaningful parameters. The proposed analysis has been applied to the nano-crystallization of amorphous FINEMET-type compositions.

Low Temperature Magnetic Transition of $BiFeO_3$ Ceramics Sintered by Electric Field-Assisted Methods: Flash and Spark Plasma Sintering

Manchón-Gordón, AF; Perejón, A; Gil-González, E; Kowalczyk, M; Sánchez-Jiménez, PE; Pérez-Maqueda, LA
Materials, **16** (2023) 189
Enero, 2023 · DOI: 10.3390/ma16010189

Low temperature magnetic properties of $BiFeO_3$ powders sintered by flash and spark plasma sintering were studied. An anomaly observed in the magnetic measurements at 250 K proves the clear existence of a phase transition. This transformation, which becomes less well-defined as the grain sizes are reduced to nanometer scale, was described with regard to a magneto-elastic coupling. Furthermore, the samples exhibited enhanced ferromagnetic properties as compared with those of a pellet prepared by the conventional solid-state technique, with both a higher coercivity field and remnant magnetization, reaching a maximum value of 1.17 kOe and 8.5 10^{-3} emu/g, respectively, for the specimen sintered by flash sintering, which possesses the smallest grains. The specimens also show more significant exchange bias, from 22 to 177 Oe for the specimen prepared by the solid-state method and flash sintering technique, respectively. The observed increase in this parameter is explained in terms of a stronger exchange interaction between ferromagnetic and antiferromagnetic grains in the case of the pellet sintered by flash sintering.

New Types and Dosages for the Manufacture of Low-Energy Cements from Raw Materials and Industrial Waste under the Principles of the Circular Economy and Low-Carbon Economy

Martinez-Martinez, S; Pérez-Villarejo, L; Eliche-Quesada, D; Sánchez-Soto, PJ
Materials, **16** (2023) 802
Enero, 2023 · DOI: 10.3390/ma16020802

The cement manufacturing industry is one of the main greenhouse gas emission producers and also consumes a large quantity of raw materials. It is essential to reduce these emissions in order to comply with the Paris Agreement and the principles of the circular economy. The objective of this research was to develop different types of cement clinker blends using industrial waste and innovative design to produce low-energy cement. Several types of waste have been studied as alternative raw materials. Their main characteristics have been analyzed via X-ray fluorescence (XRF), X-ray diffraction (XRD), Attenuated total reflectance Fourier trans-form infrared spectroscopy (ATR-FTIR), thermal analysis (TG-DTG-DSC) and scanning electron microscopy and energy dispersive X-ray spectroscopy analysis (SEM-EDS). The results obtained from the experimental work carried out in this research focused on the study of crude blends for low-energy cement created from industrial waste. The effect of the addition of different industrial waste types, as a substitution for raw materials, in the production of low-energy cement with high dicalcium silicate content has been investigated. Thus, the dosage design has been performed using modified Bogue equations and quality indexes (LSF, AM, and SM). The calculations of both the modified Bogue equations and quality indexes necessitate knowledge of the weight percentages of CaO, SiO_2, Al_2O_3, and Fe_2O_3, determined via XRF. In this theoretical design of the different blends, it has been established that a dicalcium silicate ratio of 60-65 wt % and an LSF of 78-83% as the limit are values common to all of them. The calculation basis for the crude blends has been based on calcined materials. Therefore, the chemical composition was established, following this premise. Thus, it was possible to develop cement clinker blends with compositions of 50 wt % and 100 wt % using industrial wastes. This research has shown that the clinkerization process is one of the main options for the valorization of waste and its consideration for inclusion as a raw material within the circularity of the cement industry's production process. Thus, waste is used as a raw material for the production of a more useful substance, taking into account the fundamental principles of the circular economy.

Structural, Vibrational, and Magnetic Characterization of Orthoferrite $LaFeO_3$ Ceramic Prepared by Reaction Flash Sintering

Manchón-Gordón, AF; Sánchez-Jiménez, PE; Blázquez, JS; Perejón, A; Pérez-Maqueda, LA
Materials, **16** (2023) 1019
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$LaFeO_3$ perovskite ceramics have been prepared via reaction flash technique using Fe_2O_3 and La_2O_3 as precursors. The obtained pellets have been investigated using several techniques. The formation of $LaFeO_3$ has been clearly confirmed by X-ray diffraction. The scanning electron microscopy micrographs have shown the microporous character of the obtained pellets due to the low temperature and dwell time used in the synthesis process (10 min at 1173 K). The orthorhombic-rhombohedral phase transition has been observed at approximately 1273 K in differential thermal analysis measurements, which also allows us to determine the Neel temperature at 742 K. The fitted Mossbauer spectra exposed the presence of a single sextet ascribed to the Fe^{+3} ions in the tetrahedral site. Finally, magnetic measurements at room temperature indicate the antiferromagnetic character of the sample.

Effect of L-Glutamic Acid on the Composition and Morphology of Nanostructured Calcium Phosphate as Biomaterial

Takabait, F; Martinez-Martinez, S; Mahtout, L; Graba, Z; Sánchez-Soto, PJ; Pérez-Villarejo, L
Materials, **16** (2023) 1262
Febrero, 2023 · DOI: 10.3390/ma16031262

Calcium phosphate (CaP) with several chemical compositions and morphologies was prepared by precipitation using aqueous solutions of L-Glutamic acid (H_2G) and calcium hydroxide, both mixed together with an aqueous solution (0.15 M) of phosphoric acid. Plate-shaped dicalcium phosphate dihydrate (brushite) particles were obtained and identified at a lower concentration of the solution of the reactants. The Ca/P ratio deduced by EDS was similar to 1, as expected. The nanoscale dimension of carbonate apatite and amorphous calcium phosphate, with variable Ca/P ratios, were revealed by X-ray diffraction (XRD) and scanning electron microscopy and energy dispersive X-ray spectroscopy analysis (SEM-EDS). They were characterized in medium and high concentrations of calcium hydroxide (0.15 M and 0.20 M). The equilibria involved in all the reactions in aqueous solution were determined. The thermodynamic calculations showed a decrease in the amount of chelate complexes with an increase in pH, being the opposite of [$CaPO_4^-$] and [$CaHG^+$]. This fluctuation showed an evident influence on the morphology and polymorphism of CaP particles obtained under the present experimental conditions, with potential use as a biomaterial.

ICTAC Kinetics Committee recommendations for analysis of thermal decomposition kinetics

Koga, N; Vyazovkin, S; Burnham, AK; Favergeon, L; Muravyev, NV; Pérez-Maqueda, LA; Saggese, C; Sánchez-Jiménez, PE
Thermochimica Acta, **719** (2023) 179384
Enero, 2023 · DOI: 10.1016/j.tca.2022.179384

In this review article, the Kinetics Committee of the International Confederation for Thermal Analysis and Calorimetry (ICTAC) delivers a collection of recommendations for the kinetic analysis of thermal decomposition processes. These recommendations specifically focus on the thermal decomposition processes in inorganic, organic, and polymeric materials, as well as biomass and solid fuels. A general introduction to the kinetic analysis of thermal decompositions studied by thermal analysis techniques is followed by individual sections that discuss thermal decomposition of specific classes of materials and respective kinetic approaches. In each section, various kinetic analysis procedures are introduced with regard to specific features of the reactions and explained pro-gressively from simple to complex reactions with examples of practical kinetic analysis. These recommendations are expected to provide a guidance for performing reliable and meaningful kinetic analysis in terms of practical usefulness and physico-chemical significance of the results.

Flexible Kinetic Model Determination of Reactions in Materials under Isothermal Conditions

Arcenegui-Troya, J; Perejón, A; Sánchez-Jiménez, PE; Pérez-Maqueda, LA
Materials, **16** (2023) 1851
Febrero, 2023 · DOI: 10.3390/ma16051851

Kinetic analysis remains a powerful tool for studying a large variety of reactions, which lies at the core of material science and industry. It aims at obtaining the kinetic parameters and model that best describe a given process and using that information to make reliable predictions in a wide range of conditions. Nonetheless, kinetic analysis often relies on mathematical models derived assuming ideal conditions that are not necessarily met in real processes. The existence of nonideal conditions causes large modifications to the functional form of kinetic models. Therefore, in many cases, experimental data hardly obey any of these ideal models. In this work, we present a novel method for the analysis of integral data obtained under isothermal conditions without any type of assumption about the kinetic model. The method is valid both for processes that follow and for those that do not follow ideal kinetic models. It consists of using a general kinetic equation to find the functional form of the kinetic model via numerical integration and optimization. The procedure has been tested both with simulated data affected by non-uniform particle size and experimental data corresponding to the pyrolysis of ethylene-propylene-diene.

Seville history insight through their construction mortars

Pérez-Rodríguez, JL; Pérez-Maqueda, LA; Franquelo, ML; Duran, A
Journal of Thermal Analysis and Calorimetry, **148** (2023) 13157-13174
Julio, 2023 · DOI: 10.1007/s10973-023-12313-y

Seville is intimately linked to its historic role and extensive cultural heritage. The city has been occupied by Romans, Arabs and Christians, who built important historical buildings. Roman (first-second centuries) and Arabic (eleventh century) buildings, medieval Shipyard (thirteenth century), San Isidoro and Santa Maria de las Cuevas monasteries (fifteenth century), Santa Maria de las Cuevas (fifteenth century modified in eighteenth century), El Salvador Church (eighteenth century), the Royal Ordenance building (eighteenth century) and Santa Angela de la Cruz convent (twentieth century) performed with lining mortars, and mortars used in building stones (City Hall and Marchena Gate), all of them located in Seville (Spain), have been studied. Ninety-four mortar samples (employed as structural, plaster, coating) originally used or applied in restoration processes have been collected to perform an archaeometry study. The ratio of CO_2 mass loss to hydraulic water (H_2O) mass loss, and the mineralogical characterization by X-ray diffraction has been used to compare the mortars used in the different historical periods. Mainly hydraulic mortars were widely used in all these studied monuments as most mortars showed CO_2/H_2O ratios within the 4-10 range. Moreover, the thermal analysis curves also showed a broad temperature range for the thermal decomposition of the carbonate fraction of the mortars.

Determination of the activation energy under isothermal conditions: revisited

Arcenegui-Troya, J; Sánchez-Jiménez, PE; Perejón, A; Pérez-Maqueda, LA
Journal of Thermal Analysis and Calorimetry, **148** (2023) 1679-1686
Febrero, 2023 · DOI: 10.1007/s10973-022-11728-3

The kinetic analysis of solid-state processes aims at obtaining fundamental information that can be used for predicting the time evolution of a process within a wide range of conditions. It is an extended belief that the determination of the kinetic parameters from the analysis of curves recorded under isothermal conditions is strongly conditioned by the kinetic model used to fit the experimental data. Thus, much effort is devoted to finding the model that truly describes a process in order to calculate the kinetic parameters with accuracy. In this work, we demonstrate that the value of activation energy determined

from kinetic analysis of isothermal curves is independent of the kinetic model used to fit the experimental data and, taking advantage of the underlying reason for this, a method for determining the activation energy with two isothermal curves is proposed.

Thermal arrest analysis of the reverse martensitic transformation in a $Ni_{55}Fe_{19}Ga_{26}$ Heusler alloy obtained by melt-spinning

Vidal-Crespo, A; Manchón-Gordón, AF; Blázquez, JS; Ipus, JJ; Svec, P; Conde, CF
Journal of Thermal Analysis and Calorimetry, **148** (2023) 2367-2375
Enero, 2023 · DOI: 10.1007/s10973-022-11889-1

$Ni_{55}Fe_{19}Ga_{26}$ ribbons obtained by melt-spinning technique exhibit a martensitic transformation from $L2_1$ cubic austenite phase to 14 M martensite phase above room temperature. We have taken advantage of the existence of thermal hysteresis of the martensitic phase transition (~11 K) to analyze the effect of isothermal treatments on the reverse martensitic transformation, which has been analyzed by means of interrupted heating using differential scanning calorimetry. The experimental findings clearly indicate a time-depending effect in the martensitic transformation at temperatures between the austenite start and finish temperatures. Moreover, it has been observed that two successive martensitic transformations take place after the isothermal arrest was performed.

Sintering behaviour of a clay containing pyrophyllite, sericite and kaolinite as ceramic raw materials: Looking for the optimum firing conditions

Sánchez-Soto, PJ; Garzon, E; Pérez-Villarejo, L; Eliche-Quesada, D
Boletin de la Sociedad Española de Ceramica y Vidrio, **62** (2023) 26-39
Enero, 2023 · DOI: 10.1016/j.bsecv.2021.09.001

The sintering behaviour of a pyrophyllite clay has been investigated. The mineralogical composition by X-ray diffraction (XRD) of this sample was ~35 wt.% pyrophyllite, ~25 wt.% sericite/illite, ~15 wt.% kaolinite and ~20 wt.% quartz. The chemical composition was consistent with these results, with a total flux content of 4.18 wt.%. Prismatic bars were prepared by dry pressing using this sample and fired in the range 800-1500 °C with 0.5-5 h of soaking times. Sintering diagrams were obtained using the results of linear firing shrinkage, water absorption capacity, bulk density and apparent porosity determined in the ceramic bodies as a function of firing temperatures. It was found a trend of slight variations of bulk density values firing in the range 1000-1150 °C, with marked decreases of these values for these bodies fired at 1200 °C and 1300 °C. The temperature of maximum bulk density was determined as ~1200 °C and the vitrification temperature was ~1300 °C where the apparent porosity becomes almost zero. The vitrification process of the pyrophyllite clay sample was investigated using a method previously described in the literature, which considered an Arrhenius approach under isothermal conditions and a first order kinetic. It was determined an activation energy *(Ea) of* ~45 kJ/mol with a linear correlation coefficient of 0.998. The relative rates of vitrification were calculated. It was found that the contribution of vitrification due to the heating was relatively small compared to the vitrification during soaking. Mullite and quartz are forming the ceramic bodies besides a vitreous or glassy phase. The thermally treated pyrophyllite clay showed a dense network of rod-shaped and elongated needle-like crystals, being characteristic features of mullite as a dense felt. The vitrification rate equation, as deduced in this study by first time, can be a useful tool to estimate the optimum firing conditions of the pyrophyllite clays applied as ceramic raw materials.

Effect of Alkaline Salts on Pyrolyzed Solid Wastes in Used Edible Oils: An Attenuated Total Reflectance Analysis of Surface Compounds as a Function of the Temperature
Romero-Sarria, F; Real, C; Córdoba, JM; Hidalgo, C; Alcalá, MD
Spectroscopy Journal, **1** (2023) 98-110
Septiembre, 2023 · DOI: 10.3390/spectroscj1020009

Biochars obtained via the pyrolysis of biomass are very attractive materials from the point of view of their applications and play key roles in the current energy context. The characterization of these carbonaceous materials is crucial to determine their field of application. In this work, the pyrolysis of a non-conventional biomass (solid wastes in used edible oils) was investigated. The obtained biochars were characterized using conventional techniques (TG, XRD, and SEM-EDX), and a deep analysis via ATR-FTIR was performed. This spectroscopic technique, which is a rapid and powerful tool that is well adapted to study carbon-based materials, was employed to determine the effect of temperature on the nature of functional groups on the surface. Moreover, the water washing of the raw sample (containing important quantities of inorganic salts) before pyrolysis evidenced that the inorganic salts act as catalysts in the biomass degradation and influence the degree of condensation (DOC) of PAH. Moreover, it was observed that these salts contribute to the retention of oxygenated compounds on the surface of the solid.

ARTICULOS PUBLICADOS EN REVISTAS (NO SCI) / PAPERS IN NON-SCI JOURNALS

Simultaneous Biocementation and Compaction of a Soil to Avoid the Breakage of Cementitious Structures during the Execution of Earthwork Constructions
L. Morales, E. Garzón, P.J. Sánchez-Soto, E. Romero
Geotechnics, 3 (2023) 224-253

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

47th International Conference and Exposition on Advanced Ceramics and Composites ICACC2023
22-27 enero [Florida, Estados Unidos de América]

On the development of multifunctional ceramic composites – Fracture resistance. *C. Muñoz-Ferreiro, H. Reveron, J. Chevalier, A. Morales-Rodríguez, R. Poyato, A. Gallardo-López.* COMUNICACIÓN ORAL

Fabrication of Al_2O_3-Y_2O_3-ZrO_2 composites using spark plasma sintering. *M. Vakhshouri, A. Najafzadeh, A. Talimian, A. Gallardo-López, R. Poyato, F. Gutiérrez-Mora, A. Prnová, D. Galusek.* COMUNICACIÓN ORAL

Congreso Español Iberoamericano de Pulvimetalurgia · CEIPM2023
29-31 mayo [San Sebastián, España]

Manufacture and characterization of porous TiNbZrTa samples for bone replacements: conventional PM vs space holder technique. *L.M. Rodríguez-Albelo, J.E. de la Rosa, P. Navarro, D. Mena, R. Cañete, F.J. Gotor, E.J. Delgado-Pujol, F.J. García García, A. Alcudia, A.M. Beltran, Y. Torres*. COMUNICACIÓN ORAL

XVIII Conference & Exhibition of the European Ceramic Society · ECerS
02-06 julio [Lyon, Francia]

Tuning the mechanical and electrical properties of structural zirconia ceramics with graphene-based nanostructures. *A. Gallardo-López, C. Muñoz-Ferreiro, C. López-Pernía, H. Reveron, J. Chevalier, R. Moriche, A. Morales-Rodríguez, R. Poyato*. CONFERENCIA INVITADA

Piezoelectric properties of BZT-BCT ceramics obtained by mechanosynthesis and their dependence on processing parameters. *R. Moriche, M.J. Sayagués, F.J. Gotor, R. Poyato, R. Donate, M. Monzón, R. Paz*. COMUNICACIÓN ORAL

A multiscale characterization of tetragonal zirconia reinforced with 2D nanomaterials. *C. Muñoz-Ferreiro, H. Reveron, J. Chevalier, A. Morales-Rodríguez, R. Poyato, A. Gallardo-López*. COMUNICACIÓN ORAL

Additives for densification of fine-grained Y_2O_3: from solid state to liquid phase sintering. *A. Najafzadeh, A. Talimian, V. Girman, R. Poyato, A. Gallardo-López, F. Gutiérrez-Mora, P. Hvizdos, K. Maca, D. Galusek*. COMUNICACIÓN ORAL

8YCSZ/rGO composites for components in SOFC: Microstructure and electrical conductivity. *R. Poyato, F.J. Coto, A. de la Cruz-Blanco, R. Moriche, C. López-Pernía, A. Morales-Rodríguez, A. Gallardo-López*. COMUNICACIÓN ORAL

Optimization of the piezoelectric and dielectric properties of BST-BCT ceramics obtained by mechanosynthesis. *R. Poyato, A. Otero, F.J. Gotor, M.J. Sayagués, A. Morales-Rodríguez, R. Moriche*. COMUNICACIÓN ORAL

Tribological behavior of few-layered graphene / zirconia composites. *C. Muñoz-Ferreiro, E. Guisado-Arenas, R. Moriche, A. Morales-Rodríguez, R. Poyato, A. Gallardo-López, F. Gutiérrez-Mora*. PÓSTER

7th Central and Eastern European Conference on Thermal Analysis and Calorimetry · CEE-TAC7
28-31 agosto [Brno, República Checa]

Chemical, mechanical and thermal characterization of gypsum samples from quarries in the Tabernas desert (Almería, Spain). *V. García-Garzón, F. Peiró, J.A. Sánchez-Garrido, E. Garzón, L.A. Pérez-Maqueda, P.J. Sánchez-Soto*. PÓSTER

Characterization of crushed brick waste from the Alhabia Ceramic Plant (Almería, Spain). J.D. Ayala, V. García-Garzón, F. Peiró, J.A. Sánchez-Garrido, S. Martínez, P.J. Sánchez-Soto, E. Garzón. PÓSTER

Jornada ACerS Materiales vítreos y cerámicos para aplicaciones de alta tecnología
26 octubre [Sevilla, España]

Composites circona/grafeno para componentes en celdas SOFC. *F.J. Coto, A. de la Cruz-Blanco, R. Moriche, A. Gallardo-López, A. Morales-Rodríguez, R. Poyato*. COMUNICACIÓN ORAL

Flash sintering of ceramic materials. *P.E. Sánchez-Jiménez, L.A. Pérez Maqueda, A. Perejón, E. Gil González, S. Molina*. COMUNICACIÓN ORAL

Graphene-based nanostructures to improve the mechanical and electrical performance of zirconia ceramics. *C. Muñoz-Ferreiro, C. López-Pernía, H. Reveron, J. Chevalier, R. Moriche, F. Gutiérrez-Mora, A. Morales-Rodríguez, R. Poyato, A. Gallardo-López*. COMUNICACIÓN ORAL

Vitrification and Geopolimerization of Wastes for Inertizing and/or Recycling · Vitro-GeoWaste III
09-10 noviembre [Sofia, Bulgaria]

Study of gypsum wastes as by-product from several quarries examined in the Tabernas desert (Almería, Spain). *V. García-Garzón, F. Peiró, J.A. Sánchez-Garrido, P.J. Sánchez-Soto, E. Garzón*. PÓSTER

Rejected brick waste from an industrial ceramic plant (Alhabia, Almería, Spain) as raw material for plant substrates. *E. Garzón, J.D. Ayala, V. García-Garzón, R.M. Chica-Moreno, M.T. Lao-Arenas, F. Peiró, J.A. Sánchez-Garrido, S. Martínez-Martínez, P.J. Sánchez-Soto*. PÓSTER

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

Jornada de Jóvenes investigadores en Materiales Funcionales (UCO-SECV)
11-12 mayo [Córdoba, España]

Caracterización mediante espectroscopía de impedancia de composites circona/grafeno para electrolitos en SOFC. *F.J. Coto, A. de la Cruz-Blanco, R. Moriche, R. Poyato*. COMUNICACIÓN ORAL

Aplicación del método de distribución de tiempos de relajación para el análisis de espectros de impedancia en composites de circona/grafeno. *A. de la Cruz-Blanco, F.J. Coto, Á. Gallardo-López, R. Poyato*. COMUNICACIÓN ORAL

V Jornadas de Jóvenes Científicos en Materiales de Construcción. Wokshop "Situación actual y perspectiva de los materiales de construcción"
27-28 noviembre [Madrid, España]

Manufacture and study of low energy cement clinkers under the concept of circular economy. S. Martínez-Martínez, L. Pérez-Villarejo, D. Eliche-Quesada, P.J. Sánchez-Soto. PÓSTER

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Processing and characterization of ceramic composites with two dimensional layered nanomaterials**
Autor:	Carmen Muñoz Ferreiro
Directores:	Ángela Gallardo López, Rosalía Poyato Galán, Jérôme Chavalier
Centro:	Universidad de Sevilla
Fecha Defensa:	22 de septiembre de 2023

FORMACIÓN DE GRADUADOS / BACHELOR DEGREE THESIS

Título:	**Optimización de materiales nanocompuestos de matriz polimérica cargados con cerámicas piezoeléctricas para su aplicación en nanogeneradores flexibles**
Autor:	Andrea Otero Pino
Directoras:	María Jesús Sayagués de Vega, Rocío Moriche Tirado
Grado:	Trabajo de Investigación · Prácticas en empresa
Centro:	Universidad de Sevilla
Fecha Defensa:	23 de mayo de 2023

Título:	**Análisis de espectroscopía de impedancia compleja en electrolitos para celdas de combustible de óxido sólido**
Autor:	Ana de la Cruz Blanco
Tutora:	Rosalía Poyato Galán
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	21 de junio de 2023

Título:	**Caracterización de sistemas rGO/8YCSZ para su uso como componentes en celdas de combustible de óxido sólido**
Autor:	Francisco Javier Coto Ruiz
Tutora:	Rosalía Poyato Galán
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	28 de junio de 2023

Título:	**Síntesis y caracterización del sistema (Ba, Ca)(Sn, Ti)O_3 para su uso en nanogeneradores piezoeléctricos flexibles**
Autor:	Andrea Otero Pino
Tutora:	María Jesús Sayagués de Vega, Rocío Moriche Tirado
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	21 de julio de 2023

DOCENCIA / TEACHING

MÁSTER EN CIENCIA Y TECNOLOGÍA DE NUEVOS MATERIALES

Modelización Aplicada a la Caracterización Estructural de Medios Condensados Dra. Regla Ayala Espinar
Química del Estado Sólido Dr. Pedro Enrique Sánchez Jiménez
Recuperación y Transformación de Materiales Dr. Antonio Perejón Pazo

El personal del ICMS imparte docencia en titulaciones de Grado y doble Grado de la Universidad de Sevilla. La docencia se desarrolla en diversos centros: Facultad de Física, Facultad de Biología, Facultad de Química, Facultad de Farmacia y Escuela Técnica Superior de Ingeniería Informática.

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Microdurómetro FM700 Future-Tech
- Máquina de ensayo universal AGS-J, Shimadzu
- 3 Termobalanzas CI Electronics
- 2 molinos planetarios PULVERISETTE 7 (Fritsch)
- 1 molino planetario PULVERISETTE 7 Premium Line (Fritsch)
- 1 molino planetario PULVERISETTE 4 (Fritsch)
- 1 molino planetario PM100 (Retsch)
- 1 molino vibratorio MM301 (Retsch)

- 1 molino vibratorio SPEX 8000
- 1 molino centrífugo PULVERISETTE (Fritsch)
- 1 molino de atrición O1HD (Union Process)
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- Horno horizontal alta temperatura 1600 oC Carbolite
- Horno horizontal 1200 oC Carbolite
- Microcortadora metalográfica manual EVOLUTION (REMET)
- Microcortadora metalográfica MICROMET (REMET)
- Prensa automática metalográfica IPA30 (REMET)
- Pulidora automática LS2 (REMET)
- Analizador Termomecánico TMA 1000 (Linseis)
- Calorímetro diferencial de barrido DSC (TA instruments Q200)
- Horno horizontal 1150 oC Hobersal
- Impedancímetro Agilent 4294ª
- Multímetro Keysight B2901A
- Equipo de Hot-Press TERMOLAB HP2500

MATERIALES FUNCIONALES NANOESTRUCTURADOS
NANOSTRUCTURED FUNCTIONAL MATERIALS

GRUPOS DE INVESTIGACIÓN

Materiales Nanoestructurados y Microestructura | 642015
Nanostructured Materials and Microstructure
http://nanomatmicro.icmse.csic

Materiales para Bioingeniería y Regeneración Tisular |642014
Materials for Bioengineering and Tissue Regeneration

Nanotecnología en Superficies y Plasma |642012
Nanotechnologies on Surfaces and Plasma
http://sincaf.icms.us-csic.es

Tribología y Protección de Superficies |861494
Tribology and Protection of Surfaces

PERSONAL / PERSONNEL

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Profesores "Ad Honorem"	Agustín Rodríguez González-Elipe
Investigadores Honorarios	José Cotrino Bautista
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Doctores Contratados	Jorge A. Budagosky Marcilla Lidia Contreras Bernal Víctor López Flores Carmen López Santos José Manuel Luque Centeno Manuel Oliva Ramírez
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Programa Investigo	Melania Sánchez Villa

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Descongelación inteligente y sostenible mediante ingeniería de ondas acústicas aplicadas a superficies
Sustainable Smart De-Icing by Surface Engineering of Acoustic Waves · SOUNDOFICE

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
H2020-FET-OPEN	01-11-2020 31-10-2024	Comisión Europea	690.602 €

Investigador Principal Research Head	Componentes Research Group
Ana Isabel Borrás Martos	Agustín R. González-Elipe Juan Pedro Espinós Manzorro Francisco Yubero Valencia Ángel Barranco Quero Víctor J. Rico Gavira María del Carmen López Santos

RESUMEN / ABSTRACT

Icing on surfaces is commonplace in nature and industry and too often causes catastrophic events. SOUNDofICE ultimate goal is to overcome costly and environmentally harmful de-icing methods with a pioneering strategy based on the surface engineering of MHz Acoustic Waves for a smart and sustainable removal of ice. This technology encompasses the autonomous detection and low-energy-consuming removal of accreted ice on any material and geometry. For the first time, both detection and de-icing will share the same operating principle. The visionary research program covers the modeling of surface wave atom excitation of ice aggregates, integration of acoustic transducers on large

areas, and the development of surface engineering solutions to stack micron-size interdigitated electrodes together with different layers providing efficient wave propagation, anti-icing capacity, and aging resistance. We will demonstrate that this de-icing strategy surpasses existing methods in performance, multifunctionality, and capacity of integration on industrially relevant substrates as validated with proof of concept devices suited for the aeronautic and wind power industries. SOUNDofICE high-risks will be confronted by a strongly interdisciplinary team from five academic centers covering both the fundamental and applied aspects. Two SMEs with first-hand experience in icing will be in charge of testing this technology and its future transfer to key EU players in aeronautics, renewable energy, and household appliances. An Advisory Board incorporating relevant companies will contribute to effective dissemination and benchmarking. The flexibility of the R&D plan, multidisciplinarity, and assistance of the AdB guarantee the success of this proposal, bringing up a unique opportunity for young academia leaders and SMEs from five different countries to strengthen the EU position on a high fundamental and technological impact field, just on the moment when the climate issues are of maxima importance.

Diseño de nanomateriales tridimensionales para la solución todo en uno a la recolección de energía ambiental de fuentes múltiples

Three-dimensional nanoscale design for the all-in-one solution to environmental multisource energy scavenging | 3DSCAVENGERS

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
H2020-ERC-STG/0655	01-03-2020 / 28-02-2025	Comisión Europea	1.498.414 €

Investigador Principal Research Head
Ana Isabel Borrás Martos

ABSTRACT

Thermal and solar energy as well as body movement are all sources of energy. They can be exploited by advanced technology, obviating the need for battery recharging. These local ambient sources of energy can be captured and stored. However, their low intensity and intermittent nature reduces the recovery of energy by microscale instruments, highlighting the need for an integrated multisource energy harvester. Existing methods combine different single source scavengers in one instrument or use multifunctional materials to concurrently convert various energy sources into electricity.

The EU-funded 3DScavengers project proposes a compact solution based on the nanoscale architecture of multifunctional three-dimensional materials to fill the gap between the two existing methods. These nanoarchitectures will be able to simultaneous and individual harvesting from light,

movement and temperature fluctuations. 3DScavengers ultimate goal is to apply a scalable and environmental friendly one-reactor plasma and vacuum approach for the synthesis of this advanced generation of nanomaterials.

Dispositivos fotónicos y optoelectrónicos de alta estabilidad basados en perovskitas de haluro mediante tecnologías de vacío y plasma Stable halide perovskite-based photonic and optoelectronic devices by vacuum and plasma technologies · PVSkite

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2022-143120OB-100	01-09-2023 31-08-2026	Ministerio de Ciencia e Innovación	175.000 €

Investigador Principal Research Head	Componentes Research Group
Ángel Barranco Quero Juan Ramón Sánchez Valencia	Vanda Fortio Godinho, Victor López Flores, José Cotrino Bautista, Ricardo Molina (IQAC), Victor J. Rico Gavira, Juan Pedro Espinós Manzorro, Ana I. Borrás Martos, Francisco J. Aparicio Rebollo, Carmen López Santos, Agustín Rodríguez González-Elipe

RESUMEN / ABSTRACT

PVSkite es un proyecto multidisciplinar que tiene como principales objetivos incorporar las técnicas de plasma de deposición y de procesado de materiales y un conjunto de técnicas sintéticas de vacío al desarrollo de materiales, nanoestructuras y dispositivos basados en perovskitas de haluro. En el caso de las técnicas de plasma, buscamos explorar aproximaciones, como la técnica RPAVD (deposición en vacío asistida por plasmas remotos), a desarrollo de sistemas optimizados de encapsulación de celdas, pasivación de electrodos, ingeniería de intercaras, y diseño de nuevas formulaciones de electrodos para celdas de perovskita de haluro. Esta aproximación queda avalada por algunos resultados recientes y muy prometedores del grupo, sobre la encapsulación de celdas de perovskita y la pasivación de electrodos inorgánicos con películas poliméricas conformales ultradelgadas mediante procesos de plasma. En el caso de los procesos de vacío, el proyecto se centrará en la aplicación de la técnica de deposición en ángulo rasante (GLAD) al diseño de perovskitas cristalinas anisotrópicas para el control de la polarización de la luz, así como en la estructuración de electrodos de transporte de carga. También aquí se parte de algunos resultados iniciales muy recientes que muestran el enorme potencial de esta aproximación en al campo de la síntesis de nanoestructuras de perovskitas de haluro anisotrópicas. Las aproximaciones experimentales propuestas no han sido abordadas en la literatura actual, pero creemos que

pueden tener un impacto muy importante en desarrollo de estos materiales y dispositivos. En ambos casos, el grupo cuenta con más de dos décadas de experiencia internacional reconocida en la fabricación de materiales funcionales por estas técnicas y en su aplicación final en dispositivos (fotónicos, sensores, captadores de energía, etc.).

El proyecto abarca actividades fundamentales y aplicadas a diferentes niveles, como la simulación de procesos de crecimiento, la síntesis de nuevos materiales bajo diseño, la caracterización avanzada de propiedades y la interrogación de dispositivos. El desarrollo de una serie de prototipos a escala de laboratorio es un aspecto fundamental de la propuesta, que servirá para validar la viabilidad de los materiales desarrollados. Con este fin se diseñarán las plataformas y los protocolos de medida adecuados. El primer tipo de dispositivo a desarrollar serán celdas de perovskitas estables frente al agua y la humedad que incorporen todas las modificaciones de intercaras, nuevos electrodos y elementos de encapsulación desarrollados en el proyecto. El segundo tipo de dispositivos serán dispositivos optoelectrónicos de perovskita sensibles a la polarización. Se estudiarán dos tipos a) dispositivos emisores de luz polarizada y b) detectores de luz polarizada. El proyecto se completa con una evaluación preliminar de la estabilidad a vacío y en presencia de fuentes de ionización de dispositivos seleccionados.

Además, se cuenta con la colaboración y el interés expreso de cuatro empresas directamente relacionadas con la propuesta: Arquimea, a través de su división de energía, Lasing SA con una amplia experiencia en el uso y desarrollo de elementos y dispositivos fotónicos y Fluxim, líder mundial en el estudio y el desarrollo de equipamiento para el estudio de la estabilidad ambiental de celdas solares. La cuarta, ALTER Tech, está interesada en la potencial aplicación de celdas estables de perovskita en el espacio.

PVSkite is a multidisciplinary project whose main objective is to exploit advanced vacuum and plasma techniques for the development of materials, nanostructures, and devices based on halide perovskites. In the case of plasma techniques, we seek to explore proprietary approaches, such as the RPAVD (remote plasma-assisted vacuum deposition) technique, for the development of encapsulation systems, electrode passivation, interfacial engineering, and new electrode formulations for perovskite solar cells. This approach is supported by some very promising recent results of the group on perovskite cell encapsulation and passivation of inorganic electrodes with ultra-thin conformal polymeric films. In the case of vacuum processes, the project will focus on applying the glancing angle deposition technique (GLAD) to the design of anisotropic crystalline perovskites for light polarization control and the structuring of charge transport electrodes.

We also start from some very recent initial results that demonstrate the enormous potential of this approach. The proposed approaches have not been addressed in the current literature, but we believe can have a very important impact on the development of halide perovskite-based materials and devices. The group has more than two decades of internationally recognized experience in the fabrication of functional materials by these techniques and their application in very diverse fields including the development of functional devices (photonics, sensors, energy sensors, etc.).

The project encompasses activities at different levels, combining fundamental and applied research, growth process and materials simulations, synthesis of new materials under design, advanced functional characterization, and device interrogation. The development of a series of laboratory-scale prototypes is a fundamental aspect of the proposal, which will validate the feasibility of the approach. To this end, appropriate platforms and measurement protocols will be designed. The first type of device to be developed will be perovskite cells, stable against water and humidity incorporating all the modifications of interfaces, novel electrodes, and encapsulation elements developed in the project. The second type of device will be polarization-sensitive perovskite optoelectronic devices, also incorporating selected plasma layers to increase their stability. Two types of polarization-sensitive devices will be studied a) polarized light emitting devices and b) polarized light detectors. The project is completed

with a preliminary evaluation of the stability in vacuum and in the presence of ionization sources of some selected devices.

For the achievement of PVskites objectives, we count on the collaboration and the express interest of four companies that are directly related to each of the aspects of the proposal. These companies are Arquimea, through its energy division, Lasing SA with a wide experience in the use and development of photonic elements and devices, and Fluxim, a world leader in the study of the environmental stability of solar cells. The fourth company, ALTER TÜV NORD, is interested in the potential application of stable perovskite cells in space.

Desarrollo de plasmas intermitentes operados con electricidad renovable para la eliminación y revalorización de CO_2 Development of intermittent plasmas ignited by renewable electricity for the CO_2 splitting and revalorization processes · RENOVACO2

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
TED2021-130124A-100	01-12-2022 30-11-2024	Ministerio de Ciencia e Innovación	148.925 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

La emisión de CO_2 representa actualmente un 77% de las emisiones totales de gases de efecto invernadero con origen antropogénico, propiciando un aumento paulatino del calentamiento global del planeta con las consecuentes y nefastas repercusiones medioambientales que ello supone. Por tanto, es indudable la necesidad de propiciar una transición hacia una economía donde el uso intensivo de combustibles fósiles no sea el eje prioritario, favoreciendo el desarrollo de procedimientos de transformación y aprovechamiento químicos respetuosos con el medio ambiente mediante el uso de fuentes energéticas alternativas. El proyecto "Desarrollo de plasmas intermitentes operados con electricidad renovable para la eliminación y revalorización de CO_2", RENOVACO2, pretende el desarrollo de tecnologías de plasma atmosférico que usan la electricidad como vector energético directo para llevar a cabo pro-

cesos químicos convencionalmente abordados mediante técnicas catalíticas, que involucran altas presiones y temperaturas y usan catalizadores térmicos con elementos contaminantes y de difícil reciclado.

CO_2 emissions currently represent the 77% of the total greenhouse gas emissions of anthropogenic origin. It provokes a gradual increase in global warming of our planet with catastrophic environmental consequences. There is no doubt about the need to promote a transition toward an economy avoiding the intensive use of fossil fuels, i.e., using the electricity generated from renewable sources as primary source of energy, and favoring alternative and more sustainable chemical processes. The project "Development of intermittent plasmas ignited by renewable electricity for the CO_2 splitting and revalorization processes", RENOVACO2, aims at developing atmospheric plasma technologies that use electricity as a direct energy vector to induce chemical processes that are currently carried out through catalytic techniques (i.e., at high pressures and temperatures, using harmful and non-recyclable catalysts). RENOVACO2 is a multidisciplinary project that pursuits the development of novel physical processes for the elimination and revalorization of CO_2, especially designed and optimized for their activation by means of renewable energy sources. The proposed technology consist of using atmospheric pressure plasmas to induce chemical reactions in non-equilibrium conditions at atmospheric pressure and in a distributed way.

Nanogeneradores triboeléctricos para la recolección de energía renovable de gotas de lluvia

Triboelectric nanogenerators for raindrop renewable energy harvesting · DropEner

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
TED2021-130916B-100	01-12-2022 30-09-2025	Ministerio de Ciencia e Innovación	253.000 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

DropEner tiene como objetivo el desarrollo de paneles de lluvia, es decir, recolectores de energía proveniente de gotas que, basados en el principio del nanogenerador triboeléctrico (TENG), funcionan en condiciones exteriores y pueden fabricarse a través de tecnologías escalables y de alto rendimiento. El proyecto demostrará la aplicación de un concepto innovador patentado recientemente por el grupo Nanotecnología en Superficies y Plasma (CSIC-US), "Tixel", sobre la recolección de energía cinética proveniente de gotas de líquido en contacto instantáneo con una superficie triboeléctrica integrada en una arquitectura de tipo condensador. Por lo tanto, el principal objetivo es desarrollar un panel de recolección de energía basado en el primer TENG de arquitecturas nano y microestructuradas capaces de generar alta densidad de potencia mediante la implementación de matrices de nanogeneradores triboeléctricos en la microescala, donde cada generador produzca cientos de microvatios de potencia cuando una gota de lluvia con alta velocidad y alta energía golpee su superficie. La potencia de salida total sería equivalente a la suma de la potencia producida por los generadores individuales y podría alcanzar potencialmente cientos de vatios por metro cuadrado cuando se fabrique una matriz de alta densidad bien diseñada. Además, en un paso más allá en el estado del arte para la explotación de captadores de energía de contacto entre sólido-líquido, DropEner persigue el desarrollo de Tixels duraderos y transparentes totalmente compatibles con celdas solares, incluidas las tecnologías de Silicio y de Tercera Generación (como celdas solares de colorantes y celdas solares de perovskita). Los avances esperados abarcan aspectos como el desarrollo de superficies con super-mojabilidad, la explotación de rutas de producción escalables y procesado de materiales, la fabricación de recolectores de energía de gotas transparentes, la prueba de concepto de diseños novedosos de nanogeneradores triboeléctricos y la gestión de energía en sistemas multifuente de recolección de energía intermitente.

DropEner aims to develop rain panels, that is, energy collectors from drops that, based on the principle of the triboelectric nanogenerator (TENG), work in outdoor conditions and can be manufactured through scalable and high-performance technologies. The project will demonstrate the application of an innovative concept recently patented by the group Nanotechnology on Surfaces and Plasma (CSIC-US), "Tixel", on the collection of kinetic energy from drops in instant contact with a triboelectric surface integrated into a condenser-like architecture. Therefore, the main objective is to develop a drop energy harvesting panel based on the first TENG of nano and microstructured architectures capable of generating high power density by implementing triboelectric nanogenerator arrays at the microscale, where each nanogenerator produces hundreds of microwatts of power when a high-velocity, high-energy raindrop strikes its surface. The total power output would be equivalent to the sum of the power produced by the individual systems and could potentially reach hundreds of watts per square meter when a well-designed high density array is manufactured. In addition, in a step further in the state of the art for the exploitation of solid-liquid drop energy harvesters, DropEner pursues the development of durable and transparent Tixels fully compatible with solar cells, including Silicon and Third Generation technologies. (such as dye solar cells and perovskite solar cells). The expected advances cover aspects such as the development of surfaces with super-wettability, the exploitation of scalable production routes and processing of materials, the manufacture of transparent drop energy harvesters, the proof of concept of novel designs of triboelectric nanogenerators and the management of energy in multi-source intermittent energy collection systems.

Plasmas atmosféricos de arco deslizante para procesos sostenibles Atmospheric Pressure Gliding-Arc Plasmas for Sustainable Applications | FIREBOW

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2020-114270RA-100	01-09-2021 31-08-2024	Ministerio de Ciencia e Innovación	108.900 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

La necesidad de propiciar una transición efectiva desde una economía basada en el uso intensivo de combustibles fósiles a otra donde los criterios de desarrollo se basen en procesos sostenibles que no impliquen la generación de CO_2 hace necesaria la puesta a punto de nuevos procesos, donde la fuente de energía primaria sea la electricidad generada a partir de fuentes renovables. El proyecto "Plasmas Atmosféricos de Arco Deslizante para Procesos Sostenibles", FIREBOW en adelante, pretende el desarrollo de tecnologías de plasma atmosférico que usan la electricidad como vector energético directo para llevar a cabo procesos químicos convencionalmente abordados mediante técnicas catalíticas (a altas presiones y temperaturas, con bajos rendimientos y obtención de subproductos no deseados). En concreto se persigue la puesta a punto de un reactor de Plasma Atmosférico de Arco Deslizante (PAAD) para inducir tres procesos de gran impacto industrial y medioambiental, como son la síntesis de amoniaco (NH_3), la producción de hidrógeno (H_2) y la descontaminación de agua. El amoniaco es la sustancia base de los fertilizantes usados en agricultura, y su demanda aumenta conforme las necesidades de alimentación mundiales. En cuanto al hidrógeno, es conocido que el camino hacia una economía basada en dicho combustible es uno de los retos del siglo XXI. Por otro lado, el desarrollo de técnicas novedosas para la depuración de aguas es cada vez más necesaria, debido al aumento de contaminantes emergentes, sustancias tales como pesticidas, compuestos derivados de la industria farmacéutica y química, microorganismos e incluso productos de higiene personal que los métodos convencionales no son capaces de eliminar en su totalidad. FIREBOW propone, en una primera etapa, desarrollar la tecnología PAAD mediante el diseño, construcción, modelización y puesta a punto de un reactor de arco deslizante. Se explorarán posibles modificaciones sobre los modelos de reactores PAAD actuales, contemplándose el efecto de la incorporación de materiales piezoeléctricos para inducir fenómenos de emisión

secundaria de electrones, la modificación de las características superficiales de los electrodos o la geometría del sistema a fin de propiciar en el futuro una mejora en el rendimiento de los procesos estudiados. La complejidad de los procesos básicos involucrados en este tipo de reactores implicará un estudio fundamental de su respuesta eléctrica y de los fenómenos de transporte de masa y carga, así como una caracterización exhaustiva y diagnosis del plasma en función de parámetros como flujo de gases, interacción entre especies excitadas, tiempo de residencia y otros parámetros básicos de operación. Tanto la caracterización experimental como la simulación teórica del reactor, esta última llevada a cabo mediante métodos computacionales, serán fundamentales para su correcto funcionamiento y optimización de los procesos propuestos. En una segunda etapa se abordará el estudio de las reacciones de obtención de H_2 y NH_3, con el objetivo de maximizar el rendimiento energético de dichos procesos, así como de la purificación de agua. El desarrollo científico-tecnológico propuesto en FIREBOW es de gran interés para diferentes actores socio-económicos, planteándose actividades de transferencia a las empresas y entidades que ya han mostrado su interés en el desarrollo del mismo.

The need to promote an effective transition from an economy based on the intensive use of fossil fuels to another where the development criteria are based on sustainable processes that do not involve the generation of CO_2 makes it necessary to develop new processes using the electricity generated from renewable sources as primary source of energy. The project "Atmospheric Pressure Gliding-Arc Plasmas for Sustainable Applications", FIREBOW hereinafter, aims at developing atmospheric plasma technologies that use electricity as a direct energy vector to induce chemical processes that are currently carried out through catalytic techniques (i.e., at high pressures and temperatures, with low yields and harmful by-products). Specifically, FIREBOW pursues the development of a Gliding Arc Atmospheric Plasma reactor (GA) to induce three processes of great industrial and environmental impact, such as the synthesis of ammonia (NH_3), the production of hydrogen (H_2) and the decontamination of water. Ammonia is the main source to produce fertilizers, which are used in agriculture with an increasing demand according to the increasingly higher needs of foods at global scale. In the case of hydrogen, it is well-known that the path to an economy based on this fuel is one of the challenges of the 21st century. Research in novel techniques for water purification is also increasingly necessary, due to its scarcity and the increase in emergent contaminants, polluting substances such as pesticides, compounds derived from the pharmaceutical and chemical industry, microorganisms and even personal hygiene products that conventional methods are unable to remove completely. FIREBOW proposes, in a first stage, to develop the GA technology through the design, construction, modelling and commissioning of a GA reactor. Possible modifications on the current GA reactors will be explored, considering the effect of the incorporation of piezoelectric materials to induce phenomena of secondary emission of electrons, the modification of the electrode surface materials or the geometry of the system in order to improve the performance of the analysed processes with respect to the current state of the art. The complexity of the basic mechanisms involved in this type of reactors will require a fundamental study of their electrical response and the phenomena of mass and charge transport, as well as an exhaustive characterization and diagnosis of the plasma as a function of operating parameters such as gas flow, interaction between excited species, residence time and other basic operating conditions. Both the experimental and theoretical characterization of the reactor, the latter carried out using computational methods, will be crucial for its correct operation and for the optimization of the proposed processes. In a second stage, the study of the reactions to obtain H_2 and NH_3 will be approached, with the aim of maximizing the energy efficiency, as well as that for the case of the purification of water. The scientific-technological developments proposed in FIREBOW are of the outmost interest to different socio-economic sectors and in the project they are considered knowledge-transfer actions to companies and entities that have already shown their interest in the proposal.

Procesos de Nucleación y Crecimiento en Superficies Piezoeléctricas Excitadas Acústicamente en Atmósferas de Plasma/Vacío

Nucleation and growth mechanisms on piezoelectric surfaces under acoustic excitation in plasma/vacuum environments

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2020-112620GB-100	01-09-2021 31-08-2024	Ministerio de Ciencia e Innovación	106.480 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

Este proyecto aborda el estudio de los fenómenos de nucleación atómica y crecimiento de películas delgadas sobre materiales piezoeléctricos sometidos a excitación acústica en atmósferas de plasma y vacío. Los materiales piezoeléctricos se caracterizan por la aparición de una polarización eléctrica no nula al someterlos a una deformación mecánica, y por el efecto contrario, la aparición de una deformación mecánica al someterlos a una excitación eléctrica y, en la actualidad, se emplean en multitud de aplicaciones y dispositivos, tales como sensores de lluvia, pantallas táctiles o manipulación de líquidos en la microescala, entre otros. En un trabajo seminal publicado por el grupo investigador se demostró que, al crecer una película delgada mediante técnicas de plasma sobre este tipo de superficies excitadas, ésta se estructuraba de acuerdo al patrón definido por las ondas. Este resultado inicial demostraba que la interacción entre la onda/película delgada en crecimiento podría utilizarse como nueva metodología de nanoestructuración de superficies. En este proyecto se aborda esta problemática de tipo fundamental, estudiando específicamente dos mecanismos principales de interacción: i) la transferencia directa de energía/momento de la onda acústica a las especies depositadas, y ii) la interacción entre la onda de polarización eléctrica que se propaga por el material piezoeléctrico y las líneas de campo eléctrico en el plasma, con incidencia directa en el transporte de especies cargadas y al bombardeo superficial selectivo del piezoeléctrico durante el crecimiento de la película. De esta manera, este proyecto se centra en la descripción, desarrollo y comprensión de una nueva fenomenología, y en el desarrollo de todo el marco teórico y conceptual que permita entender dicha interacción. Se espera que la activación acústica de piezoeléctricos y su efecto en atmósferas de plasma se convierta en un nuevo procedimiento para inducir la formación de centros de nucleación para la micro- y nano-estructuración de películas delgadas, permitiendo nuevos desarrollos en el campo de la física de superficies. Asimismo, en el campo de la física del plasma, la posibilidad de modular la interacción entre el plasma y una superficie de acuerdo a un patrón definido por ondas electro-acústicas podría abrir procedimientos alternativos para operar dispositivos de microplasmas o pantallas de plasma.

This project aims at studying atomic nucleation and thin film growth phenomena on piezoelectric surfaces under acoustic excitation in vacuum/plasma environments. Piezoelectric materials are characterized by a non-zero polarization vector when subjected to mechanical deformation and the reverse, a mechanical deformation when subjected to an electrical excitation. While piezoelectric surfaces under acoustic excitation are being used for numerous applications, e.g. raindrop sensors, touch-sensitive screens, or handling of liquids at the microscale, among others, a systematic survey of the literature reveals that only a seminal work published by the research team addresses the effect of acoustic waves in nucleation and growth processes in a plasma environment. There, we demonstrated a strong correlation between the features of the acoustic wave, the associated polarization pattern on the piezoelectric material and the structural features of a surface grown in the presence of a plasma, suggesting that this interaction can be employed as a new methodology to tailor the film nanostructure. Two main sources of interaction are analyzed in this project: i) the mechanical influence of the propagating acoustic wave on the surface-induced mobility processes of ad-atoms, ii) the interaction between the polarization wave on the piezoelectric and the plasma electric field lines, that may affect the transport of charged species and their impingement on the piezoelectric material during growth. In this way, this project focusses on the description, development and understanding of a new phenomenology, and on the provision of the fundamental and theoretical framework to describe this interaction. It is expected that acoustic waves activation and its effect on surrounding plasmas represents a radically new procedure to activate thin film growth and nuclei formation and that the proposed methodology goes beyond any present paradigm in the field of surface physics, envisaging new routes of nanostructuration. Similarly, in the field of plasma dynamics, the possibility of modulating the plasma/surface interaction by acoustic waves is an option that may open alternative procedures for the operation of advanced microplasmas devices or flat plasma displays.

Recubrimientos innovadores preparados por magnetron sputtering para absorción solar selectiva

MAGnetron sputtered Innovative COatings for Solar Selective absorption MAGICOS2

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2019-104256RB-I00	01-06-2020 31-05-2024	Ministerio de Ciencia e Innovación	121.000 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El cambio climático ocasionado por las emisiones de gases con efecto invernadero y el agotamiento de los combustibles fósiles a corto-medio plazo hacen necesaria la búsqueda de nuevas fuentes de energía alternativas, limpias y renovables. De entre ellas, la energía solar es una de las mejores opciones por su gran disponibilidad para la generación de calor y electricidad.

El objetivo de este proyecto va encaminado al desarrollo de nuevos recubrimientos absorbedores solares selectivos crecidos en forma de multicapas basados en nitruros metálicos de cromo y aluminio (CrAlN). Las propiedades de resistencia a la oxidación y estabilidad térmica del CrAlN unidas a un diseño nanoestructurado adecuado permitirán mantener unas buenas prestaciones ópticas (alta absorbancia y baja emitancia) y mejorar su durabilidad a alta temperatura. El incremento de la temperatura de trabajo (T>550 ºC) conllevará una mejora de la eficiencia y una reducción de costes de las plantas de concentración de solar térmica, haciéndolas más competitivas. Para su preparación se utilizará la técnica de pulverización catódica mediante impulsos de alta intensidad (HiPIMS), una variante reciente de la pulverización catódica convencional que permite mejorar la densidad y compacidad de las capas gracias a un mayor grado de ionización del plasma. Estas propiedades son de interés para mejorar la adhesión al sustrato y ralentizar los procesos de degradación térmica. Además de los nitruros se ensayarían otras configuraciones cambiando el tipo de material absorbedor (oxinitruros y nanocomposites de carburos metálicos).

El proyecto comprenderá todas las etapas, desde la síntesis de los materiales componentes de las estructuras solares selectivas, diseño y simulación de su comportamiento óptico, a su validación en condiciones similares a la aplicación final (a nivel de laboratorio y ensayos de campo). La caracterización estructural, química y de estabilidad térmica y resistencia a la oxidación discurrirá en paralelo con el fin de optimizar los recubrimientos solares selectivos con mejores prestaciones y durabilidad.

The climatic change produced by the gas pollutants emissions and the greenhouse effect along to the short mid-term depletion of the energy fossil fuels make necessary the search of alternative energy sources, clean and renewable. Among them, the solar energy is one the best options due to the major availability to generate heat and electricity.

The goal of the present project is the development of new solar multilayered absorber coatings based on chromium and aluminum nitride (CrAlN). The good oxidation resistance and thermal stability of CrAlN, together with a nanostructured design will ensure a good optical performance (high absorbance and low emissivity) and increase their durability at high temperature. The increment of the working temperature (T>550 °C) will improve the efficiency and reduce the costs of the solar thermal power plants, make them more competitive. The High Power Impulse Magnetron Sputtering technique (HiPIMS) will be used for the preparation of the coatings. This recent innovation of the conventional magnetron sputtering technology allows increasing the film density and compactness thanks to an increased ionization of the plasma. These properties are interesting for the improvement of the adhesion to the substrate and decrease the thermal degradation. In addition to abovementioned strategy, other alternative configurations changing the nature of the material absorber (metal oxynitrides and carbides nanocomposites) would be tried.

The project will comprise all the stages, from the synthesis of the material components of the solar selective structures, design and simulation of the optical behaviour, to the validation in conditions similar to the final application (both in lab and field tests). The structural and chemical characterization, the evaluation of the thermal stability and oxidation resistance will run simultaneously with the aim of optimizing the solar absorber selective coatings with the best performance and durability.

Tecnología de plasma para la fabricación de celdas solares de perovskita eficientes y duraderas a prueba de agua

Plasma technology for efficient and DURAble waterproof perovskite SOLar cells · DuraSol

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2019-109603RA-I00	01-06-2020 31-05-2023	Ministerio de Ciencia e Innovación	96.800 €

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RESUMEN / ABSTRACT

Las celdas solares –dispositivos que transforman directamente la luz solar en electricidad- son de vital interés para el futuro sostenible del planeta. Durante los últimos años y conscientes de este hecho, la comunidad científica ha realizado un gran esfuerzo por mejorar la eficiencia de estos dispositivos. Un ejemplo particular de celda solar que contiene una perovskita de haluro organometálico como absorbedor de luz han centrado la atención de la comunidad científica durante la última década debido, sobre todo, a su alta eficiencia y bajo coste. Esta tecnología de celda solar supone una alternativa prometedora a las celdas actuales (basadas en Si y en calcogenuros), aunque se enfrentan a un reto científico y tecnológico que no ha sido resuelto en 10 años desde su descubrimiento: para que la realización final y comercial de las celdas de perovskita sea posible, necesitan alcanzar una mayor estabilidad, durabilidad y reproducibilidad. El principal problema radica en la alta sensibilidad que presentan estas perovskitas al oxígeno y humedad ambiental, que producen una rápida degradación del comportamiento de la celda en un tiempo extremadamente corto, haciendo inviable su comercialización.

DuraSol persigue abordar este gran reto científico y tecnológico mediante la fabricación de componentes de la celda mediante tecnología de vacío y plasma. Estas metodologías son escalables industrialmente y presentan grandes ventajas con respecto a las metodologías en disolución (las más usadas), entre las que destacan: su alta versatilidad, control de composición y microestructura, bajo coste, que son respetuosas con el medio ambiente ya que no precisan disolventes, no producen emisiones contaminantes y son compatibles con la tecnología actual de semiconductores.

El objetivo principal de DuraSol es la fabricación de celdas solares de perovskita “a prueba de agua” mediante integración de componentes fabricados por metodologías de vacío y plasma en forma

de películas delgadas y nanoestructuras, que actúan como sellantes hidrofóbicos. La viabilidad de DuraSol se basa en resultados recientes que demuestran que la fabricación asistida por plasma de distintos componentes de la celda solar puede ser una de las vías más prometedoras para aumentar su estabilidad y durabilidad, que es hoy en día el cuello de botella que impide su comercialización. Cabe señalar que no hay ningún ejemplo en la literatura de este enfoque sintético, y se espera que esta oportunidad demuestre las ventajas y la versatilidad de esta metodología innovadora en un campo de muy alto impacto. La investigación propuesta en DuraSol se enmarca dentro de las áreas prioritarias del programa Horizon 2021-2027 de la Unión Europea y responden a varios de los retos propuestos en la presente convocatoria de "Energía segura, eficiente y limpia" (Reto 3) y de "Cambio climático y utilización de recursos y materias primas" (Reto 5).

Solar cells – devices that transform sunlight into electricity – are of vital interest for the sustainable future of the planet. During the last years and aware of this fact, the scientific community has made a great effort to improve the efficiency of these devices. A particular example of a solar cell that contains an organometallic halide perovskite as light absorber has focused the attention of the scientific community during the last decade due, above all, to its high efficiency and low cost. This solar cell technology is a promising alternative to currently existing ones (based on Si and chalcogenides), although they face a scientific and technological challenge that has not been solved in 10 years since its discovery: for the commercial realization of the perovskite cells possible, they need to achieve higher stability, durability and reproducibility. The main problem lies in the high sensitivity of these perovskites to oxygen and environmental humidity, which produce a rapid degradation of the cell's behaviour in an extremely short time, making commercialization unfeasible.

DuraSol seeks to address this great scientific and technological challenge by manufacturing cell components using vacuum and plasma technology. These methodologies are industrially scalable and present great advantages over solution methods (the most used), among which are: their high versatility, control of composition and microstructure, low cost, environmentally friendly since they do not require solvents, do not produce pollutant emissions and are compatible with current semiconductor technology.

The main objective of DuraSol is the fabrication of waterproof perovskite solar cells by integrating components manufactured by vacuum and plasma methodologies in the form of thin films and nanostructures, which act as hydrophobic sealants. The viability of DuraSol is based on recent results that demonstrate that plasma-assisted synthesis of different components of the solar cell can be one of the most promising ways to increase its stability and durability, which is today the bottleneck that prevents their commercialization. It is worth to highlight that there is no example in the literature about this synthetic approach, and this opportunity is expected to demonstrate the advantages and versatility of this innovative methodology in a field of very high impact. The research proposed in DuraSol falls within the priority areas of the European Union Horizon 2021-2027 program and responds to several of the challenges proposed in this call for "Energía segura, eficiente y limpia" (Challenge 3) and "Cambio climático y utilización de recursos y materias primas" (Challenge 5).

Estructuras adaptativas multiresponsivas para fotónica integrada, piezo/tribotrónica y monitorización optofluídica

Adaptive multiresponsive nanostructures for integrated photonics, piezo/tribotronics and optofluidic monitoring |AdFunc

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2019-110430GB-C21	01-06-2020 31-05-2023	Ministerio de Ciencia e Innovación	211.750 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

AdFunc es un proyecto muy interdisciplinar que tiene como principal objetivo conseguir un progreso significativo en dos temáticas en la frontera de la Ciencia de Materiales: el desarrollo de sensores con capacidad multirespuesta y de sistemas de energía activados por luz. Los denominadores comunes de AdFunc son el diseño inteligente de arquitecturas complejas en la nanoescala y el desarrollo de demostradores a escala de laboratorio.

Estamos convencidos de que el proyecto nos abre una ventana de oportunidad para realizar investigaciones que podemos clasificar en cuatro áreas: i) Aplicaciones y dispositivos: Desarrollaremos los recientemente descubiertos efectos tribotrónicos y piezotrónicos para fabricar dispositivos sensores autoalimentados. Con estos materiales, en combinación con varias tecnologías avanzadas de sensado fotónico y espectro-electroquímico, expandiremos la eficiencia, multiactuación y multirespuesta de sistemas adaptativos optofluídicos. Estos sistemas, manteniendo una arquitectura común, presentarán una respuesta diferenciada frente a escenarios reales diversos y complejos, que se simularán en el proyecto (alteraciones medioambientales como vertidos, accidentes, amenazas químicas o de explosivos). También se plantean dispositivos captadores de energía solar en condiciones de baja iluminación, captadores de energía mecánica y dispositivos que sean capaces de acoplar luz y movimiento a la activación de procesos de descomposición electroquímica del agua. ii) Nanomateriales: Adfunc es un proyecto donde concurren un equipo de especialistas en el desarrollo de nanoestructuras soportadas por distintas tecnologías. Esto nos permitirá, por primera vez, implementar un conjunto de nanoarquitecturas 3D (nanohilos, nanotubos, core@shell) y el diseño de materiales con estructuras nanoporosas controladas

(capas esculturales, nanocanales, porosidad asociada en varias escalas, multicapas ópticas porosas, desarrollos pioneros de redes metaloorgánicas (MOFs) en estructuras fotónicas porosas) directamente a la mejora de los componentes activos de los dispositivos del proyecto. iii) Estrategia. El proyecto nos da la oportunidad de trabajar simultáneamente en rutas sintéticas nuevas, caracterización avanzada de materiales y propiedades, integración de materiales en dispositivos, y esto a la vez que se tiene información de modelado y simulación. iv) Perspectiva de escalabilidad: En todos los casos se utilizarán métodos y técnicas compatibles con procesos industriales establecidos, como el plasma y el vacío típicos de la industria optoelectrónica y microelectrónica, y procesos de síntesis en disolución. Otro aspecto interesante, es la posibilidad de introducir plásticos y polímeros para fabricar dispositivos, lo que puede permitir revalorizar residuos de la industria del plástico, en un esfuerzo de economía circular en el que investigadores del proyecto están comprometidos.

AdFunc sólo es posible gracias al esfuerzo conjunto de un gran número de investigadores, en su mayoría del ICMS-CSIC y la Universidad Pablo de Olavide, que se completa con un grupo de investigadores de otros centros y colaboradores internacionales con experiencia e interés complementarios. Es precisamente la coordinación de un número tan elevado de especialistas (25 doctores en los dos subproyectos) lo que nos permite plantear el desarrollo de un conjunto de actividades tan completo y ambicioso.

AdFunc is a highly interdisciplinary project whose main objective is to achieve significant progress in two areas at the frontier of Materials Science: the development of multi-response sensors and light-activated energy systems. The common denominators of AdFunc are the intelligent design of complex architectures at the nanoscale and the development of laboratory scale demonstrators.

We are convinced that the project opens a window of opportunity for us to carry out research that can be classified into four areas: i) Applications and devices: We will develop the recently discovered tribotronic and piezotronic effects to manufacture self-powered sensor devices. With these materials, in combination with several advanced photonic sensing and spectro-electrochemical technologies, we will expand the efficiency, multiactuation and multiresponse of optofluidic adaptive systems. These systems, maintaining a common architecture, will present a differentiated response to diverse and complex real scenarios, which will be simulated in the project (environmental alterations such as spills, accidents, chemical or explosive threats).

Another fundamental aspect of the project are the photovoltaic devices, which will be optimized to be able to work in low light conditions, and mechanical energy collectors and devices that are capable of coupling light and movement to the activation of the water electrochemical decomposition. ii) Nanomaterials: AdFunc is a project where a team of specialists in the development of supported nanostructures by different technologies come together. This will allow us, for the first time, to implement a set of 3D nanoarchitectures (nanowires, nanotubes, core@shell) and the design of materials with controlled nanoporous structures (sculptural layers, nanochannels, porosity associated in several scales, porous optical multilayers, pioneering developments of metalloorganic networks (MOFs) in porous photonic structures) directly to the improvement of the active components of the project devices. Iii) Strategy: The project gives us the opportunity to work simultaneously on new synthetic routes, advanced characterization of materials and properties, integration of materials into devices, and this while simultaneously obtaining modeling and simulation information. iv) Perspective of scalability: In all cases, methods and techniques compatible with established industrial processes will be used, such as plasma and vacuum, typical of the optoelectronic and microelectronic industry, and synthesis processes in solution. Another interesting aspect is the possibility of introducing plastics and polymers to manufacture devices, which may allow the valorization of waste from the plastic industry, in an effort of circular economy in which researchers of the project are committed.

AdFunc is only possible thanks to the joint effort of a large number of researchers, mostly from ICMS-CSIC and the Pablo de Olavide University, which is completed by a group of researchers from

other national and international institutions with complementary experience and interest. It is precisely the coordination of such a large number of specialists (25 doctors in the two subprojects) that allows us to propose the development of such a complete and ambitious set of activities.

Películas delgadas nanoestructuradas crecidas por pulverización catódica con plasmas de Helio y otros gases ligeros

Nanostructured thin films grown by magnetrón sputtering deposition with plasmas of Helium and other light gases

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2021-124439NB-100	01-09-2022 31-08-2026	Ministerio de Ciencia e Innovación	114.950 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

La pulverización catódica (magnetron sputtering-MS) es una metodología de deposición física desde fase vapor (PVD) muy usada para la fabricación de películas delgadas y recubrimientos. En la técnica MS se emplean comúnmente mezclas de Ar ó Ar/N_2-O_2 (MS reactivo) como gas de proceso que se ionizará en una descarga para crear el plasma adecuado y pulverizar el material del blanco. El grupo NanoMatMicro ha sido pionero en la introducción de plasmas de helio en la tecnología de pulverización catódica. Aunque la tasa de deposición puede bajar, demostramos la formación en condiciones controladas de nanoporosidad y/o gas atrapado (nanoburbujas de He y N_2) en las películas producidas. En particular las láminas sólidas que contienen nanoporos llenos de gas tienen características únicas: permiten atrapar una gran cantidad de gas en un estado condensado con alta estabilidad y proporcionan una ruta para modificar las propiedades del material preparado. La técnica MS es fácil de escalar y mucho más barata que las tecnologías alternativas basadas en la implantación de iones de alta energía. Sobre esta base, proponemos seguir desarrollando una metodología bottom-up innovadora y versátil para fabricar películas delgadas (Si, C, otros metaloides y metales) que promueva la porosidad abierta o, por el contrario, permita estabilizar las "nanoburbujas" atrapadas del gas de proceso (He, Ne, N_2, H_2 y sus isótopos).

La metodología se investigará principalmente para fabricar blancos sólidos y estándares del gas atrapado para estudios de reacciones nucleares. Nuestro trabajo permitirá que los gases ligeros y sus isótopos estén disponibles en un estado condensado y en un formato fácil de manejar sin necesidad de celdas de alta presión o dispositivos criogénicos. Junto con una red de investigadores colaboradores de

las áreas de Física Nuclear y Astrofísica, nuestro objetivo es llevar esta aplicación desde la prueba de concepto hasta los experimentos finales en grandes instalaciones. También cabe mencionar que el control del proceso desde estructuras con gas atrapado a nanoporosas permitirá estudiar aplicaciones adicionales en el proyecto como dispositivos ópticos, emisores de luz UV o recubrimientos catalíticos. El proyecto incluye el diseño y control de proceso en nuestras cámaras de MS para trabajar con los diferentes gases ligeros aquí propuestos. Se seguirán implementando metodologías de bajo consumo para isótopos escasos (por ejemplo, 3He). El objetivo final es implementar una configuración mejorada de MS y desarrollar la metodología bottom-up propuesta en términos de combinaciones de matriz y gas, mezclas de gases, variedad de soportes y diseños autosoportados o multicapa que permitan las aplicaciones innovadoras.

Una tarea importante es también determinar el mecanismo de crecimiento de las láminas. La caracterización del plasma durante el proceso de deposición y el uso de la herramienta de simulación SRIM pueden contribuir en gran medida a una mejor comprensión y control de los procesos de crecimiento. Para comprender la microestructura, composición y propiedades físico-químicas de los nuevos materiales, se llevará a cabo una caracterización química y microestructural en la nanoescala con una variedad de técnicas. Destacan las microscopías electrónicas (TEM y SEM) que incluyen la espectroscopia de pérdida de energía de electrones y las técnicas de análisis por haz de iones para la determinación de la composición elemental en profundidad.

Magnetron Sputtering (MS) is a Physical Vapour Deposition (PVD) methodology typically used for thin films and coatings fabrication. MS commonly employs Ar or Ar/N_2-O_2 (reactive MS) mixtures as the process gas to be ionized in a glow discharge to create the adequate plasma to sputter a target material. Among a few laboratories we pioneered the introduction of Helium plasmas in the magnetron sputtering technology. Although the deposition rate may be reduced we demonstrated the formation under controlled conditions of nanoporosity and/or trapped gas (He and N2 nanobubbles) in the produced films. In particular solid-films containing gas filled nanopores have several unique characteristics: They allow a large amount of gas to be trapped in a condensed state with high stability, and will provide a route to tailor the over-all films properties. Magnetron sputtering is easy to scale and much cheaper than alternative technologies based on high energy ion implantation. Building on this, we propose to further develop an innovative and versatile bottom-up methodology to fabricate thin films (e.g. Si, C, other metalloids and metals) promoting open porosity or in the opposite stabilizing trapped nanobubbles of the process gas (He, Ne, N_2, H_2 and their isotopes).

The methodology will be mainly investigated to fabricate unique solid targets and standards of the trapped gas for nuclear reactions studies. Our work will make light gases and their isotopes available in a condensed state and easy-to-handle format without the need for high pressure cells or cryogenic devices. Together with a network of collaborative researchers from the Nuclear Physics and Astrophysics domain we are aiming to bring this application from proof-of-concept to final experiments in large installations facilities. It is also worth to mention that the control of the process from gas filled to nanoporous structures will open additional applications to be investigated in the project such as optical devices, vacuum-UV emitters or catalytic coatings.

The project will introduce innovative process design and control in our magnetron sputtering chambers to work with the different light weight gases newly proposed. Low gas consumption methodologies will be further implemented for scarce isotopes (e.g. 3He). The final goal is to implement an improved MS experimental set-up and to develop the proposed bottom-up methodology in terms of matrix-gas combinations, gas mixtures, variety of supports (e.g. flexible), and self-supported or multilayer designs looking for the innovative applications. An important task is also to determine the MS film growth mechanism. The plasma characterization during the deposition process and the use of the SRIM simulation tool may strongly contribute to a better understanding and control of the growth processes. To understand the microstructure, composition and physical-chemical properties of the novel materials,

a complete microstructural and chemical characterization at the nano-scale will be undertaken with a variety of techniques. Of special mention are the advanced electron microscopies (TEM and SEM) including the Electron Energy Loss Spectroscopy and the Ion Beam Analysis techniques for the in-depth elemental composition determination.

Dispositivo optofluídico NIR para análisis de líquidos
NIR Optofluidic device for liquid analysis · NIRFLOW

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PDC2021-121379-I00	01-12-2021 30-11-2023	Ministerio de Ciencia e Innovación	144.900 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

NIRFLOW es un proyecto I+D+i para la realización de una Prueba de Concepto en el que se plantea desarrollar un prototipo precomercial para análisis óptico en el infrarrojo cercano de fluidos en condiciones de flujo en entornos industriales relevantes. El proyecto se basa en varias innovaciones no contempladas en equipos comerciales basados en análisis NIR hoy en el mercado. De un lado, sustituir la óptica de análisis NIR convencional operada por espectrómetros NIR basados en redes de difracción o óptica de Fourier por una selección de la longitud de onda de análisis basada en combinaciones de filtros ópticos de paso alto y paso bajo variables de forma continua con respuesta sintonizada (centro y anchura de banda) a voluntad en el NIR. De otro lado, la celda optofluídica a desarrollar, operada en modo transflectancia, se caracteriza por tener camino óptico de análisis variable y sintonizable a los sobretonos de las absorciones características de las moléculas presentes en el fluido problema. De esta manera, los análisis estadísticos característicos de la espectroscopía NIR se van a ver apoyados por variables independiente (medidas correspondientes no sólo a variaciones de longitud de onda, sino también a distintos caminos ópticos de análisis), lo cual va a propiciar análisis estadísticos más robustos que los convencionales. Finalmente, el equipo se va a desarrollar con una concepción microfluídica de análisis automática, para su operación en remoto mediante tecnología wireless. Estas tres innovaciones hacen de NIRFLOW un proyecto I+D+i en el que parte de los conocimientos y uno de los desarrollos reali-

zado en un proyecto de investigación previo del Plan Estatal (MAT2016-79866-R), parcialmente protegido con una patente, se pretende transferir a la sociedad a través del desarrollo de un equipo precomercial que demuestre sus capacidades de análisis en entornos operacionales significativos, en particular para el seguimiento de procesos de fermentación ligados a la producción de vinos.

NIRFLOW is a R+D+i Project for the realization of a Proof of Concept in which it is aimed to develop a pre-commercial prototype for the optical analysis in the near infrared of fluids in flow conditions in relevant industrial environments. The project is based on several innovations that are not implemented in conventional NIR apparatus in the market so far. First, to substitute the conventional NIR optics mainly operated by spectrometers based on diffraction gratings or Fourier optics by a selection of the wavelength of analysis based on combinations of continuously variable short and long pass filters designed to tune a NIR passband (regarding center and width). Second, to develop an optofluidic cell, operated in transflectance mode, characterized by a tunable optical pathlength to optimize the info obtained by the different overtones of the characteristic molecules present in the fluid under analysis. This innovation will offer the possibility of more robust statistical analysis than conventional NIR spectroscopy operated with single optical pathlength. Finally, the prototype will be developed within a microfluidic approach with automate analysis concept, for its operation within a wireless remote technology. These three innovations make NIRFLOW a R&D+i project in which part of the knowledge and one of the developments done in previous research project from the Spanish Plan Estatal (MAT2016-79866-R), partially protected by a patent claim, is aimed to be transferred to the society through the development of a precommercial prototype that showed ability of analysis in industrial operational environments, in particular to follow the evolution of fermentation processes linked to wine production.

Nuevos recubrimientos nanoestructurados para absorción eficiente de la radiación solar en dispositivos de concentración New nanostructured coatings for efficient absorption of solar radiation in concentrated devices

Junta de Andalucía

Unión Europea
Fondo Europeo de Desarrollo Regional

Andalucía se mueve con Europa

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P18-RT-2641	01-02-2020 31-03-2023	Junta de Andalucía	102.268 €

Investigador Principal Research Head	Componentes Research Group
Juan Carlos Sánchez López	T. Cristina Rojas Ruiz Belinda Sigüenza Carballo

RESUMEN / ABSTRACT

La mejora de los materiales empleados en los dispositivos usados en el campo de las energías renovables permitirá incrementar la eficiencia de los mismos haciéndolos más competitivos y rentables. El presente proyecto pretende desarrollar nuevos recubrimientos absorbedores selectivos de la energía solar aptos para trabajar a temperaturas superiores a las posibles con los materiales actualmente en uso en dispositivos de concentración solar térmica (500 °C en vacío – media concentración; 800 °C al aire – alta concentración). Los sistemas serán preparados en forma de multicapas por la novedosa tecnología de pulverización catódica donde los materiales son evaporados mediante impulsos de alta energía (HiPIMS - High Power Impulse Magnetron Sputtering). Los materiales preparados deberán cumplir los requisitos ópticos y de estabilidad química para soportar las condiciones de alta irradiación solar y temperaturas de trabajo. Este ambicioso proyecto se llevará a cabo mediante la colaboración de dos grupos de investigación pertenecientes al Instituto de Ciencia de Materiales de Sevilla CSIC-ICMS (grupo TEP958) y a la plataforma solar de Almería CIEMAT-PSA (Grupo TEP247). El grupo CSIC-ICMS se encargará del diseño, preparación y caracterización de los recubrimientos. Por su parte CIEMAT-PSA, diseñará y desarrollará los ensayos de campo, validando los recubrimientos en condiciones de trabajo similares a las de la aplicación final en términos de flujo solar concentrado incidente y temperaturas de operación. Dichos ensayos incluirán tanto determinación de parámetros térmicos y ópticos en condiciones nominales de operación, así como ciclado térmico de alta frecuencia (tratamiento térmico y envejecimiento).

The improvement of the materials employed in the devices used in the renewable energy sector will enable to increase the efficiency of these systems to become more competitive and profitable. The current project aims to develop new solar selective coatings able to operate at temperatures beyond the working temperature limits of the materials currently being used in concentrated solar systems (500 °C in vacuum- mid concentration; 800 °C in air –high concentration). The systems will be prepared in the form of multilayers using the novel technology of magnetron sputtering where the materials are evaporated by means of high energy pulses (HiPIMS - High Power Impulse Magnetron Sputtering). The developed materials should fulfill the optical requirements and thermal stability to withstand the high solar irradiance flux and working temperatures. This project will be carried out through the collaboration of two research groups belonging to the "Instituto de Ciencia de Materiales de Sevilla", CSIC-ICMS (TEP958 group) and the "Plataforma Solar de Almería", CIEMAT-PSA (TEP247 group). The ICMS-CSIC group will perform the design, preparation and characterization of the coatings. Meanwhile, the CIEMAT-PSA group will be in charge of designing the bench tests, validating the coatings in working conditions similar to the final application in terms of high incident solar flux and operation temperatures. Such tests will include both the determination of thermal and optical parameters in nominal operating conditions, as well as the thermal cycling at high frequency (thermal treatment and aging).

Recubrimientos termocrómicos inteligentes para la climatización eficiente y el control ambiental Smart thermochromic coatings for smart windows and environmental control TOLERANCE

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P18-RT-2641	01-01-2020 31-03-2023	Junta de Andalucía	119.800 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

La Agencia Internacional de la Energía considera que el uso sistemático de procedimientos autónomos de control ambiental representa una de las mejores apuestas tecnológicas para reducir el consumo energético asociado a la climatización de edificios (más del 40% del consumo global en países desarrollados, muy superior al porcentaje debido al transporte), reduciendo el impacto ambiental y mejorando además el confort habitacional. TOLERANCE persigue introducir y desarrollar en Andalucía la tecnología de los recubrimientos termocrómicos como elemento inteligente y autónomo de control de la irradiación solar en edificios. El interés de la propuesta se centra en nichos de aplicación como el cerramiento de edificios, el mobiliario urbano, la mejora de sistemas de producción de agua caliente sanitaria o la mejora de invernaderos. Un recubrimiento termocrómico se caracteriza por transmitir todo el espectro solar a bajas temperaturas y reflejar selectivamente parte de éste (el infrarrojo) a altas temperaturas. En esta línea, el proyecto propone diversas acciones de I+D para el desarrollo de capas delgadas con composición VO2, óxido termocrómico caracterizado con una temperatura de transición cercana a la temperatura ambiente, sobre vidrio y plásticos mediante técnicas escalables industrialmente, así como su nanoestructuración, dopado e integración en sistemas multicapas a fin de mejorar sus características y prestaciones multifuncionales.

The International Energy Agency considers that the systematic use of autonomous procedures for environmental control is one of the best technological approaches to minimize the energy employed to cool down buildings and other urban structures (it represents more than 40% of the global energy use in developed countries, much above the use in transportation, for instance), thus reducing the environmental impact and improving human comfort. TOLERANCE aims at introducing and developing a

technology based on thermochromic materials in Andalusia as a smart and autonomous element to control the penetration of solar radiation in buildings. This project focusses on various applications such as smart windows in buildings and urban furniture, improvement of sanitary water systems or environmental control in greenhouses. While at low temperatures, a thermochromic coating transmits most solar spectrum, it selectively filters out the infrared region of this spectrum at high temperatures. In this research, TOLERANCE proposes several R+D actions to grow thin films with composition VO2, a thermochromic oxide with transition temperature near room temperature, on glass and plastic by means of industrial scalable techniques, as well as its nanostructuration, doping and integration in multilayer systems to improve its features and multifunctional properties.

Nanoscopías y Espectroscopías integradas para el análisis en la nano-escala de nuevos materiales funcionales

Integrated nanoscopies and spectroscopies for the analysis of novel functional materials at the nano-scale

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P20_00239	05-10-2021 30-06-2023	Junta de Andalucía	46.695 €

Investigador Principal Research Head	Componentes Research Group
Asunción Fernández Camacho	María del Carmen Jiménez de Haro

RESUMEN / ABSTRACT

El desarrollo de los nanomateriales y materiales funcionales, así como sus aplicaciones nanotecnológicas, vienen determinados por las capacidades actuales para la caracterización de la microestructura, la composición y las propiedades de los materiales en la nano-escala. El proyecto propone potenciar una investigación de frontera en la caracterización microestructural de materiales. Se integrarán las técnicas nanoscópicas y espectroscópicas, ligadas a la microscopía electrónica (sonda de electrones), con las técnicas asociadas a las sondas de fotones (rayos-X) y de haces de iones (técnicas IBA en general). La caracterización se asociará a materiales funcionales seleccionados de alto interés actual en la temática de recubrimientos y láminas delgadas en las que el equipo de trabajo es experto.

Será objetivo central el desarrollo y aplicación de manera integrada de las técnicas disponibles con múltiples sondas, tanto en el ICMS, como en otros centros de las Universidades de Sevilla (CITIUS, CNA) y Cádiz (servicios centrales). Igualmente, a través de colaboraciones y solicitudes de medidas se tendrá acceso a otras instalaciones internacionales.

En el proyecto se dispondrá de materiales seleccionados en dos tecnologías emergentes: i) Láminas delgadas y recubrimientos nanoporosos que estabilizan gases a ultra-alta densidad y presión. ii) Catalizadores para los procesos de almacenamiento y generación de hidrógeno en líquidos orgánicos portadores de hidrógeno (LOHCs). La caracterización avanzada que se propone contribuirá a la comprensión fundamental de las relaciones síntesis-microestructura-propiedades con el objetivo de alcanzar un diseño racional de nuevos materiales funcionales en las líneas seleccionadas. El proyecto incide directamente en las tecnologías facilitadoras o emergentes como son "la nanotecnología" y "los materiales avanzados". Incide también en los retos sociales y objetivos RIS3 de Andalucía en relación al almacenamiento de energías renovables.

The current development of nanomaterials and functional materials in general, as well as their nanotechnological applications, are determined to a large extent by the current capacities on the characterization of microstructure, composition and even properties of the materials at the nano-scale. The project is proposed to promote an innovative research in the microstructural characterization of materials. The nanoscopic and spectroscopic techniques linked to the electron microscopes (electron beam probe), will be integrated together with techniques associated with photon beam (X-rays) and ion beam (IBA techniques) probes. This characterization will be associated with selected functional materials, also within advanced research lines of high current interest, in the topic of coatings and thin films in which the work team has strong experience.

The development and application of the available techniques with multiple probes will be a first central objective, both in the ICMS and in other centers of the Universities of Seville (CITIUS, CNA) and Cádiz (TEM central services). Likewise, through collaborations and measurement time applications, access to other international facilities will be achieved. In the project, selected materials will be available in two emerging technologies: i) Nanoporous thin films and coatings that stabilize gases at ultra-high density and pressure. ii) Catalysts for hydrogen storage and on demand hydrogen generation through the use of liquid organic hydrogen carriers (LOHCs). The advanced characterization proposed in the nano-scale will contribute to the fundamental understanding of the synthesis-microstructure-properties relationships with the final objective of achieving a rational design of new functional materials in the selected priority lines. The project has a direct impact on enabling or emerging technologies such as "nanotechnology" and "advanced materials", as well as on the Andalusian societal challenges and RIS3 objectives in relation to the storage of renewable energies "Topic: Hydrogen and fuel cells".

Nanorecubrimientos dieléctricos para dispositivos electrónicos Flexibles por tecnología de plasma

Dielectric Nanocoatings for Flexible Electronic Devices by Plasma Technology FLEXDIELEC

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
EMERGIA20_00346	01-09-2021 30-08-2025	Junta de Andalucía	256.000 €

Investigador Principal Research Head
Francisco Javier Aparicio Rebollo

RESUMEN / ABSTRACT

Dadas sus características físicas y mecánicas de la tecnología de dispositivos electrónicos flexibles emergentes combina estructuras multicapas de láminas delgadas flexibles, nanomateriales 2D, o nanoconductores 1D, como son los nanotubos de carbono y los nanohilos. Sin embargo, estos presentan diferentes limitaciones relacionadas con su degradación frente a agentes ambientales e incompatibilidad con las técnicas de fabricación convencionales más presentes a nivel industrial. El proyecto FlexDielec persigue el desarrollo de una nueva generación de materiales dieléctricos para el desarrollo de dispositivos electrónicos flexibles avanzados, superando estas limitaciones. Con este fin, se empleará una técnica pionera de plasma remotos, desarrollada por el IP, que regula en un amplio rango la composición y propiedades de nanocomposites orgánicos funcionales. Esta es una metodología de vía seca (ausencia de disolventes) y a temperatura ambiente, lo que asegura su completa compatibilidad con el uso de sustratos sensibles, como muchos de los que tienen mayores perspectivas de implementación en campo de la electrónica flexible (materiales poliméricos, tejidos, papel, nanomateriales 2D, nanofibras orgánicas…).

Due to its physical and mechanical characteristics, the emerging technology of flexible electronic devices combines multilayer structures of flexible thin films, 2D nanomaterials, or 1D nanoconductors, such as carbon nanotubes and nanowires. However, these present different limitations related to their degradation against environmental agents and incompatibility with the conventional manufacturing techniques. FLEXDIELEC pursues the development of a new generation of dielectric materials for the development of advanced flexible electronic devices, overcoming these limitations. To this end, a pioneering remote plasma technique will be used, developed by the IP, which regulates the composition and properties of functional organic nanocomposites over a wide range, will be used. This is a dry and room temperature method that ensures complete compatibility with sensitive substrates, such as those with high prospects for implementation in the field of flexible electronics (polymeric materials, fabrics, paper, 2D nanomaterials, organic nanofibers…).

Nueva generación de nanorecubrimientos dieléctricos conformales para dispositivos electrónicos emergentes por tecnología de plasma

New Generation of Conformal Dielectric Nanocoating for Emerging electronic Devices by Plasma Technology · PLASMADIELEC

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-1381057	01-01-2022 31-05-2023	Junta de Andalucía	30.000 €

Investigador Principal Research Head	Componentes Research Group
Francisco Javier Aparicio Rebollo	Ana Isabel Borrás Martos Jorge Budagosky

RESUMEN / ABSTRACT

Los recientes avances en nanomateriales están conduciendo al desarrollo de nanodispositivos de elevada miniaturización y nuevas funcionalidades en el campo de los dispositivos electrónicos. La tecnología emergente combina transistores orgánicos de láminas delgadas nanomateriales 2D y arquitecturas coaxiales que emplean conductores 1D como son los nanotubos de carbono y nanohilos como electrodos. En este contexto, el proyecto persigue el desarrollo de procesos de deposición por plasma para la síntesis de una nueva generación de materiales dieléctricos para su integración conformal sobre este tipo de nanoarquitecturas. La metodología de deposición por plasma propuesta permitirá regular de manera controlada las propiedades dieléctricas de estos recubrimientos, así como su deposición conformal sobre nanoestructuras de elevada relación de aspecto como son los nanohilos conductores. Dada la versatilidad de la técnica de deposición propuesta se sintetizarán materiales dieléctricos de alta y baja permitividad.

Recent developments in nanomaterials are leading to the development of highly miniaturized nanodevices and new functionalities in the field of electronic devices. Emerging technology combines organic thin-film transistors with 2D nanomaterials and coaxial architectures that employ 1D conductors such as carbon nanotubes and nanowires as electrodes. In this context, the project pursues the development of plasma deposition processes for the synthesis of a new generation of dielectric materials for their conformal integration on this type of nanoarchitectures. The proposed plasma deposition methodology will make it possible to regulate in a controlled manner the dielectric properties of these coatings, as well as their conformal deposition on high aspect ratio nanostructures such as conductive nanowires. Given the versatility of the proposed deposition technique, high and low permittivity dielectric materials will be synthesized.

OTROS PROYECTOS / OTHER PROJECTS

Ondas acústicas superficiales y su transferencia para aplicaciones de relevancia industrial

Periodo/Period: 01-02-2021 / 31-01-2024
Entidad Financiadora: CSIC (Intramural)
Importe total/Total amount: 47.640 €
Investigador responsable/Research head: Ana Isabel Borrás Martos

Electrodos nanoestructurados para el desarrollo de procesos electroquímicos de detección y aprovechamiento energético

Código/Code: 202260E110
Periodo/Period: 01-08-2022 / 31-07-2025
Organismo Financiador/Financial source: CSIC (Intramural)
Importe total/Total amount: 138.185 €
Investigador responsable/Research head: Jorge Gil Rostra

Caracterización de dispositivos optoelectrónicos basados en perovskitas organometálicas fabricadas por métodos de vacío y plasma

Periodo/Period: 03-11-2022 / 31-12-2023
Entidad Financiadora: CSIC
Importe total/Total amount: 5.000 €
Investigador responsable/Research head: Juan Ramón Sánchez Valencia

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Caracterización superficial de membranas de ósmosis inversa

Periodo/Period: 01-05-2020 / 05-04-2023
Organismo Financiador/Financial source: ACCIONA AGUA, S.A.U.
Importe total/Total amount: 24.738,45 €
Investigador responsable/Research head: Juan Pedro Espinós Manzorro

Fabricación, caracterización y análisis de eficiencia de electrocatalizadores para electrolizadores de intercambio aniónico

Periodo/Period: 13-12-2021 / 31-12-2024
Organismo Financiador/Financial source: H2B2 ELECTROLYSIS TECHNOLOGIES, S.L.
Importe total/Total amount: 178.620,20 €
Investigador responsable/Research head: Francisco Yubero Valencia

Recubrimientos y caracterización de láminas delgadas bajo tecnologías de alto vacío

Periodo/Period: 29-03-2022 / 28-03-2023
Organismo Financiador/Financial source: VALEO ILUMINACIÓN ESPAÑA, S.A
Importe total/Total amount: 5.082 €
Investigador responsable/Research head: Francisco Yubero Valencia

Caracterización de materiales, componentes y dispositivos para aplicaciones espaciales

Periodo/Period:: 10-10-2022 / 10-10-2025
Organismo Financiador/Financial source: Alter Technology TÜV Nord SAU
Importe total/Total amount: 30.250 €
Investigador responsable/Research head: Ángel Barranco Quero

Estudio de materiales y tratamientos superficiales para mejora del comportamiento tribológico de un sistema de transmisión por fricción

Periodo/Period:: 02-03-2023 / 31-12-2024
Organismo Financiador/Financial source: ARQUIMEA Centro de Investigaciones Avanzadas S.L.U.
Importe total/Total amount: 81.634 €
Investigador responsable/Research head: Juan Carlos Sánchez López
Componentes/Research Group: T. Cristina Rojas Ruiz, Agustín R. González-Elipe, José Manuel Moreno de la Vega

Mitigación de los efectos de carga utilizando materiales innovadores

Código/Code: ESA 4000139513/22/NL/CRS
Periodo/Period:: 09-03-2023 / 15-12-2024
Organismo Financiador/Financial source: Agencia Espacial Europea (ESA)
Importe total/Total amount: 121.000 € (CSIC)
Investigador responsable/Research head: Francisco Javier Aparicio Rebollo y Ángel Barranco Quero
Componentes/Research Group: Vanda Godinho, Juan Ramón Sánchez-Valencia, Ana Borrás
Participantes/Partners: Fundación Centro Tenológico de Componentes (CTC), Agencia Estatal Consejo Superior de Investigaciones Científicas CSIC, Spain, DHV Technologies, Spain y Alter Technology TUV NORD

PATENTES / PATENTS

BAUELEMENT
Inventores: Agustín R. González-Elipe, Ana Isabel Borrás Martos, Jaime del Morán Jalón
Tipo de Patente: Patente Solicitada Prioritaria
Número de Solicitud: 102023115696
Fecha Solicitud: 15 junio 2023
Entidades Titulares: Leibniz Institute for Baltic Sea Research, Consejo Superior de Investigaciones Científicas

Dispositivo de Eliminación y Prevención de Formación de Hielo en Superficies
Inventores: Manuel Oliva Ramírez, Victor J. Rico Gavira, Ana Isabel Borrás Martos, Agustín R. González-Elipe, Laura Montes Montañez, Aurelio García Valenzuela, Carmen López Santos
Tipo de Patente: Patente
Número de Solicitud: 18/571530
Fecha Solicitud: 18 diciembre 2023
Entidades Titulares: Universidad de Sevilla, Consejo Superior de Investigaciones Científicas

Self-Powered Triboelectric Touch Contact Transductor Device
Inventores: Juan Ramón Sánchez Valencia, Xabier García Casas, Ali Ghaffarinejad, Angel Barranco Quero, Ana Isabel Borrás Martos
Tipo de Patente: Patente Solicitada Prioritaria
Número de Solicitud: 23382177
Fecha Solicitud: 27 febrero 2023
Entidad Titular: Consejo Superior de Investigaciones Científicas

Self-Powered Triboelectric Transductor Device for Drops and Liquids
Inventores: Juan Ramón Sánchez Valencia, Xabier García Casas, Ali Ghaffarinejad, Angel Barranco Quero, Ana Isabel Borrás Martos
Tipo de Patente: Patente Solicitada Prioritaria
Número de Solicitud: 23382176
Fecha Solicitud: 27 febrero 2023
Entidad Titular: Consejo Superior de Investigaciones Científicas

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

A Holistic Solution to Icing by Acoustic Waves: De-Icing, Active Anti-Icing, Sensing with Piezoelectric Crystals, and Synergy with Thin Film Passive Anti-Icing Solutions
Del Moral, J; Montes, L; Rico-Gavira, VJ; López-Santos, C; Jacob, S; Oliva-Ramirez, M; Gil-Rostra, J; Fakhfouri, A; Pandey, S; Del Val, MG; Mora, J; García-Gallego, P; Ibanez-Ibanez, PF; Rodríguez Valverde, MA; Winkler, A; Borras, A; González-Elipe, AR
Advanced Functional Materials, **33** (2023) 2209421

Enero, 2023 · DOI: 10.1002/adfm.202209421

Icing has become a hot topic both in academia and in the industry given its implications in transport, wind turbines, photovoltaics, and telecommunications. Recently proposed de-icing solutions involving the propagation of acoustic waves (AWs) at suitable substrates may open the path for a sustainable alternative to standard de-icing or anti-icing procedures. Herein, the fundamental interactions are unraveled that contribute to the de-icing and/or hinder the icing on AW-activated substrates. The response toward icing of a reliable model system consisting of a piezoelectric plate activated by extended electrodes is characterized at a laboratory scale and in an icing wind tunnel under realistic conditions. Experiments show that surface modification with anti-icing functionalities provides a synergistic response when activated with AWs. A thoughtful analysis of the resonance frequency dependence on experimental variables such as temperature, ice formation, or wind velocity demonstrates the application of AW devices for real-time monitoring of icing processes.

Paper-based ZnO self-powered sensors and nanogenerators by plasma technology

Garcia-Casas, X; Aparicio, FJ; Budagosky, J; Ghaffarinejad, A; Orozco-Corrales, N; Ostrikov, K; Sánchez-Valencia, JR; Barranco, A; Borras, A

Nano Energy, **114** (2023) 108686
Septiembre, 2023 · DOI: 10.1016/j.nanoen.2023.108686

Nanogenerators and self-powered nanosensors have shown the potential to power low-consumption electronics and human-machine interfaces, but their practical implementation requires reliable, environmentally friendly and scalable processes for manufacturing and processing. Furthermore, the emerging flexible and wearable electronics technology demands direct fabrication onto innovative substrates such as paper and plastics typically incompatible with high process temperatures. This article presents a plasma synthesis approach for the fabri-cation of piezoelectric nanogenerators (PENGs) and self-powered sensors on paper substrates. Polycrystalline ZnO nanocolumnar thin films are deposited by plasma-enhanced chemical vapour deposition on common paper supports using a microwave electron cyclotron resonance reactor working at room temperature yielding high growth rates and low structural and interfacial stresses. Applying Kinetic Monte Carlo simulation, we elucidate the basic shadowing mechanism behind the characteristic microstructure and porosity of the ZnO thin films, relating them to an enhanced piezoelectric response to periodic and random inputs. The piezoelectric devices are assembled by embedding the ZnO films in polymethylmethacrylate (PMMA) and using Au thin layers as electrodes in two different configurations, namely laterally and vertically contacted devices. We present the response of the laterally connected devices as a force sensor for low-frequency events with different answers to the applied force depending on the impedance circuit, i.e. load values range, a behaviour that is theoretically analyzed. The characterization of the vertical devices in cantilever-like mode reaches instantaneous power densities of 80 nW/ cm^2 with a mean power output of 20 nW/cm^2. Besides, we analyze their actual-scenario performance by acti-vation with a fan and handwriting. Overall, this work demonstrates the advantages of implementing plasma deposition for piezoelectric films to develop robust, flexible, stretchable, and enhanced-performance nano-generators and self-powered piezoelectric sensors compatible with inexpensive and recyclable supports.

Improved strain engineering of 2D materials by adamantane plasma polymer encapsulation

Carrascoso, F; Li, H; Obrero-Pérez, JM; Aparicio, FJ; Borras, A; Island, JO; Barranco, A; Castellanos-Gómez, A
NPJ 2D Materials and Applications, **7** (2023) 24
Marzo, 2023 · DOI: 10.1038/s41699-023-00393-1

Two-dimensional materials present exceptional crystal elasticity and provide an ideal platform to tune electrical and optical properties through the application of strain. Here we extend recent research on strain engineering in monolayer molybdenum disulfide using an adamantane plasma polymer pinning layer to achieve unprecedented crystal strains of 2.8%. Using micro-reflectance spectroscopy, we report maximum strain gauge factors of -99.5 meV/% and -63.5 meV/% for the A and B exciton of monolayer MoS_2, respectively, with a 50 nm adamantane capping layer. These results are corroborated with photoluminescence and Raman measurements on the same samples. Taken together, our results indicate that adamantane polymer is an exceptional capping layer to transfer substrate-induced strain to a 2D layer and achieve higher levels of crystal strain.

Photoelectrochemical Water Splitting with ITO/WO_3/$BiVO_4$/CoPi Multishell Nanotubes Enabled by a Vacuum and Plasma Soft- Template Synthesis

Gil-Rostra, J; Castillo-Seoane, J; Guo, Q; Sobrido, ABJ; González-Elipe, AR; Borras, A
ACS Applied Materials & Interfaces, **15** (2023) 9250-9262
Febrero, 2023 · DOI: 10.1021/acsami.2c19868

A common approach for the photoelectrochemical (PEC) splitting of water relies on the application of WO_3 porous electrodes sensitized with $BiVO_4$ acting as a visible photoanode semiconductor. In this work, we propose a new architecture of photoelectrodes consisting of supported multishell nanotubes (NTs) fabricated by a soft-template approach. These NTs are formed by a concentric layered structure of indium tin oxide (ITO), WO_3, and $BiVO_4$, together with a final thin layer of cobalt phosphate (CoPi) co-catalyst. The photoelectrode manufacturing procedure is easily implementable at a large scale and successively combines the thermal evaporation of single crystalline organic nanowires (ONWs), the magnetron sputtering deposition of ITO and WO_3, and the solution dripping and electrochemical deposition of, respectively, $BiVO_4$ and CoPi, plus the annealing in air under mild conditions. The obtained NT electrodes depict a large electrochemically active surface and outperform the efficiency of equivalent planar-layered electrodes by more than one order of magnitude. A thorough electrochemical analysis of the electrodes illuminated with blue and solar lights demonstrates that the characteristics of the WO_3/$BiVO_4$ Schottky barrier heterojunction control the NT electrode efficiency, which depended on the $BiVO_4$ outer layer thickness and the incorporation of the CoPi electrocatalyst. These results support the high potential of the proposed soft-template methodology for the large-area fabrication of highly efficient multishell ITO/WO_3/$BiVO_4$/CoPi NT electrodes for the PEC splitting of water.

Plasmas and acoustic waves to pattern the nanostructure and chemistry of thin films

Rico, V; Regodon, GF; Garcia-Valenzuela, A; Alcaide, AM; Oliva-Ramirez, M; Rojas, TC; Alvarez, R; Palomares, FJ; Palmero, A; González-Elipe, AR
Acta Materialia, **255** (2023) 119058
Agosto, 2023 · DOI: 10.1016/j.actamat.2023.119058

In this work, piezoelectric AWs and plasmas have been brought together during the growth of a thin film as a novel methodology of plasma-assisted thin film structuration. The ensuing effects have been investigated on a model system where SiO_2 and SiO_x ($x<2$) thin films have been deposited by magnetron sputtering at oblique angles (MS-OAD) on an electro-acoustically excited $LiNbO_3$ piezoelectric substrate under resonant conditions. The microstructure of the resulting films was 2D patterned and depicted submillimeter size intermingled zones with different optical characteristics, compositions (SiO_2 and SiO_x) and porosity, from highly porous to dense and compact regions. The 2D nanostructural pattern mimics the AW distribution and has been accounted for by means of a specific simulation model. It is concluded that the morphological and chemical film pattern replicates the distribution of polarization potential on the surface of the AW activated substrate immersed in the plasma. Moreover, we show that the main mechanism responsible for the appearance of domains with different morphology and chemical composition is the focused impingement of Ar^+plasma ions on certain regions of the substrate. The general character of this patterning process, the underlying physics and its possibilities to tailor the composition and microstructure of dielectric thin film materials are discussed.

Preparation, characterization and activation of Pd catalysts supported on CNx foam for the liquid phase decomposition of formic acid

Arzac, GM; Rojas, TC; Real, C; Fernández, A
International Journal of Hydrogen Energy, **48** (2023) 31899-31613
Septiembre, 2023 · DOI: 10.1016/j.ijhydene.2023.04.244

In this work, we have prepared a series of Pd catalysts on a CNx support for the liquid phase decomposition of formic acid. The structured CNx support was obtained through thermal pyrolysis of melamine foam and the pyrolysis conditions were optimized to achieve high surface area. The resulting support contains high amount of nitrogen with a contribution of pyridinic component. Several Pd catalysts were prepared and under optimized conditions, we were able to obtain small (2.7 ± 0.9) nm Pd particles by using the oxidized support in powdery form. The activity of the optimized catalyst was studied under different conditions in the fresh and the used form. The fresh catalyst did not show significant activity. However, we found that the catalyst activated after use. Activation was understood in terms of the variation of surface Pd oxidation states under the effect of formic acid/sodium formate solutions. We found that the best activity is achieved under an optimal proportion of Pd^0/Pd^{II} surface states according to previous reports. Under the best conditions, the activity of the best catalyst ($8.6Pd/CN_{0.3}$) was as high as 9245 h^{-1}, attributable to the small particle size, the Pd0/PdII ratio, the amount of pyridinic nitrogen, and the testing conditions, which included the preadsorption of sodium formate

Microstructure and activity of Pd catalysts prepared on commercial carbon support for the liquid phase decomposition of formic acid

Arzac, GM; Montes, O; Fernández, A
International Journal of Hydrogen Energy, **48** (2023) 2628-2639
Enero, 2023 · DOI: 10.1016/j.ijhydene.2022.10.149

In this work, a series of Pd catalysts supported on commercially available activated carbon (Norit (R)) were prepared by employing different metal precursors ($Pd(NO_3)_2$ and Na_2PdCl_4) by the impregnation-reduction method at different pH. Catalysts were tested for the liquid phase decomposition of formic acid to generate hydrogen. The best results, in terms of small particle size and high catalytic activity were achieved for the Pd/C sample prepared by using $Pd(NO_3)_2$ salt impregnated at pH = 2.5, and

reduced with sodium borohydride. The particle size of the best Pd/C catalyst is (4.1±1.4) nm with initial TOFs of 2929 and 683 h^{-1} at 60 and 30 °C respectively and an apparent activation energy of 40 kJ mol-1. Samples prepared by using Na_2PdCl_4 precursor, consisted of particles with higher size and thus lower activity than the ones prepared with $Pd(NO_3)_2$. Regardless the Pd precursor employed, the best results in terms of particle size and activity were achieved at the point of zero charge of the support when the Pd species and the carbon surface were both neutral. The impregnation pH not only determines the particle size, but also the nature of the reducing agent does. The catalytic activity was shown to be size-dependent and it was shown that a mixture of surface Pd^0 and Pd^{II} oxidation states is beneficial for the activity. When comparing with literature catalysts with similar composition, we found that our best catalyst is competitive enough and that Norit (R) support could be promising for future studies on this reaction.

Plasma assisted dry reforming of methane: Syngas and hydrocarbons formation mechanisms

Navascues, P; Cotrino, J; González-Elipe, AR; Gómez-Ramirez, A
Fuel Processing Technology, **248** (2023) 107827
Septiembre, 2023 · DOI: 10.1016/j.fuproc.2023.107827

Plasma reactions of CO_2+CH_4 mixtures have been proposed as a suitable process for the dry reforming of methane. Without specific catalysts, most studies report the formation of CO and H_2 as main reaction products and arise the question whether CHx radicals coming from CH_4 may interact with intermediate species formed by electron impact dissociation of CO_2, a critical step for the formation of high added value oxygenated compounds. We have addressed this question studying the CO_2+CH_4 plasma reaction in a ferroelectric-moderated packed -bed reactor varying the reactants ratio. Analysis of the reaction products by mass spectrometry and the plasma reaction intermediates by optical emission spectroscopy suggest that few direct cross-link interactions exist between intermediate plasma species issued from CH_4 or CO_2. This preliminary evidence is corroborated by experiments using $^{13}CO_2$ instead $^{12}CO_2$ as reactant. The isotope labeling procedure has proved that plasma reaction mechanisms of CO_2 and CH_4 molecules proceed almost independently, with the formation of small amounts of water and the removal of carbon deposits resulting CH_4 plasma decomposition as sole evidences of cross reactions. These results highlight the need of using catalysts to promote specific surface reactions for a better control of the selectivity of the process.

Incorporation of a Metal Catalyst for the Ammonia Synthesis in a Ferroelectric Packed-Bed Plasma Reactor: Does It Really Matter?

Navascues, P; Garrido-Garcia, J; Cotrino, J; González-Elipe, AR; Gómez-Ramirez, A
ACS Sustainable Chemistry & Engineering, **11** (2023) 3621-3632
Febrero, 2023 · DOI: 10.1021/acssuschemeng.2c05877

Plasma-catalysis has been proposed as a potential alternative for the synthesis of ammonia. Studies in this area focus on the reaction mechanisms and the apparent synergy existing between processes occurring in the plasma phase and on the surface of the catalytic material. In the present study, we approach this problem using a parallel-plate packed-bed reactor with the gap between the electrodes filled with pellets of lead zirconate titanate (PZT), with this ferroelectric material modified with a coating layer of alumina (i.e., Al_2O_3/PZT) and the same alumina layer incorporating ruthenium nanoparticles (i.e., Ru-Al_2O_3/PZT). At ambient temperature, the electrical behavior of the ferroelectric packed-bed

reactor differed for these three types of barriers, with the plasma current reaching a maximum when using Ru-Al_2O_3/PZT pellets. A systematic analysis of the reaction yield and energy efficiency for the ammonia synthesis reaction, at ambient temperature and at 190 °C and various electrical operating conditions, has demonstrated that the yield and the energy efficiency for the ammonia synthesis do not significantly improve when including ruthenium particles, even at temperatures at which an incipient catalytic activity could be inferred. Besides disregarding a net plasma-catalysis effect, reaction results highlight the positive role of the ferroelectric PZT as moderator of the discharge, that of Ru particles as plasma hot points, and that of the Al_2O_3 coating as a plasma cooling dielectric layer.

Surface Acoustic Waves Equip Materials with Active De-Icing Functionality: Unraveled Glaze Ice De-Icing Mechanisms and Application to Centimeter-Scale Transparent Surfaces

Jacob, S; Pandey, S; Del Moral, J; Karimzadeh, A; Gil-Rostra, J; González-Elipe, AR; Borras, A; Winkler, A
Advanced Materials Technologies, **8** (2023) 2300263
Mayo, 2023 · DOI: 10.1002/admt.202300263

Enabling active de-icing functionality on low heat conductive and transparent materials is a requirement for several seminal industries in critical economic sectors. However, developing efficient and environmentally friendly de-icing methods still fails because of compatibility problems with large-scale devices and real-world conditions. In this paper, de-icing several square centimeters covered with thick layers of glaze ice is approached through nanoscale activation by surface acoustic waves (SAWs). De-icing functionality is demonstrated with a self-supported piezoelectric material ($LiNbO_3$) and a piezoelectric film (ZnO) deposited on fused silica, the latter system proving the compatibility of the method with materials of practical relevance. Its applicability to large and transparent substrates is demonstrated by placing the interdigitated electrodes (IDTs) required for activation close to the substrate's edges, leaving most of the surface unaltered. The de-icing mechanism of glaze ice by SAW activation is revealed by simulating the SAW propagation on ice-covered surfaces and by experimental analysis of the ice melting process. This involves a combination of ice mechanical stress activation and heating through the initially formed water/ice front. Possible Joule effects due to ohmic losses in the IDTs have been discarded, monitoring local temperature variations during SAW activation at and out of resonance conditions.

Strontium/zinc phytate-based self-assembled monolayers on titanium surfaces enhance osteogenesis and antibacterial performance in vitro

Asensio, G; Hernández-Arriaga, AM; Martin-del-Campo, M; Prieto, MA; González-Elipe, AR; Rojo, L; Vázquez-Lasa, B
Applied Surface Science, **620** (2023) 156818
Mayo, 2023 · DOI: 10.1016/j.apsusc.2023.156818

The accumulation of bacteria over implant surfaces is still the first cause of failure, and the development of antimicrobial surfaces constitutes a first line in implant research. Besides, the durability and mechanical performance of implants, in special in the dental area, are mainly determined by their osseointegration capacity into the maxillofacial bone and the appearance of infections. Consequently, implant osseointegration and infection prophylaxis remain as big challenges to attain so a huge investigation is being developed on the production of bioactive surfaces to achieve improvements in these aspects. In this work we propose the functionalization of titanium surfaces (Ti Cp) with self-assembled monolayers

(SAMs) of bioactive organophosphate compounds: phytic acid (Ti-PA) and its metallic phytate de- rivatives bearing Sr^{2+} and/or Zn^{2+} (Ti-SrPhy, Ti-ZnPhy and Ti-SrPhy/ZnPhy) which exhibited tunable in vitro osteogenic, antimicrobial and antioxidant properties in a previous work. Thus, phytate compounds are chemically anchored onto Ti discs through a simple procedure consisting of a condensation reaction promoted by heat treatment. EDS and XPS spectroscopies confirm the obtaining of the modified surfaces and the topographic properties and wettability analysed by SEM, AFM, profilometry and contact angle measurements, respectively, are explored. Additionally, phytate-SAMs do not release any cytotoxic compound after 14 days and stimulate in vitro adhesion and proliferation of human osteoblast cells after 14 days of culture. The osteogenic ability of the modified surfaces evaluated by the quantification of ALP activity and matrix mineralization degree shows a significant improvement with respect to unmodified surfaces. Furthermore, the antimicrobial activity of phytate-SAMs against Streptococcus mutans cultures is evaluated. The count of viable cells and the quantification of produced biofilm are significantly reduced by all phytate-SAMs groups ($p < 0.001$). Cell membrane integrity studies by LIVE/DEAD staining and SEM imaging confirm a decreased viability of adhered bacteria when phytate-based surfaces are tested, due to a disruption in the function and permeability of the cell membrane. Therefore, phytate-SAMs exhibit suitable in vitro features suggesting their promising potential as bioactive coatings of dental implants.

Exalted dual-scale surface roughening in laser ablated aluminum capped with a transparent thin film: Wetting and anti-icing behavior

Ghemras, I; Montes, L; López-Santos, C; González-Elipe, AR; Rico, V
Applied Surface Science, **630** (2023) 157357
Septiembre, 2023 · DOI: 10.1016/j.apsusc.2023.157357

Near infrared laser ablation of metals, specifically aluminum, has been systematically applied to generate surface roughness. Very high laser fluences may even lead to a so called "explosive" ablation regime where roughness becomes dramatically enhanced. In the present work we have developed an alternative methodology that, uti-lizing milder laser irradiation conditions (i.e. laser fluences from 0.37 to 0.72 J/cm^2), renders aluminum surfaces with a dual-scale roughness character and Sp parameter values twice or even trice the value found in reference samples. This has been possible for aluminum substrates coated with a highly transparent aluminum oxynitride capping layer. The resulting surfaces, consisting of very rough partially oxidized aluminum with negligible amounts of nitrogen species, resulted highly hydrophobic and depicted long icing delay times as required for anti-icing applications. A correlation has been found between the wetting and anti-icing behaviors, the use of a capping layer and the laser irradiation conditions. To account for this exalted roughening phenomenon, we propose that the transparent capping layer confines the laser energy within the aluminum shallow zones, delays the formation of the plasma plume and produces an enhancement in the aluminum ablation, even at relatively low laser fluences.

Effect of the effective refractive index on the radiative decay rate in nanoparticle thin films

Romero, M; Sánchez-Valencia, JR; Lozano, G; Míguez, H
Nanoscale, **15** (2023) 15279-15287
Septiembre, 2023 · DOI: 10.1039/d3nr03348a

In this work, we theoretically and experimentally study the influence of the optical environment on the radiative decay rate of rare-earth transitions in luminescent nanoparticles forming a thin film. We use electric dipole sources in finite-difference time-domain simulations to analyze the effect of modifying the effective refractive index of transparent layers made of phosphor nanocrystals doped with rare earth cations, and propose a correction to previously reported analytical models for calculating the radiative decay rate. Our predictions are tested against an experimental realization of such luminescent films, in which we manage to vary the effective refractive index in a gradual and controllable manner. Our model accurately accounts for the measurements attained, allows us to discriminate the radiative and non-radiative contributions to the time-resolved photoluminescence, and provides a way to rationally tune the spontaneous decay rate and hence the photoluminescence quantum yield in an ensemble of luminescent nanoparticles.

Ti6Al4V coatings on titanium samples by sputtering techniques: Microstructural and mechanical characterization

Sánchez-López, JC; Rodríguez-Albelo, M; Sánchez-Pérez, M; Godinho, V; López-Santos, C; Torres, Y
Journal of Alloys and Compounds, **952** (2023) 170018
Agosto, 2023 · DOI: 10.1016/j.jallcom.2023.170018

Although titanium is widely used as biomaterial, the control of the interface properties between its surface and the surrounding physiological environment (like bone, other tissues or biofluids) results crucial to achieve a successful osseointegration and good biomechanical and functional performance. In this work, commercially pure titanium (Grade IV) discs obtained by conventional powder metallurgy were coated with 1-3 μm of Ti6Al4V (Grade V) alloy using DC-pulsed or high-power impulse magnetron sputtering (HiPIMS) technique with the aim of improving their biomedical performance. SEM, confocal microscopy, X-ray diffraction, nanoindentation and wetting measurements are used to evaluate the bio-interface role of the titanium-coated implants. Conformal Ti6Al4V coatings with controlled nano-roughness can be deposited with enhanced mechanical (H = 5-8 GPa; E = 140-160 GPa) and hydrophobic properties thanks to a dense columnar structure. The increased Ti-O bonding at the interface helps to prevent the corrosion due to the formation of a surface passivation layer. Particularly in the case of the HiPIMS process, the surface modification of titanium implants (chemistry, morphology and structure) appears as an effective strategy for satisfying the biomedical requirements and functionality, with enhanced mechanical properties and nanostructuration for prevention of bacteria colonization.

Setting a comprehensive strategy to face the runback icing phenomena

Mora, J; García, P; Carreño, F; González, M; Gutiérrez, M; Montes, L; Rico Gavira, V; López-Santos, C; Vicente, A; Rivero, P; Rodríguez, R; Larumbe, S; Acosta, C; Ibáñez-Ibáñez, P; Corozzi, A; Raimondo, M; Kozera, R; Przybyszewski, B; González-Elipe, AR; Borrás, A; Redondo, F; Agüero, A
Surface & Coatings Technology, **465** (2023) 129585
Julio, 2023 · DOI: 10.1016/j.surfcoat.2023.129585

The development of anti-icing robust surfaces is a hot topic nowadays and particularly crucial in the aeronautics or wind energy sectors as ice accretion can compromise safety and power generation efficiency. However, the current performance of most anti-icing strategies has been proven insufficient for such demanding applications, particularly in large unprotected zones, which located downstream from

thermally protected areas, may undergo secondary icing. Herein, a new testing methodology is proposed to evaluate accretion mechanisms and secondary icing phenomena through, respectively, direct impact and running-wet processes and systematically applied to anti-icing materials including commercial solutions and the latest trends in the state-of-the-art. Five categories of materials (hard, elastomeric, polymeric matrix, SLIPS and superhydrophobic) with up to fifteen formulations have been tested. This Round-Robin approach provides a deeper understanding of anti-icing mechanisms revealing the strengths and weaknesses of each material. The conclusion is that there is no single passive solution for anti-ice protection. Thus, to effectively protect a given real component, different tailored materials fitted for each particular zone of the system are required. For this selection, shape analysis of such a component and the impact characteristics of water droplets under real conditions are needed as schematically illustrated for aeronautic turbines.

Spherosilicate-modified epoxy coatings with enhanced icephobic properties for wind turbines applications

Kozera, R; Zietkowska, K; Przybyszewski, B; Boczkowska, A; Sztorch, B; Paku, D; Przekop, RE; Trzcinski, J; Borras, A
Colloids and Surfaces A-Physicochemical and Engineering Aspects, **679** (2023) 132475
Diciembre, 2023 · DOI: 10.1016/j.colsurfa.2023.132475

Industries around the world use active methods, which include thermal, mechanical and chemical approaches, to reduce icing on aerodynamic surfaces such as wind turbines and aircraft. However, they are often inefficient, costly, and pollute the environment. For years, new coatings with anti-icing properties (so-called icephobic coatings) have been developed to either replace or work in tandem with active systems. In this study, coatings were designed based on an epoxy gelcoat commonly used for wind turbines through chemical modification with spherosilicate derivatives. Di- and tri-functional spherosilicates have both groups that increase the degree of hydro-/icephobicity of composites , groups capable of interacting with epoxy resin and amine hardener. The icephobicity of the surface was determined using ice adhesion. The lowest value of this parameter reached a value of 186 kPa, a 30 % reduction compared to the unmodified coating. In addition, the hydrophobicity of the surface was determined (the highest water contact angle was equal to 103°). A correlation was observed, proven in many works, that as the surface roughness increases, the anti-icing properties deteriorate. For individual modifications, it was also shown that hydrophobicity has a positive effect on ice adhesion. The work also examined the surface zeta potential and determined the durability of the properties after 100 icing/deicing cycles.

Advanced Cellulose-Nanocarbon Composite Films for High-Performance Triboelectric and Piezoelectric Nanogenerators

González, J; Ghaffarinejad, A; Ivanov, M; Ferreira, P; Vilarinho, PM; Borras, A; Amorin, H; Wicklein, B
Nanomaterials, **13** (2023) 1206
Abril, 2023 · DOI: 10.3390/nano13071206

Natural polymers such as cellulose have interesting tribo- and piezoelectric properties for paper-based energy harvesters, but their low performance in providing sufficient output power is still an impediment to a wider deployment for IoT and other low-power applications. In this study, different types of celluloses were combined with nanosized carbon fillers to investigate their effect on the enhancement of the electrical properties in the final nanogenerator devices. Cellulose pulp (CP), microcrystalline cellulose

(MCC) and cellulose nanofibers (CNFs) were blended with carbon black (CB), carbon nanotubes (CNTs) and graphene nanoplatelets (GNPs). The microstructure of the nanocomposite films was characterized by scanning electron and probe microscopies, and the electrical properties were measured macroscopically and at the local scale by piezoresponse force microscopy. The highest generated output voltage in triboelectric mode was obtained from MCC films with CNTs and CB, while the highest piezoelectric voltage was produced in CNF-CNT films. The obtained electrical responses were discussed in relation to the material properties. Analysis of the microscopic response shows that pulp has a higher local piezoelectric d(33) coefficient (145 pC/N) than CNF (14 pC/N), while the macroscopic response is greatly influenced by the excitation mode and the effective orientation of the crystals relative to the mechanical stress. The increased electricity produced from cellulose nanocomposites may lead to more efficient and biodegradable nanogenerators.

Determination of the Primary Excitation Spectra in XPS and AES

Pauly, N; Yubero, F; Tougaard, S
Nanomaterials, **13** (2023) 339
Enero, 2023 · DOI: 10.3390/nano13020339

This paper reviews a procedure that allows for extracting primary photoelectron or Auger electron emissions from homogeneous isotropic samples. It is based on a quantitative dielectric description of the energy losses of swift electrons travelling nearby surfaces in presence of stationary positive charges. The theory behind the modeling of the electron energy losses, implemented in a freely available QUEELS-XPS software package, takes into account intrinsic and extrinsic effects affecting the electron transport. The procedure allows for interpretation of shake-up and multiplet structures on a quantitative basis. We outline the basic theory behind it and illustrate its capabilities with several case examples. Thus, we report on the angular dependence of the intrinsic and extrinsic Al 2s photoelectron emission from aluminum, the shake-up structure of the Ag 3d, Cu 2p, and Ce 3d photoelectron emission from silver, CuO and CeO_2, respectively, and the quantification of the two-hole final states contributing to the $L_3M_{45}M_{45}$ Auger electron emission of copper. These examples illustrate the procedure, that can be applied to any homogeneous isotropic material.

Microstructural characterization and thermal stability of He charged amorphous silicon films prepared by magnetron sputtering in helium

Fernández, A; Sauvage, T; Diallo, B; Hufschmidt, D; de Haro, MCJ; Montes, O; Martínez-Blanes, JM; Caballero, J; Godinho, V; Ferrer, FJ; Ibrahim, S; Brault, P; Thomann, AL
Materials Chemistry and Physics, **301** (2023) 127674
Junio, 2023 · DOI: 10.1016/j.matchemphys.2023.127674

Sputtering of silicon in a Helium magnetron discharge has been reported as a bottom-up procedure to obtain amorphous Si films containing high amounts of gas-filled nanopores. Here we compare the microstructure and composition of Si-He nanocomposite films deposited by magnetron sputtering (MS) with ^{4}He in DC or RF and ^{3}He in RF operation modes. Electron microscopy (SEM and TEM), X-ray diffraction (XRD) and ion beam analysis (IBA) have been used to analyze the films and to investigate the in-situ and ex-situ thermal evolution. Depending on deposition conditions different in depth compositions, nanopore size and shape distributions, porosity and He content could be obtained. The presence of impurities (i.e. oxygen) has shown to promote He diffusivity reducing He accumulation. The start temperature of He-release varied in the range 473-723 K without films crystallization. Films grown in

RF mode reached contents of 32 and 29 at% of ^{4}He and ^{3}He and were respectively stable up to 573 and 723 K both in vacuum and under inert gas flow. In-situ p-EBS (proton Elastic Back Scattering) allowed monitoring the He release accompanied by blistering/delamination effects visualized by SEM. These results show the potentiality of annealing to hold nano-porous structures after liberation of trapped gas.

Sol–Gel Technologies to Obtain Advanced Bioceramics for Dental Therapeutics

X. Song; J.J. Segura-Egea; A.Díaz-Cuenca
Molecules, **28** (2023) 6967
Octubre, 2023 · DOI: 10.3390/molecules28196967

The aim of this work is to review the application of bioceramic materials in the context of current regenerative dentistry therapies, focusing on the latest advances in the synthesis of advanced materials using the sol–gel methodology. Chemical synthesis, processing and therapeutic possibilities are discussed in a structured way, according to the three main types of ceramic materials used in regenerative dentistry: bioactive glasses and glass ceramics, calcium phosphates and calcium silicates. The morphology and chemical composition of these bioceramics play a crucial role in their biological properties and effectiveness in dental therapeutics. The goal is to understand their chemical, surface, mechanical and biological properties better and develop strategies to control their pore structure, shape, size and compositions. Over the past decades, bioceramic materials have provided excellent results in a wide variety of clinical applications related to hard tissue repair and regeneration. Characteristics, such as their similarity to the chemical composition of the mineral phase of bones and teeth, as well as the possibilities offered by the advances in nanotechnology, are driving the development of new biomimetic materials that are required in regenerative dentistry. The sol–gel technique is a method for producing synthetic bioceramics with high purity and homogeneity at the molecular scale and to control the surfaces, interfaces and porosity at the nanometric scale. The intrinsic nanoporosity of materials produced by the sol–gel technique correlates with the high specific surface area, reactivity and bioactivity of advanced bioceramics.

Optical monitoring of detergent pollutants in greywater

Lahoz, F; de Armas-Rillo, S; Hernandez-Rodríguez, C; Gil-Rostra, J; Yubero, F
Optics Express, **31** (2023) 15227-15238
Mayo, 2023 · DOI: 10.1364/OE.466194

Large amount of wastewater is produced by washing machines and dishwashers, which are used in a daily basis. This domestic wastewater generated in households or office buildings (also called greywater) is drained directly to the drainpipes without differentiation from that with fecal contamination from toilets. Detergents are arguably the pollutants most frequently found in greywater from home appliances. Their concentrations vary in the successive stages in a wash cycle, which could be taken into account in a rational design of home appliances wastewater management. Analytical chemistry procedures are commonly used to determine the pollutant content in wastewater. They require collecting samples and their transport to properly equipped laboratories, which hampers real time wastewater management. In this paper, optofluidic devices based on planar Fabry-Perot microresonators operating in transmission mode in the visible and near infrared spectral ranges have been studied to determine the concentration of five brands of soap dissolved in water. It is found that the spectral positions of the

optical resonances redshift when the soap concentration increases in the corresponding solutions. Experimental calibration curves of the optofluidic device were used to determine the soap concentration of wastewater from the successive stages of a washing machine wash cycle either loaded with garments or unloaded. Interestingly, the analysis of the optical sensor indicated that the greywater from the last water discharge of the wash cycle could be reused for gardening or agriculture. The integration of this kind of microfluidic devices into the home appliances design could lead to reduce our hydric environmental impact.

Tribological Response of delta-Bi_2O_3 Coatings Deposited by RF Magnetron Sputtering

Rodil, SE; Depablos-Rivera, O; Sánchez-López, JC
Lubricants, **11** (2023) 207
Mayo, 2023 · DOI: 10.3390/lubricants11050207

Bismuth oxide (Bi_2O_3) coatings and composite coatings containing this oxide have been studied due to their potential applications in gas sensing, optoelectronics, photocatalysis, and even tribology. Two parametric models based on chemical features have been proposed with the aim of predicting the lubricity response of oxides. However, such models predict contradictory values of the coefficient of friction (COF) for Bi_2O_3. In this study, we deposited Bi_2O_3 coatings, via magnetron sputtering, on AISI D2 steel substrates to evaluate the tribological responses of the coatings and determine which parametric model describes them better. Experimentally, only coatings presenting the cubic defective fluorite-like delta-Bi_2O_3 phase could be evaluated. We performed pin-on-disk tests at room temperature and progressively increasing temperatures up to 300 °C using alumina and steel counter-bodies. Low wear and COFs (0.05 to 0.15) indicated that the delta-phase behaves as a lubricious solid, favoring the validity of one of the models. An alternative explanation is proposed for the low COF of the defective fluorite-like structure since it is well known that it contains 25% of anionic vacancies that can be ordered to form low shear-strength planes, similar to the Magneli phases. Two challenges for future potential applications were observed: one was the low adhesion strength to the substrate, and the other was the thermal stability of this phase.

Structure and Void Connectivity in Nanocolumnar Thin Films Grown by Magnetron Sputtering at Oblique Angles

Alvarez, R; Regodon, G; Acosta-Rivera, H; Rico, V; Alcala, G; González-Elipe, AR; Palmero, A
Coatings, **13** (2023) 991
Junio, 2023 · DOI: 10.3390/coatings13060991

The morphology and void connectivity of thin films grown by a magnetron sputtering deposition technique at oblique geometries were studied in this paper. A well-tested thin film growth model was employed to assess the features of these layers along with experimental data taken from the literature. A strong variation in the film morphology and pore topology was found as a function of the growth conditions, which have been linked to the different collisional transport of sputtered species in the plasma gas. Four different characteristic film morphologies were identified, such as (i) highly dense and compact, (ii) compact with large, tilted mesopores, (iii) nanocolumns separated by large mesopores, and (iv) vertically aligned sponge-like coalescent nanostructures. Attending to the topology and connectivity of the voids in the film, the nanocolumnar morphology was shown to present a high pore volume and area connected with the outside by means of mesopores, with a diameter above 2 nm, while the sponge-

like nanostructure presented a high pore volume and area, as well as a dense network connectivity by means of micropores, with a diameter below 2 nm. The obtained results describe the different features of the porous network in these films and explain the different performances as gas or liquid sensors in electrochromic applications or for infiltration with nanoparticles or large molecules.

Low temperature nucleation of thermochromic VO_2 crystal domains in nanocolumnar porous thin films

Alcaide, AM; Regodon, G; Ferrer, FJ; Rico, V; Alvarez, R; Rojas, TC; González-Elipe, AR; Palmero, A
Nanotechnology, **34** (2023) 255702
Junio, 2023 · DOI: 10.1088/1361-6528/acc664

The low temperature formation of monoclinic VO_2 crystal domains in nanocolumnar vanadium/oxygen thin films prepared by magnetron sputtering at oblique angles is analyzed. The synthesis procedure involved the deposition of amorphous nanocolumnar $VO_{1.9}$ thin films at room temperature and its subsequent annealing at temperatures between 250 °C and 330 °C in an oxygen atmosphere. The thermochromic transition of these films was found at a temperature of 47 °C when the annealing temperature was 270 °C and 58 °C when the annealing temperature was 280 °C and 290 °C, presenting a clear drop of the optical transmittance in the infrared region of the spectrum. The significant downshift in the temperature window to obtain VO_2 in comparison with compact films and other strategies in literature is explained by the particular morphology of the nanocolumnar structures, which contains numerous defects along with open and embedded porosity.

H_2 Production from NH_3 in a $BaTiO_3$ Moderated Ferroelectric Packed-Bed Plasma Reactor

Ruiz-Martín, M; Marín-Meana, S; Megías-Sánchez, A; Oliva-Ramírez, M; Cotrino, J; González-Elipe, AR; Gómez-Ramírez, A
Plasma Chemistry and Plasma Processing, **43** (2023) 2093-2110
Noviembre, 2023 · DOI: 10.1007/s11090-023-10427-7

Plasma decomposition reactions are used for various gas phase chemical processes including the decomposition of ammonia. In this work we show that pure ammonia can be effectively decomposed at atmospheric pressure and ambient temperature using a packed-bed plasma reactor moderated with $BaTiO_3$ ferroelectric pellets without catalyst. The decomposition rate and energy efficiency of this ferroelectric barrier discharge reactor have been monitored as a function of applied voltage (up to a maximum value of 2.5 kV) and flow rate. For each operating condition reaction efficiencies have been correlated with the parameters defining the electrical response of the reactor. It is found that plasma current and volume inside the reactor and hence the energy efficiency of the process and the decomposition rate vary with the applied voltage and the flow of ammonia (a maximum decomposition rate of 14% and an energy efficiency of 150 LH_2/kWh has been determined under optimized operation conditions). The role of back reactions (i.e. $N_2 + 3H_2 \rightarrow 2NH_3$) in decreasing reactor performance is another key effect affecting the overall efficiency for the ammonia decomposition. The possibilities of ferroelectric barrier discharge reactors to induce the decomposition of ammonia and the importance of keeping the operating temperature below the Curie temperature of the ferroelectric material are highlighted.

Understanding the Problem of Hydrogen Storage Using a Demonstration: Coupling a Hydrogen Generator Based on the Hydrolysis of Sodium Borohydride to a Fuel-Cell Kit

Arzac, GM; Calvo, ME; Fernández, A
Journal of Chemical Education, 100 (2023) 4554-4558
Octubre, 2023 | DOI: 10.1021/acs.jchemed.3c00590

In the context of a green global energy paradigm, hydrogen (H_2) is a very promising energy carrier. In fuel cells, hydrogen can be used to generate electricity to drive an electric motor, producing water as its only byproduct. However, to implement hydrogen as an energy vector, developing methods for its production, storage, distribution, and use is essential. Sodium borohydride is a potential hydrogen source capable of releasing H_2 through catalytic hydrolysis. Herein, we present a demonstration that couples a hydrogen generator based on the hydrolysis of sodium borohydride to a commercial fuel-cell kit. The commercial fuel-cell kit operates using the hydrogen generated by an electrolyzer and includes a small fan to prove the successful generation of electricity. The performance of the fuel cell coupled with the borohydride-based reactor is compared to the performance achieved using the hydrogen produced by the electrolyzer. The borohydride-based reactor is designed to power the fan for 300 s and demonstrates efficient and safe hydrogen storage within a small volume of sodium borohydride. This study showcases the hydrogen cycle, the hydrogen storage problem, and the potential of sodium borohydride as a hydrogen storage material in a simple and useful way, contributing to science education and dissemination in the field of energy sustainability.

Germination and First Stages of Growth in Drought, Salinity, and Cold Stress Conditions of Plasma-Treated Barley Seeds

Perea-Brenes, A; Garcia, JL; Cantos, M; Cotrino, J; González-Elipe, AR; Gómez-Ramirez, A; López-Santos, C
ACS Agricultural Science & Technology, **3** (2023) 760-770
Septiembre, 2023 · DOI: 10.1021/acsagscitech.3c00121

Numerous works have demonstrated that cold plasma treatments constitute an effective procedure to accelerate seed germination under nonstress conditions. Evidence also exists about a positive effect of plasmas for germination under environmental stress conditions. For barley seeds, this work studies the influence of cold plasma treatments on the germination rate and initial stages of plant growth in common stress environments, such as drought, salinity, and low-temperature conditions. As a general result, it has been found that the germination rate was higher for plasma-treated than for untreated seeds. Plasma also induced favorable changes in plant and radicle dimensions, which depended on the environment. The obtained results demonstrate that plasma affects the biochemical metabolic chains of seeds and plants, resulting in changes in the concentration of biochemical growing factors, a faster germination, and an initially more robust plant growth, even under stress conditions. These changes in phenotype are accompanied by differences in the concentration of biomarkers such as photosynthetic pigments (chlorophylls a and b and carotenoids), reactive oxygen species, and, particularly, the amino acid proline in the leaves of young plants, with changes that depend on environmental conditions and the application of a plasma treatment. This supports the idea that, rather than an increase in seed water imbibition capacity, there are clear beneficial effects on seedling of plasma treatments.

Microstructural Characterization and Self-Propagation Properties of Reactive Al/Ni Multilayers Deposited onto Wavelike Surface Morphologies: Influence on the Propagation Front Velocity
Camposano, YHS; Bartsch, H; Matthes, S; Oliva-Ramirez, M; Jaekel, K; Schaaf, P
Physica Status Solidi A-Applications and Materials Science, **220** (2023) 2200765
Marzo, 2023 · DOI: 10.1002/pssa.202200765

Reactive multilayer systems are nanostructures of great interest for various technological applications because of their high energy release rate during the self-propagating reaction of their components. Therefore, many efforts are aimed at controlling the propagation velocity of these reactions. Herein, reactive multilayer systems of Al/Ni in the shape of free-standing foils with a wavelike surface morphology prepared by using sacrificial substrates with well-aligned waves are presented and the propagation of the reaction along different directions of the reproduced waves is analyzed. During the ignition test, the propagation front is recorded with a high-speed camera, and the maximum temperature is measured using a pyrometer. The propagation of the reaction is favored in the direction of the waves, which points out the influence of the anisotropy generated by this morphology and how it affects the propagation dynamics and the resulting microstructure. Furthermore, compared to their counterparts fabricated on flat substrates, these reactive multilayers with wavelike morphology exhibit a remarkable reduction in the propagation velocity of the reaction of about 50%, without significantly affecting the maximum temperature registered during the reaction.

Dielectric multilayers for broadband optical rotation enhancement
Pellegrini, G; Mogni, E; Gil-Rostra, J; Yubero, F; Fossati, S; Dostálek, J; Vázquez, RM; Osellame, R; Celebrano, M; Finazzi, M; Biagioni, P
Nuovo Cimento C-Colloquia and Communications in Physics, **46** (2023) 111
Julio, 2023 · DOI: 10.1393/ncc/i2023-23111-1

We design a simple dielectric multilayer capable of sustaining broadband superchiral surface waves. We show that the platform can produce large optical chirality enhancements in a wavelength range of hundreds of nanometers. We finally demonstrate that these properties result in the enhancement of the optical rotation signal well above two orders of magnitude, thus extending surface-enhanced chiral spectroscopies beyond the traditionally addressed circular dichroism signals.

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

49th EPS Conference on Plasma Physics
03-07 julio [Bordeaux, Francia]

Ana Isabel Borrás Martos · MIEMBRO DEL COMITÉ CIENTÍFICO

FEMS EUROMAT 23
03-07 septiembre [Frankfurt am Main, Alemania & Online]

Juan Carlos Sánchez López · ORGANIZADOR DEL SIMPOSIO C07 – Coatings and Surface Modification Technologies

19th International Conference on Thin Films · ICTF2023
26-29 septiembre [Burgos, España]

Francisco Yubero Valencia · CHAIR

COMUNICACIONES / COMMUNICATIONS

The European Space Components Conference · ESCCON 2023
07-09 marzo [Toulouse, Francia]

OSIP activity: Assesing pseudo-hermeticity on ICs with plastic encapsulated materials. *L. Arriaga, G. Fernández, D. Fraser, S. Bernardsky, F.J. Aparicio, A. Barranco*. COMUNICACIÓN ORAL

2023 MRS Spring Meeting & Exhibit
10-14 abril [San Francisco, Estados Unidos de América]

Vacuum and plasma synthesis and processing of surfaces, multifunctional thin films and 3D nanoarchitectures - A platform for the development of energy harvesting system. X. García-Casas, J. Castillo-Seoane, L. Montes, J. Del Moral, F. Aparicio, A. Ghaffarinejad, L. Contreras-Bernal, J. Gil-Rostra, J. Budagosky, C. López-Santos, J. Sánchez-Valencia, A. Barranco, A. Borrás. CONFERENCIA INVITADA

Effect of pulsed bias on the deposition of multi-layered $Cr_xAl_{1-x}N_y/Al_2O_3$ solar selective coatings tandem for high temperature applications. *M. Sánchez-Pérez, T.C. Rojas, F.J. Ferrer, A. Morales, R. Escobar-Galindo, J.C. Sánchez-López*. COMUNICACIÓN ORAL

Theoretical and experimental study of self-powered piezoelectric sensors response to applied force. *X. García-Casas, J. Budagosky, F.J. Aparicio, J. Sánchez Valencia, A. Barranco, A. Borrás*. PÓSTER

Plasma Processing and Technology International Conference · PLASMA TECH 2023
26-28 abril [Lisboa, Portugal]

Characterization and modelling of surface plasma devices. *S. Marín-Meana, G. Regodón-Harkness, A. Palmero, J. Cotrino, A.R. González-Elipe, A. Gómez Ramírez, M. Oliva-Ramírez*. COMUNICACIÓN ORAL

Fourth Workshop on Size-Dependent Effects in Materials for Environmental Protection and Energy Application · SizeMat4
10-14 mayo [Pomorie, Bulgaria]

Synthesis and optimization to improve setting performance of a Sr-doped bioactive endodontic cement. *D. Flores-Barnett, X. Song, A. Díaz-Cuenca*. CONFERENCIA-ONLINE

Sol-gel synthesis of Zn-doped bioactive endodontic cements: effect of Zn content on crystal phase formation. *X. Song, D. Flores-Barnett, A. Díaz-Cuenca*. PÓSTER

Synthesis and spectroscopic characteristics of new poorly crystalline hydroxyapatite-polycarboxy/sulfo betaine hybrid materials. *D. Rabadjieva, A. Díaz-Cuenca, R. Gergulova, K. Ruseva, E. Vassileva*. PÓSTER

25th International Symposium on Plasma Chemistry · ISPC25
21-26 mayo [Kyoto, Japón]

Ammonia synthesis: on the effect of adding a metal catalyst in a ferroelectric packed-bed plasma reactor. *A. Gómez-Ramírez, P. Navascués, J. Garrido-García, M. Oliva-Ramírez, J. Cotrino, A.R. González-Elipe*. COMUNICACIÓN ORAL

Unraveling surface for improving the germination of barley seeds: from drying to air plasma treatments. *A. Perea-Brenes, A. Gómez-Ramírez, C. López-Santos, M. Oliva-Ramírez, R. Molina, J. Cotrino, J.L. García, M. Cantos, A.R. González-Elipe*. PÓSTER

15th International Conference on Hybrid and Organic Photovoltaics · HOPV23
12-14 junio [Londres, Reino Unido]

Effect of 1D nanostructured electrodes in dye sensitized solar cells for indoor light harvesting. *L. Contreras-Bernal, J. Castillo-Seoane, A. Riquelme-Expósito, J. Gil-Rostra, G. Lozano, A. Barranco, R. Demadrille, J.R. Sánchez-Valencia, A. Borrás*. COMUNICACIÓN ORAL

Environmental stability of perovskite solar cells with water-repellent fluorinated surfaces by plasma assisted technology. *F. Núñez Gálvez, A. Descalzo, X. García-Casas, J.M. Obrero-Pérez, L. Contreras Bernal, J.R. Sánchez-Valencia, C. López-Santos*. PÓSTER

Workshop on Ion Exchange Membranes for Energy Applications · EMEA 2023
20-22 junio [Bad Zwischenahn, Alemania]

Ionomer-free electrodes for efficient AEM water electrolysis. *F. Yubero, J. Gil-Rostra, P.J. Lloreda, A.R. González-Elipe, E. López-Fernández, V. Rodríguez-Pintor, A. de Lucas Consuegra, J. Brey*. PÓSTER

International Conference on Icing of Aircraft, Engines, and Structures · SAE
20-22 junio [Viena, Austria]

Could superhydrophobic surfaces be a realistic solution for running-wet areas?. *F. Carreño, L. Montes, C. López-Santos, V. Rico, A. Borrás, F. Redondo, A.R. González-Elipe, A. Agüero*. COMUNICACIÓN ORAL

23rd International Conference on Transparent Optical Network · ICTON2023
02-06 julio [Bucarest, Rumania]

Photonic multilayers for broadband and large area superchiral surface waves. *G. Pelligrini, E. Mogni, J. Gil-Rostra, F. Yubero, G. Simone, S. Fossati, J. Dostalek, M. Celebrano, M. Finazzi, R. Martínez-Vázquez, R. Osellame, P. Biagioni*. CONFERENCIA INVITADA

49th EPS Conference on Plasma Physics
03-07 julio [Burdeos, Francia]

Recent results on the development of advanced plasma assisted vacuum deposition. *F.J. Aparicio, G.P. Moreno, T. Czermak, J. Obrero, C. López-Santos, J.R. Sánchez-Valencia, F. Carrascoso, A. Castellanos-Gómez, A. Borrás, A. Barranco*. COMUNICACIÓN ORAL

Photonics & Electromagnetics Research Symposium · PIERS 2023
03-06 julio [Praga, República Checa]

Plasma technology for the development of nanogenerators based in multifunctional thin films and 3D nanoarchitectures. *J.R. Sánchez-Valencia, X. García-Casas, J. Castillo-Seoane, F.J. Aparicio, A. Ghaffarinejad, L. Contreras-Bernal, J. Gil-Rostra, J. Budagosky, V. López-Flores, A. Barranco, A. Borrás*. CONFERENCIA INVITADA

International Conference on Phenomena in Ionized Gases · ICPIG 2023
09-14 julio [Egmond aan Zee, Países Bajos]

On the role of reaction mechanisms and metal catalysts during the plasma-assisted ammonia synthesis. *A. Gómez-Ramírez, P. Navascués, J. Garrido-García, M. Oliva-Ramírez, J. Cotrino, A.R. González-Elipe*. COMUNICACIÓN INVITADA

Unraveling surface effects for improving the germination of barley seeds: from drying to air plasma treatments. *A. Perea-Brenes, A. Gómez-Ramírez, C. López-Santos, M. Oliva-Ramírez, R. Molina, J. Cotrino, J.L. García, M. Cantos, A.R. González-Elipe*. PÓSTER

31st International Materials Research Congress 2023 · IMRC2023
13-18 agosto [Cancún, México]

Enhancing the stability and reproducibility of perovskite solar cells by introducing ultrathin plasma polymer interlayers. *M. Nabil, L. Contreras-Bernal, G.P. Moreno, F. Núñez-Galvez, G. Oskam, M. Acosta Díaz, P. Pistor, J.A. Anta, A. Borrás, J.R. Sánchez-Valencia, A. Barranco*. PÓSTER

FEMS EUROMAT 23
03-07 septiembre [Frankfurt am Main, Alemania & Online]

Solar aging of solar selective coatings based on CrAlN multilayers for high temperature applications. *I. Cañadas, M. Sánchez-Pérez, J. Wette, M. Farchado, A. Morales, J. Rodríguez, F. Sutter, D.F. Reyes, T.C. Rojas, R. Escobar-Galindo, J.C. Sánchez-López*. COMUNICACIÓN ORAL

11th International Workshop on Functional Nanocomposites · NANOWORKSHOP 2023
12-15 septiembre [Plön Castle, Alemania]

Multifunctional plasma-enabled functional thin films low dimensional nanoarchitectures: from synthesis to devices. *X. García-Casas, J. Castillo-Seoane, J. del Moral, G.P. Moreno, T. Czermak, L. Montes, J. Gil-Rostra, V. Rico, F.J. Aparicio, C. López-Santos, J.R. Sánchez-Valencia, A. Barranco, A. Borrás*. CONFERENCIA INVITADA

19th International Conference on Thin Films · ICTF 2023
26-29 septiembre [Burgos, España]

Functional applications of nanostructured surfaces developed by plasma and vacuum technologies: from wetting to energy harvesting. *J. Castillo Seoane, X. García Casas, J. del Moral, L. Montes, F. Núñez-Gálvez, G.P. Moreno, D. Jumilla, C. López-Santos, F.J. Aparicio, V. Godinho, J. Gil Rostra, V. Rico, V. López-Flores, A.R. González-Elipe, J.R. Sánchez Valencia, A. Barranco, A. Borrás*. CONFERENCIA INVITADA

NIR optofluidic device for liquid analysis. *P.J. Lloreda Jurado, J. Gil-Rostra, A.R. González-Elipe, R. González, F. Yubero*. COMUNICACIÓN ORAL

Ultrathin plasma polymer for improved stability and reproducibility of perovskite solar cells. *L. Contreras-Bernal, J. Obrero-Pérez, F. Núñez-Galvez, J. Castillo-Seoane, K. Valez-Villalobos, F.J. Aparicio, J.A. Anta, A. Borrás, J.R. Sánchez-Valencia, A. Barranco*. COMUNICACIÓN ORAL

Environmental stability of perovskite solar cells encapsulated with water-repellent fluorinated thin films by plasma assisted technology. *F. Núñez-Gálvez, A. Descalzo, X. García-Casas, J.M. Obrero-Pérez, L. Contreras-Bernal, A. Borrás, J.R. Sánchez-Valencia, C. López-Santos*. COMUNICACIÓN ORAL

Omniphobic hierarchical stainless-steel surfaces by vacuum and plasma techniques for protective applications. *L. Montes, V. Rico, S. Bobaru, A. García-Valenzuela, M.A. Arenas, A. Conde del Campo, J.P. Espinós, A. Borrás, A.R. González-Elipe, C. López Santos*. COMUNICACIÓN ORAL

Vacuum soft-template methodology for perovskite-based core@shell nanotubes with enhanced optoelectronic properties. *J. Castillo Seoane, L. Contreras Bernal, T.C. Rojas, A. Barranco, J.R. Sánchez-Valencia, A. Borrás*. COMUNICACIÓN ORAL

Transparent drop energy harvesters based on PDMS@TiO_2 nanowires. *F. Núñez-Gálvez, X. García-Casas, V. Godinho, J.R. Sánchez-Valencia, A. Barranco, C. López-Santos, A. Borrás*. PÓSTER

Physical vapour deposition of multifunctional coatings on ASA, ASA-FC and ASA-Cu printed using additive manufacturing. *R. Escobar Galindo, J. Hernández-Saz, T.C. Rojas, M. Sánchez-Pérez, J.C. Sánchez-López, S.I. Molina*. PÓSTER

Influence of chromium oxide (CrOx)-based layers as thermal diffusion barriers on 316L steel and Inconel 625 for solar selective absorbers applications. *C.I. Parra-Montero, J.M. Montero, J.C. Sánchez-López, R. Escobar-Galindo*. PÓSTER

244th ECS Meeting

08-12 octubre [Gotemburgo, Suecia]

Multifunctional plasma-enabled low dimensional nanoarchitectures: from synthesis to devices. A. Borrás. CONFERENCIA INVITADA

76th Annual Gaseous Electronics Conference · GEC 2023

09-13 octubre [Ann Arbor, Estados Unidos de América]

Plasma assisted dry reforming of methane: Syngas and hydrocarbons formation mechanisms. *M. Oliva-Ramírez, P. Navascués, J. Cotrino, A.R. González-Elipe, A. Gómez-Ramírez*. PÓSTER

X Jornadas de I+D+i & 2nd International Workshop on STEM

19-20 octubre [Sevilla, España]

Nanoestructured ZnO@PVDF hybrid nanogenerator for multisource energy harvesting. *J. Delgado Álvarez, X. García Casas, F.J. Aparicio, V. López Flores, J.R. Sánchez Valencia, A. Barranco, A. Borrás*. COMUNICACIÓN ORAL

Efecto del tratamiento con plasma sobre los procesos de intercambio con el entorno de iones potasio y nitratos en semillas de cebada. *A. Perea Brenes, J.L. García, A.R. González-Elipe, A. Gómez Ramírez, C. López Santos*. COMUNICACIÓN ORAL

Plasma-enabled tripositive polymer for nanogenerators. *G.P. Moreno, T. Czermak, J. Obrero, F.J. Aparicio, A. Barranco*. COMUNICACIÓN ORAL

Environmental stability of perovskite solar cells with water-repellent fluorinated thin films coatings by plasma assisted technology. *F. Núñez-Gálvez, A. Descalzo, L. Contreras Bernal, J.M. Obrero, X. García Casas, A. Borrás, J.R. Sánchez Valencia, C. López-Santos*. COMUNICACIÓN ORAL

Organic nanometric thin films with tailored dielectric properties by remote plasma assisted vacuum deposition. *T. Czermak Álvarez, G.P. Moreno, J.R. Sánchez Valencia, C. López Santos, A. Barranco, F.J. Aparicio*. PÓSTER

13th Asian-European International Conference on Plasma Surface Engineering
05-08 noviembre [Busan, República de Korea]

Multifunctional plasma polymers and supported oxide nanostructures by remote plasma assisted vacuum deposition. *G.P. Moreno, T. Czermak, J. Obrero, F.J. Aparicio, J.R. Sánchez-Valencia, A. Borrás, A. Barranco*. CONFERENCIA INVITADA

Plasma fabrication of piezoelectric ZnO self-powered sensors and nanogenerators on paper. *X. García-Casas, F.J. Aparicio, J. Budagosky, A. Ghaffarinejad, N. Orozco-Corrales, K. Ostrikov, J.R. Sánchez-Valencia, A. Barranco, A. Borrás*. PÓSTER

Electronic Materials and Packaging in Space EMPS
21-23 noviembre [Noordwijk, Paises Bajos]

OSIP activity: Assesing pseudo-hermeticity on ICs with plastic encapsulated materials. *L. Arriaga, G. Fernández, D. Fraser, S. Bernardsky, F.J. Aparicio, A. Barranco*. COMUNICACIÓN ORAL

12th International Symposium on Plasma Nanoscience · iPlasmaNano-XII 2023
05-09 diciembre [Guadeloupe, Francia]

Recent results in remote plasma polymerization from advanced dielectric films to conformal aerogel-like functional oxides. *A. Barranco*. CONFERENCIA INVITADA

Advanced nanogenerators by plasma synthesis of multifunctional thin films and 3D nanoarchitectures. *J.R. Sánchez-Valencia, X. García-Casas, J. Castillo-Seoane, F.J. Aparicio, L. Contreras-Bernal, J. Gil-Rostra, J. Budagosky, V. López-Flores, A. Barranco, A. Borrás*. CONFERENCIA INVITADA

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

XII Reunión del Grupo de Física de la Materia Condensada de la RSEF · GEFES23
01-03 febrero [Salamanca, España]

Nanogenerators and self-powered sensors enabled by plasma and vacuum processing of multifunctional thin films and 3D nanoarchitectures. *X. García-Casas, J. Castillo-Seoane, F.J. Aparicio, A. Ghaffarinejad, L. Contreras-Bernal, J. Gil, J. Budagosky, V. López-Flores, J.R. Sánchez-Valencia, A. Barranco*. CONFERENCIA INVITADA

A coarse-grained approach for growth simulations of metal oxides and polymers on planar/nanostructured substrates. *J. Budagosky, X. García-Casas, J.R. Sánchez-Valencia, A. Barranco, A. Borrás*. PÓSTER

XI Congreso de Jóvenes Investigadores en Polímeros · JIP 2023
02-05 octubre [Alicante, España]

Methodologies for the fabrication of cations-dopped titanium implant coatings. *G. Asensio Martín, A.M. Hernández-Arriaga, M.A. Prieto, A.R. González-Elipe, S. Deb, M.R. Aguilar, B. Vázquez-Lasa, L. Rojo*. PÓSTER

FORMACION / TRAINING

FORMACIÓN DE POSTGRADO / MASTER DEGREE THESIS

Título:	**Desarrollo de nanoconversores de energía cinética y solar**
Autor:	Francisco Javier Martínez Castilla
Tutores:	Juan Ramón Sánchez Valencia, Lidia Contreras Bernal
Grado:	Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro:	Universidad de Sevilla
Fecha Defensa:	06 de septiembre de 2023

Título:	**Fabricación y caracterización de celdas solares de perovskita multistack**
Autor:	Elisa Guisado Arenas
Tutores:	Ángel Barranco Quero, Lidia Contreras Bernal, Rosa María Pereñíguez Rodríguez

Grado: Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro: Universidad de Sevilla
Fecha Defensa: 19 de septiembre de 2023

Título: **Fabricación, caracterización y optimización de nanoestructuras orgánicas 1D soportadas en sustratos planos mediante técnicas de vacío y plasma**
Autor: Juan Manuel Solís Vilches
Tutores: Víctor López Flores, Ana Isabel Borrás Martos
Grado: Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro: Universidad de Sevilla
Fecha Defensa: 30 de noviembre de 2023

FORMACIÓN DE GRADUADOS / BACHELOR DEGREE THESIS

Título: **Producción de hidrógeno en un reactor de plasma de lecho empaquetado**
Autor: Mateo Ruiz Martín
Tutores: Manuel Oliva Ramírez, Ana María Gómez Ramírez
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 23 de junio de 2023

Título: **Desarrollo y caracterización de filtro interferométrico de paso banda variable mediante magnetrón sputtering**
Autor: Pedro Fernández Palmero
Tutores: Pedro Javier Lloreda Jurado, Ana María Gómez Ramírez
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 23 de junio de 2023

Título: **Recubrimiento de óxidos funcionales por técnicas de vacío y plasma sobre implantes de titanio**
Autor: Álvaro Blázquez Martínez
Tutores: Vanda Fortio Godihno
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 27 de junio de 2023

Título:	**Nanopartículas basadas en volframato de manganeso y disprosio para su uso en bioimagen por MRI**
Autor:	Miguel Ángel Mayo Llamas
Tutores:	Nuria Ofelia Núñez Álvarez
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	25 de julio de 2023

Título:	**Synergistic effects of Sr and Cu on mesoporous bioactive glasses for bone regeneration**
Autor:	Diana Rosario Flores
Tutores:	María Aránzazu Díaz Cuenca
Grado:	Trabajo de Investigación · Fulbright Predoctoral Research GS-2022
Centro:	Fulbright España
Fecha Defensa:	14 de junio de 2023

DOCENCIA / TEACHING

MÁSTER EN NANOMATERIALES FUNCIONALES: APLICACIONES EN ENERGÍA, BIOTECNOLOGÍA Y MEDIO AMBIENTE

Preparación de Nanomateriales por Métodos "BOTTOM-UP" II desde fase vapor. Dr. Ángel Barranco Quero, Dr. Francisco Yubero Valencia, Dra. Vanda Cristina Fortio Godinho

Preparación de Nanomateriales por Métodos "TOP-DOWN". Dr. Francisco Javier Aparicio Rebollo, Dr. Juan Ramón Sánchez Valencia, Dra. María del Carmen López Santos

El personal del ICMS imparte docencia en titulaciones de Grado y doble Grado de la Universidad de Sevilla. La docencia se desarrolla en diversos centros: Facultad de Física, Facultad de Biología, Facultad de Química, Facultad de Farmacia y Escuela Técnica Superior de Ingeniería Informática.

ESTANCIAS DE INVESTIGADORES EN EL ICMS
PERSONNEL OF THE OTHER LABORATORIES IN THE ICMS

Universidad Federal de Pernambuco		
Brasil	**Kamilla Veronika Rodrigues de Andrade Silva**	24/11/22 – 31/05/23
Universidad Autónoma de Yucatán		
Mérida, México	**Mahmoud Nabil Hassan Mahmoud**	01/12/22 – 31/05/23

Universidad de Coimbra
Coimbra, Portugal **José David Castro Castro** 02/10/23 – 01/12/23

PREMIOS Y RECONOCIMIENTOS / PRIZES AND ACKNOWLEDGEMENTS

XIII Premios cicCartuja EBRO FOODS

Javier Castillo Seoane

Primer Premio al mejor artículo para Jóvenes Investigadores del cicCartuja por su artículo "Fabricación de nanoestructuras de perovskita altamente anisotrópicas mediante depósito por evaporación térmica en ángulo rasante"
En este estudio, se sintetizaron nanoestructuras de perovskita de haluro altamente anisotrópicas utilizando un nuevo método multietapa de fabricación en vacío. Esta aproximación tiene un gran potencial industrial y es respetuosa con el medioambiente, ya que elimina el uso de disolventes líquidos. Las nanoestructuras exhiben una fotoluminiscencia anisotrópica, con intensidades de emisión de luz polarizada superiores a las reportadas anteriormente. Estas estructuras se implementaron como detectores de polarización autoalimentados, mostrando respuestas dependientes de la polarización de la luz incidente. Este método versátil y eficiente representa un avance tecnológico en el desarrollo de dispositivos optoelectrónicos sensibles a la polarización, con aplicaciones destacables en iluminación y sensores.

Titulo: Highly Anisotropic Organometal Halide Perovskite Nanowalls Grown by Glancing-Angle Deposition
Autores: Javier Castillo Seoane, Lidia Contreras Bernal, Jose Manuel Obrero Pérez, Xabier García Casas, Francisco Lorenzo Lázaro, Francisco Jvier Aparicio, Carmen López Santos, Teresa Cristina Rojas, Juan Antonio Anta, Ana Borrás, Ángel Barranco, Juan Ramón Sánchez Valencia
Revista: *Advanced Materials*, 2022, Vol. **34**, 2107739

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Sistema de magnetron putttering para la preparación de láminas delgadas
- Potenciostato y sistema electroquímico
- Sistema de medida de ángulos de contacto (advancing and receding)
- Equipo de crecimiento en vacío de nanofibras y otros materiales nanoestructurados
- Microscopio de efecto túnel (STM)
- Sistema de desorción térmica programada

- Espectrómetro de Fotoemisión (XPS)
- Colorímetro Dr. Lange: para la medida de parámetros de color (x, y, Y/L*a*b*, etc.) de superficies y polvos
- Ellipsómetro espectroscópico Woolan VB-400 con rango de frecuencias entre 300 y 1700 nm. Medida de índices de refracción y coeficiente de extinción de capas delgadas y superficies.
- Espectrómetro visible-UV CARY-100. Medidas de coeficiente de absorción con luz normal y polarizada.
- Fluorímetro espectroscópico (HORYBA Jobin Yvon Fluorolog) con accesorio para la determinación de tiempos de vida. Microscopio de fluorescencia (HORYBA Jobin Yvon sigle photon controller: FluoroHub).
- Medidor de ángulos de contacto líquidos. Medidas ángulos de avance y retroceso, así como de energías de adhesión de líquidos sobre superficies (Dataphysics Contact Angle System SCA 20).
- Medida de cuatro puntos de conductividad eléctrica en superficies y láminas delgadas (Fuente de corriente Keithley 617 y voltímetro Keithley 2400).
- Medidas eléctricas en capas delgadas en función de la temperatura y la atmósfera
- Microscopio de Fuerzas atómicas (AFM) para la caracterización de superficies (Cervantes de Nanotec).
- Microscopio de efecto túnel (STM) con posibilidad de trabajar desde nitrógeno líquido hasta 600 oC (VT-STM de Omicrom).
- Técnicas de caracterización de plasmas: sonda de Langmuir (Plasma Consult single and double sound), espectroscopía de emisión óptica (Avantes 200-900 nm resolución 1 nm) y espectrometría de masas (Hyden)
- Espectrómetro FT-IR con celda DRIFT (Pelkin elmer Spectrum One)
- Sistema de medida de porosidades en capas delgadas.
- Sistema de desorción térmica programada dotado con espectroscopía Auger (VG-8047).
- Espectrómetro de XPS (espectrómetro VSW) con sistema REELS de alta resolución (Kimball Physics EGPS-1022B) y fuente de átomos incorporada (Oxford Scientific Osprey plasma Source).
- Sistema de tratamiento con plasmas Diener.
- Tres cámaras de deposición por la técnica de pulverización catódica (magnetrón sputtering). Con una dotación total de 7 cabezas magnetrón, 2 fuentes DC, 2 fuentes RF y 1 fuente pulsada, portamuestras girables, calentables y "biased".
- Material básico de laboratorio químico: PHmetro, agitadores, calefactores, estufa de secado a vacío, centrífuga.
- Reactores y material de vidrio convencional para síntesis de nanopartículas y catalizadores por via química.
- Rotavapor, sistemas de filtrado.
- Cámara seca MBRAUN.
- Dos campanas extractoras.
- Reactores catalíticos de lecho fijo para catálisis heterogénea sólido-gas.
- Reactores catalíticos para catálisis heterogénea sólido-líquido.
- Sistemas controladores de flujo másico (gases y líquidos evaporados), bombas peristálticas para líquidos.
- Tres cromatógrafos de gases, columnas y detectors FID y TCD.
- Sistema de medida de espectroscopía de impedancia compleja, formado por un impedancímetro Agilent modelo 4294ª, un horno Hobersal ST115020, y una celda de medida hermética para la realización de medidas en atmósfera.
- Buretas automáticas para medición de gases.
- Sistema de preparación de muestras en película delgada TXP de Leica.

- Pulidora, trípode y microscopio óptico.
- TEM de 300kV Tecnai F30 dotado de modo STEM, detector HAADF, analizador EDX Oxford Max80 y filtro de energías GIF Quantum.
- Tribómetro CSM (movimiento lineal y rotativo) para evaluación de coeficientes de fricción y desgaste.
- Tribómetro de alta temperatura (hasta 800 oC) –Microtest
- Calotest para medida de espesores y evaluación del desgaste.
- Equipo de rayado (Scratch-test) hasta 200N (Tribotechnic).
- Perfilómetro-rugosímetro (Mahr) de tipo táctil y resolución vertical nanométrica.
- Cámara de deposición PVD-Magnetron sputtering (2 magnetron).
- Fuentes DC-Pulsada (ENI) ; RF (Trumpf); HiPIMS (Solvix)
- Horno tubular 1500 oC (Carbolite)
- Pulidora
- Ultrasonidos
- Microscopio óptico (Leica)
- Microscopio óptico Interferométrico 3D (Sensofar)

MATERIALES ÓPTICOS
OPTICAL MATERIALS

GRUPOS DE INVESTIGACIÓN

Materiales Coloidales | 642011
Colloidal Materials
http://colmat.icmse.csic.es

Materiales Ópticos Multifuncionales | 642013
Multifunctional Optical Materials
http://mom.icmse.csic.es

Materiales Semiconductores para la Sostenibilidad | 6944952
Semiconductor Materials for Sustainability

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PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Materiales ópticos basados en nanofósforos para la próxima generación de dispositivos emisores de luz

Nanophosphor-based photonic materials for next generation light-emitting devices · NANOPHOM

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
H2020-ERC-STG/0259	01-04-2017 31-03-2023	Comisión Europea	1.499.739 €

Investigador Principal Research Head
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RESUMEN / ABSTRACT

El desarrollo de fuentes de luz eficientes y respetuosas con el medio ambiente constituye una parte esencial de la estrategia mundial para reducir el consumo mundial de electricidad. Los diodos emisores de luz (LED de sus siglas en inglés) emergen como la alternativa a la iluminación convencional, debido a su alta eficiencia de conversión de energía, larga vida útil, conmutación rápida, robustez y tamaño compacto. Sin embargo, su implementación en la industria electrónica de consumo se ve obstaculizada por el control limitado sobre el brillo, la calidad del color y la direccionalidad de la emisión de LED que proporcionan los elementos ópticos convencionales cuyo funcionamiento se basa en la óptica geométrica.

Este proyecto explora nuevas formas de controlar las propiedades de emisión de nanomateriales luminiscentes, superando los límites impuestos por la óptica convencional, mediante el uso de arquitecturas nanofotónicas. El desarrollo de materiales ópticos fiables y escalables basados en nanofósforos permitirá un control espectral y angular fino sobre la emisión de luz, abordando las deficiencias que los LED actuales presentan. El nuevo diseño óptico de estos dispositivos estará basado en la integración de multicapas ópticas, texturas superficiales, y nano dispersores de composición, tamaño y forma controlados, para obtener materiales que posean propiedades ópticas que faciliten un control preciso de la radiación visible.

Nanophom permitirá mejorar nuestra comprensión sobre fenómenos fundamentales como la formación de modos fotónicos en medios ópticos complejos a los que se puede acoplar la luz, así como avanzar en el desarrollo de dispositivos de iluminación de estado sólido de alta eficiencia.

Energy-efficient and environmentally friendly light sources are an essential part of the global strategy to reduce the worldwide electricity consumption. Light-emitting diodes (LEDs) emerge as a key alternative to conventional lighting, due to their high power-conversion efficiency, long lifetime, fast switching, robustness, and compact size. Nonetheless, their implementation in the consumer electronic industry is hampered by the limited control over brightness, colour quality and directionality of LED emission that conventional optical elements relying on geometrical optics provide.

This project exploits new ways of controlling the emission characteristics of nanophosphors, surpassing the limits imposed by conventional optics, through the use of nanophotonic concepts. The development of reliable and scalable nanophosphor-based photonic materials will allow ultimate spectral and angular control over the light emission properties, addressing the critical shortcomings of current LEDs. The new optical design of these devices will be based on multilayers, surface textures and nano-scatterers of controlled composition, size and shape, to attain large-area materials possessing photonic properties that will enable a precise management of the visible radiation.

Nanophom will significantly advance our comprehension of fundamental phenomena like the formation of photonic modes in complex optical media to which light can couple, as well as advancing the state of the art of high-efficiency solid-state lighting devices.

PHOTOelectrocatalytic systems for Solar fuels energy INTegration into the industry with local resources

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
HORIZON-CL5-2022-D3-02-06	01-09-2023 31-08-2027	Comisión Europea	339.200 €

Investigador Principal Research Head
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ABSTRACT

The PHOTOSINT project presents solutions to the challenges chemical industries are facing in integrating renewable energy sources into their processes. The project will deliver sustainable processes to produce hydrogen and methanol as energy vectors using only sunlight as an energy source and wastewater and CO_2 as feedstocks, making the industries more auto-sufficient. The pathway is based on solar-driven artificial photosynthesis, and aims to develop new catalytic earth-abundant materials and modifications of existing ones to improve catalytic processes. Design parameters of the PEC cell will be tuned to maximize solar to fuel (STF) efficiency. Moreover to improve the conversion for industrial

implementation, PHOTOSINT will develop a novel way to concentrate and illuminate the semiconductor surface to maximize overall energy efficiency. Perovskite solar PV cells will be integrated to harvest the light to supply the external electrical voltage.

PHOTOSINT is an ambitious project due to precedents in research conducted to date and the low production rate of the desired products. For integrating sunlight energy into the industry, the catalyst will be studied, and then the best one/s will be implemented in prototypes. The obtained results will be used for making scale-up in pilots with tandem PEC cells. These steps are necessary to assess the industrial scale-up feasibility, promoting the increased competitiveness of renewable process energy technologies and energy independence. MeOH and H_2 will be tested in engines. Also, an HTPEM fuel cell will be used for electricity generation, and hydrogen will be tested as an alternative fuel for energy generation instead natural gas in melting furnaces avoiding CO_2 emissions.

PERovskite SEmiconductors for PHOtoNics

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
H2020-MSCA-ITN-ETN/0748	01-03-2021 28-02-2025	Comisión Europea	250.904,88 €

Investigador Principal Research Head
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ABSTRACT

Funded by the Marie Skłodowska-Curie programme, PERSEPHONe is a coordinated training network that aims to equip young researchers with new skills and knowledge regarding the development of a novel photonics technological platform based on metal-halide perovskite semiconductors. These materials present unrivalled optoelectronic properties and can be engineered to achieve a large set of desirable functionalities which may change the roadmap of currently established photonic technologies. They also show great promise for their integration with silicon photonics and silicon-oxynitride-based photonics. The programme will expose 14 early-stage researchers to a wide spectrum of research activities including material synthesis, photonic (and optoelectronic) device and integrated circuit fabrication, characterisation, modelling, upscaling and manufacturing. PERSEPHONe will lay the foundation for a novel photonic technology, strengthening Europe's position in the field.

Materiales fotónicos para mejorar el proceso de aftergow en láminas delgadas transparentes con luminiscencia persistente Photonic materials boost afterglow in transparent luminescence thin films

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
EUR2023-143467	01-12-2023 30-11-2025	Ministerio de Ciencia e Innovación	100.000 €

Investigador Principal Research Head
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RESUMEN / ABSTRACT

Los materiales con luminiscencia persistente (PersL) son capaces de almacenar energía óptica en defectos estructurales que actúan como trampas y generar luz mucho después de que desaparezca la fuente de excitación, i.e. en el afterglow, lo que permite introducir el tiempo como un elemento de diseño más en nuevas soluciones de iluminación. A pesar de las ventajas asociadas a la reducción de tamaño, las propiedades de los nanomateriales persistentes distan mucho de las de sus homólogos másicos. PHLOW busca encontrar nuevas formas de controlar la PersL mediante el diseño del entorno óptico de los emisores, un camino inexplorado hasta hoy. Para ello, se propone procesar láminas delgadas transparentes con PersL para su integración en arquitecturas fotónicas con el fin de optimizar el proceso de carga y mejorar la cantidad de luz emitida durante el afterglow. Es relevante destacar que los procesos de almacenamiento de carga y emisión compiten entre sí. Es decir, a medida que las trampas se llenan, también se vacían parcialmente en un proceso dinámico. Sin embargo, no existe ninguna estrategia diseñada específicamente para alterar el proceso de carga o aumentar el nivel de ocupación de las trampas. Al mismo tiempo, la tasa de desexcitación radiativa de una transición depende del entorno óptico a través de la densidad local de estados ópticos. Por este motivo, se espera que el diseño óptico tenga un impacto, además de sobre el mecanismo de outcoupling, sobre el proceso intrínseco de generación de luz, lo que debe permitir alterar el equilibrio de población de trampas, afectando a la cinética de carga y a la intensidad de la PersL. Así, se plantea como objetivo general el estudio del impacto que los cambios en el entorno óptico producen en los procesos de almacenamiento de energía y emisión de luz persistente para señalar el potencial del diseño óptico como herramienta para controlar la PersL en láminas delgadas transparentes. Este enfoque, naturalmente interdisciplinario, tendrá un profundo impacto científico, ya que nunca se ha explorado la fotónica para controlar los mecanismos de carga y emisión que determinan la PersL, pero también tecnológico, ya que permite el desarrollo de fuentes de luz dependientes del tiempo para impulsar conversores de color más versátiles, etiquetas inteligentes, recubrimientos novedosos para la lucha contra la falsificación o el almacenamiento óptico de datos.

Persistent luminescent (PersL) materials are able to store optical energy in structural defects that act as traps and generate light long after the excitation source disappears, i.e. afterglow, allowing the introduction of time as a design element in new lighting solutions. Despite the advantages associated with size reduction, the properties of persistent nanomaterials are far from those of their bulk counterparts. PHLOW seeks to find new ways to control PersL by designing the optical environment of emitters, a path unexplored until today. To this end, it is proposed to process transparent thin films with PersL for integration into photonic architectures in order to optimize the charging process and improve the amount of light emitted during the afterglow. It is relevant to note that the charge storage and emission processes compete with each other. That is, as the traps are filled, they are also partially emptied in a dynamic process. However, there is no strategy specifically designed to alter the charging process or increase the population of the traps. At the same time, the radiative de-excitation rate of a transition depends on the optical environment through the local density of optical states. For this reason, the optical design is expected to have an impact, in addition to the outcoupling mechanism, on the intrinsic process of light generation, which should allow altering the trap population balance, affecting the charge kinetics and the intensity of the PersL. Thus, the general objective is to study the impact of changes in the optical environment on the processes of energy storage and persistent light emission in order to highlight the potential of optical design as a tool to control PersL in transparent thin films. This naturally interdisciplinary approach will have a profound scientific impact, as photonics has never been explored to control the charge and emission mechanisms that determine PersL, but also technological, as it enables the development of timedependent light sources to drive more versatile color converters, smart labels, novel coatings for anti-counterfeiting or optical data storage.

Análisis fotofísico de parámetros que afectan a la eficiencia y la estabilidad de celdas solares de perovskita procesadas en seco: procesos de activación y degradación

Photophysical análisis of parameters affecting efficiency and stability of dry processed metal halide perovskite solar cells: activation and degradation processes

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
TED2021-129679B-C22	01-12-2022 30-11-2024	Ministerio de Ciencia e Innovación	302.500 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

La caracterización fotofísica avanzada ha demostrado ser una herramienta clave en el estudio de las propiedades optoelectrónicas de las perovskitas de metal-haluro. Durante la última década, las medidas de emisión y absorción resueltas en el tiempo han revelado la fotofísica única de este material y han contribuido a explicar tanto su excelente rendimiento en dispositivos fotovoltaicos y emisores de luz como sus principales limitaciones, como la inestabilidad del material. En consecuencia, esta caracterización se ha utilizado como una guía para la fabricación de materiales más allá de los enfoques basados en prueba y error, y han contribuido a convertir las perovskitas en la tecnología fotovoltaica de más rápido crecimiento en la actualidad. En este sentido, la caracterización óptica avanzada se empleará en el presente subproyecto (ESPER2) para llevar los dispositivos fotovoltaicos de evaporación térmica un paso más cerca del rendimiento óptimo en términos de eficiencia y estabilidad. Se realizará una combinación de caracterización óptica en estado estacionario y resuelta en tiempo en films y dispositivos de perovskita para comprender los factores que afectan a su rendimiento: la presencia de defectos en la red cristalina (y los medios para evitarlos a través de cambios en la composición y agentes pasivantes), la transferencia de carga desde la perovksita a las capas transportadoras adyacentes y la presencia de procesos fotoinducidos (como degradación y fotoactivación), así como la posibilidad de utilizar estos últimos como medio para mejorar las propiedades optoelectrónicas del material. Más allá de extraer información crítica sobre la recombinación y el transporte de carga, se llevará a cabo un diseño óptico para optimizar la recolección de luz dentro del dispositivo que emplee los materiales de mejor rendimiento. La caracterización propuesta ayudará a acercar una tecnología susceptible de ser utilizada para la producción en masa, como la deposición al vacío, a las demandas del mercado en términos de eficiencia y durabilidad.

Advanced photophysical characterization has proven to be a key tool in the study of the optoelectronic properties of metal halide perovskites. Over the past decade time-resolved absorption and emission measurements have unveiled the unique photophysics of this material and have contributed to explain both, their outstanding performance in light harvesting and emitting devices but also its main limitations, such as material instability. These measurements have thus been used as a means to guide materials fabrication beyond trial and error approaches and have contributed to turning perovskites into the fastest growing photovoltaic technology. In this regard, advanced optical characterization will be employed in the present subproject (ESPER2) to bring vacuum thermal evaporated PV devices one step closer to the optimal performance in terms of efficiency as well as stability. A combination of steady state and time-resolved optical characterization experiments will be performed on perovskite films, architectures and devices in order to understand those factors affecting its performance: the presence of crystalline defects (and means to avoid them via compositional changes and passivating agents), the transfer of charges from the perovskite to adjacent charge transporting layers and the presence of photo-induced processes (such as photo activation and degradation) as well as the possibility of using the latter as a means to improve the materials optoelectronic properties. Beyond extracting critical information regarding charge recombination and transport, an optical design will be carried out in order to optimize light harvesting within the device comprising the best performing materials. The proposed characterization will thus help bringing a technology amenable to be used for mass production, such as vacuum deposition, closer to the market demands in terms of efficiency and durability.

Diseño óptico optimizado de dispositivos optoelectrónicos basados en puntos cuánticos de perovskita sin ligandos Optimized photonic design of ligand-free perovskite quantum dot based optoelectronic devices

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2020-116593RB-I00	01-09-2021 31-08-2024	Ministerio de Ciencia e Innovación	302.500 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

La motivación del proyecto FreeDot es triple. Primero, proponer soluciones a los inconvenientes específicos que obstaculizan un mayor desarrollo de la tecnología optoelectrónica de perovskita (inestabilidad, durabilidad, sensibilidad ambiental, etc.). La aproximación propuesta se basa en el desarrollo de células solares nanoestructuradas y LED basados en nuevas matrices porosas que permiten la síntesis de ensamblados de nanocristales sin ligandos con buenas propiedades de transporte de carga y, simultáneamente, minimizan su exposición a entornos degradantes. En segundo lugar, demostrar que es posible, también en el caso de dispositivos basados en puntos cuánticos, mejorar la eficiencia de conversión de energía en células solares y de extracción de luz en LEDs mediante la optimización del diseño óptico. Por último, la posibilidad de obtener nanocristales libres de ligandos abre la posibilidad de estudiar las propiedades fotofísicas fundamentales de los puntos cuánticos, lo que normalmente es obstaculizado por la presencia de capas orgánicas en el caso de puntos cuánticos coloidales.

The motivation of the FreeDot project is three-fold. First, to propose solutions to the specific drawbacks hindering further development of perovskite optoelectronic technology (instability, durability, environmental sensitivity, etc.) by developing nanostructured solar cells and LEDs based on novel porous scaffolds that permit the synthesis of ligand-free nanocrystal assemblies, which show dot-to-dot charge transport while, simultaneously, minimizing their exposure to degrading environments. Second, to prove that improved power conversion efficiency, in the case of solar cells, and enhanced outcoupling and control over the spectral and directional properties of the emitted light, in the case of LEDs, are achievable through the optimization of the optical design also for quantum dot based devices. Finally, the synthesis of ligand-free nanocrystals opens the possibility to study fundamental photophysical properties of quantum dots, which are hindered by the presence of organic cappings in colloidal nanocrystals.

Perovskitas de haluro libres de ligando en GaN poroso para aplicaciones de emisión de luz de nueva generación Ligand Free Halide Perovskites in Porous GaN for Next Generation Light Emission Applications · PEROGAN

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2022-142525OA-I00	01-09-2023 31-08-2026	Ministerio de Ciencia e Innovación	126.250 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

PEROGAN propone un material disruptivo mediante el crecimiento de emisores de perovskita de haluro dentro de los poros de GaN nanoestructurado. El proyecto estará impulsado por el modelado óptico y la visualización de las propiedades del material donde la interacción entre la fotofísica, la composición y la estructura se controlará a nanoescala. Perovskitas de haluro tolerantes a defectos se combinarán con GaN de alto rendimiento de forma monolítica. Este proyecto cimentará futuros logros científicos en los que LED operativos y rentables con emisión a la carta podrán cubrir aplicaciones fotónicas como iluminación, imagen y detección.

PEROGAN proposes a material disruption by growing halide perovskite emitters within nanostructured GaN pores. The project will be driven by the optical modelling and visualisation of the material properties where the interplay between photophysics, composition and structure will be controlled at the nanoscale. Defect tolerant, soft perovskite materials will be combined with highly performing GaN in a monolithic fashion. This project will lay the foundations for future scientific achievements where operating, cost-effective LEDs with output a la carte will be able to cover photonic applications such as lighting, imaging and sensing.

Biosondas basadas en lantánidos para la obtención de bioimagen mediante resonancia magnética y luminiscencia persistente

Lanthanide-based bioprobes for MRI and persistent luminescence imaging

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2021-122328OB-I00	01-09-2022 31-08-2025	Ministerio de Ciencia e Innovación	99.220 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El objetivo general de este proyecto es el desarrollo de nuevos agentes de contraste (CAs) para mejorar el diagnóstico médico mediante el uso de dos técnicas avanzadas de imagen como la resonancia magnética (MRI) y la imagen luminiscente. Específicamente, se planea desarrollar CAs de MRI duales (T1-T2) y sondas con luminiscencia persistente (PersL). La obtención de dos imágenes de resonancia (denominadas imagen promediada en T1 y en T2) es muy útil pues ayuda a eliminar falsos positivos mediante la validación cruzada de ambas. La ventaja de los agentes de contraste de MRI duales frente a los simples es que un único agente permite obtener los dos tipos de imágenes, evitando así la exposición del paciente a dos agentes externos. Por su parte, el empleo de sondas con PersL para la obtención de imagen luminiscente permite mejorar notablemente la relación señal ruido de la imagen puesto que, al irradiar la sonda fuera del organismo, se evita la autofluorescencia de los tejidos biológicos. Además, la eliminación de la irradiación directa (normalmente luz ultravioleta) evita daños a dichos tejidos. Ambos tipos de CAs (MRI y PersL) consistirán en nanopartículas (NPs) uniformes de diversas matrices inorgánicas cuidadosamente seleccionadas basadas en cationes lantánidos, cuyas propiedades magnéticas y luminiscentes los hacen ideales para las aplicaciones perseguidas. En cuanto a los CAs de MRI, se abordarán dos tipos de arquitecturas consistentes en NPs de fase única, donde los lantánidos activos en T2 (Dy^{3+}) y en T1 (Gd^{3+} o Mn^{2+}) se encuentran en disolución sólida, y NPs con arquitectura core-shell, donde los iones T2 se localizan en el núcleo y los T1, en la corteza. En ambos casos, se ensayarán matrices de fosfato, vanadato y molibdato, que han mostrado ser adecuadas en el caso de CAs de MRI simples. Por su parte, en el caso de las sondas para imagen luminiscente se planea sintetizar, en forma de NPs uniformes, diversos compuestos que han mostrado excelente luminiscencia persistente pero que hasta el momento solo se han fabricado en forma másica, no adecuada para aplicaciones biomédicas. Concretamente se abordarán diversas matrices de germanato y galato dopadas con iones lantánidos (Pr^{3+}, Yb^{3+}) que emiten luz infrarroja dentro de las ventanas biológicas, donde la radiación no es absorbida por los tejidos biológicos, aumentando así su capacidad de penetración y facilitando por tanto la obtención de la bioimagen. Ambos tipos de NPs (CAs duales T1-T2 y NPs con PersL) serán sometidas

a procesos de funcionalización y bioconjugación para para dotarlas de estabilidad coloidal y de capacidad de reconocimiento de tumores específicos. Se analizará asimismo su biocompatibilidad mediante el análisis de la citotoxicidad y, finalmente, los CAs óptimos se aplicarán en la obtención de imagen de resonancia magnética e imagen luminiscente, in vitro e in vivo, utilizando ratones como modelo. El equipo investigador posee sobrada experiencia en la síntesis de NPs inorgánicas basadas en elementos lantánidos y dispone de la mayoría de los medios necesarios para su caracterización morfológica, estructural y química, así como para el estudio de sus propiedades luminiscentes. Además, dicho equipo cuenta con el apoyo de investigadores de otras instituciones que colaborarán en el desarrollo de algunas tareas del proyecto relacionadas con los estudios de bioconjugación, biocompatibilidad y registro de imagen, lo que garantiza el correcto desarrollo del mismo.

The overall objective of this project is the development of new contrast agents (CAs) to improve medical diagnostics using two advanced imaging techniques such as magnetic resonance imaging (MRI) and persistent luminescence (PersL) imaging. Specifically, it is planned to develop dual MRI (T1-T2) CAs and PersL bioprobes. The advantage of dual MRI CAs over classical MRI CAs is that they allow two types of resonance images (T1-and T2 weighted images) to be obtained with a single agent. Obtaining both images is very useful as it allows avoiding false positives by cross-validation of both images. On the other hand, the use of probes with PersL significantly improves the signal-to-noise ratio of the luminescence image since, by irradiating the probe outside the organism, autofluorescence of the tissues is avoided. An additional advantage of this type of luminescent probes is that they avoid direct irradiation of living tissues with harmful ultraviolet light. Both types of CAs (MRI and PersL CAs) will consist of uniform nanoparticles (NPs) based on various carefully selected inorganic matrices containing lanthanide ions, whose excellent magnetic and luminescent properties make them ideal candidates for the pursued applications. For MRI CAs, two types of architectures will be addressed, consisting of single-phase nanoparticles (NPs), where the T2 (Dy^{3+}) and T1 (Gd^{3+} or Mn^{2+}) active cations are in solid solution, and NPs with core-shell architecture, where the T2 ions will be located in the core while the active ions for T1 imaging will be located in the shell. In both cases, phosphate, vanadate and molybdate matrices will be tested, which have been shown to be suitable in the case of T1 or T2 single MRI CAs. In the case of PersL probes, several compounds that have shown excellent luminescence properties in terms of both intensity and persistence duration as bulk materials, will be synthesized as uniform NPs. Specifically, various germanate and gallate matrices doped with lanthanide ions (Pr^{3+}, Yb^{3+}), that emit infrared light within the biological windows, where the radiation is not absorbed by biological tissues or fluids thus improving the penetration depth, will be addressed. Both types of CAs (MRI and PersL CAs) will be submitted to functionalization and bioconjugation processes to provide them with colloidal stability and tumor-specific recognition capabilities. Their biocompatibility will also be tested by studying their cytotoxicity in specific cell lines. Finally, the optimal probes obtained will be applied to MRI and PersL imaging, both in vitro and in vivo, using mice as a model. The research team has extensive experience in the synthesis of lanthanide-based inorganic NPs and has most of the necessary means for their morphological, structural and chemical characterization, as well as for the study of their luminescent properties. In addition, this team has the support of researchers from other institutions who will collaborate in the development of some of the tasks, mainly with regard to bioconjugation, biocompatibility and image recording studies, which guarantees the correct development of the project.

Nuevos agentes de contraste multimodales para el diagnóstico médico por imagen
New multimodal contrast agents for medical diagnostic imaging

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P20_00182	05-10-2021 30-06-2023	Junta de Andalucía	82.050 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El proyecto persigue el diseño de agentes de contraste (CAs) multimodales para el registro de imágenes para diagnóstico médico. Estos CAs estarán constituidos por nanopartículas inorgánicas basadas en lantánidos con propiedades adecuadas para el registro de imágenes mediante técnicas complementarias, con objeto de obtener información esencial para un diagnóstico médico más riguroso sin necesidad de inyectar al paciente CAs específicos para cada técnica. Una ventaja adicional de las sondas propuestas respecto a los CAs comerciales es que permiten controlar el tiempo de residencia en el organismo y su biodistribución y, por tanto, disminuir las dosis necesarias, resultando en un claro beneficio para el paciente. En concreto, se desarrollarán agentes de contraste para resonancia magnética (MRI) dual con funcionalidad adicional como agentes de contraste para tomografía computarizada de rayos X (CT) e imagen luminiscente en la región del infrarrojo cercano (NIR) conocida como ventana biológica (650-1800 nm), en la que las radiaciones no son dañinas para los tejidos y tienen alto poder de penetración en los mismos. Se ensayarán varias composiciones: fosfatos, vanadatos, molibdatos y wolframatos de elementos lantánidos tales como el Gd, Dy y Ho, que aportarán la funcionalidad magnética y cuyo alto número atómico es óptimo para CT. El dopado de todas ellas con Nd^{3+} permitirá la obtención de imágenes luminiscentes en el NIR. La exploración de la aplicabilidad de dichas sondas al campo del diagnóstico médico por imagen se llevará a cabo mediante la obtención de imagen "in vivo" en ratones.

The project aims to design multimodal contrast agents (CAs) for medical diagnostic imaging. The CAs will consist of lanthanide-based inorganic nanoparticles with properties suitable for different bioimaging techniques. The CAs developed will allow obtaining a more rigorous medical diagnosis without the need to inject the patient with several technique-specific CAs. An additional advantage of the proposed probes over commercial CAs is that they allow control of the residence time in the body and their biodistribution, and thus reduce the doses needed, resulting in a clear benefit for the patient. Specifically, dual magnetic resonance imaging (MRI) CAs will be developed with additional functionality

as contrast agents for X-ray computed tomography (CT) and luminescence imaging in the near-infrared (NIR) region known as the biological window (650-1800 nm), where radiation is not harmful to tissues and has high tissue penetration power. Several compositions will be tested: phosphates, vanadates, molybdates, and wolframates of lanthanide elements such as Gd, Dy, and Ho, which will provide the magnetic functionality and whose high atomic number is optimal for CT. Doping all of them with Nd^{3+} will allow luminescent imaging in the NIR. The applicability of these probes to medical imaging will be explored by in vivo imaging in mice.

Influencia del entorno óptico en nanomateriales con luminiscencia persistente: una nueva herramienta para el diseño de nanobaterías de luz Influence of the optical environment on persistent luminescence nanomaterials: A new tool for the design of nanobatteries of light

Fundación BBVA RED LEONARDO

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
2023070001	19-05-2023 19-11-2024	Fundación BBVA	40.000 €

Investigador Principal Research Head
Gabriel S. Lozano Barbero

RESUMEN / ABSTRACT

El desarrollo de las sociedades está ligado a su capacidad para generar luz artificial, desde las antorchas hasta los omnipresentes diodos emisores de luz (LED) actuales. Los materiales con luminiscencia persistente (PersL) son capaces de almacenar energía óptica en defectos estructurales y generar luz mucho después de que desaparezca la fuente de excitación, lo que los convierte en baterías de luz. Son, por ejemplo, los que se utilizan para las señales de emergencia, que se iluminan en la oscuridad; o los que se emplean para los adhesivos fluorescentes que se colocan en el paredes y techo a modo de decoración. Desde hace unos años estos materiales se pueden crear en la nanoescala, mucho más pequeños. A pesar de las ventajas asociadas a la reducción de tamaño, las propiedades de los nanomateriales persistentes distan mucho de las de sus homólogos másicos empleados en señalización u ornamentación. Esta propuesta persigue integrar nanomateriales con PersL en láminas delgadas transparentes y caracterizar de forma precisa la cinética de carga y la cantidad de luz emitida durante el afterglow en función del entorno óptico de los recubrimientos. Nunca se ha explorado la fotónica para controlar los mecanismos de carga y emisión que determinan la PersL, lo que puede tener un impacto en el desarrollo de conversores de color más versátiles, etiquetas inteligentes, elementos contra la falsificación o el almacenamiento óptico de datos.

The development of societies is linked to their ability to generate artificial light, from torches to today's ubiquitous light-emitting diodes (LEDs). Persistent luminescence (PersL) materials are able to

store optical energy in structural defects and generate light long after the excitation source disappears, making them batteries of light. Despite the advantages associated with size reduction, the properties of persistent nanomaterials are far from those of their bulk counterparts used in signaling or ornamentation. This proposal pursues to integrate PersL nanomaterials into transparent thin films and to precisely characterize the charging kinetics and the amount of light emitted during afterglow as a function of the optical environment of the coatings. Photonics has never been explored to control the charging and emission mechanisms that determine PersL, which may have an impact on the development of more versatile color converters, smart labels, anti-counterfeiting elements or optical data storage.

Detectores de Rayos X basados en compuestos de perovskita X-ray detectors based on perovskite composites

Fundación BBVA RED LEONARDO

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
LEO23-11319	01-10-2023 31-03-2025	Fundación BBVA	40.000 €

Investigador Principal Research Head
Miguel Anaya Martín

RESUMEN / ABSTRACT

Las imágenes médicas obtenidas mediante tomografía axial computarizada (TAC) podrían volverse mucho más precisas gracias a los detectores de conteo de fotones. Sin embargo, los materiales que se emplean actualmente para fabricar estos detectores, basados en el cadmio, requieren una pureza extremadamente difícil, y por tanto económicamente costosa de conseguir. El proyecto propone emplear un material alternativo – la perovskita de haluro- y encapsularlo en una red porosa para reducir considerablemente los costes de producción y facilitar la escalabilidad de estos detectores, logrando así que se vuelvan universales en las imágenes por TAC.

Photon counting detectors have the potential to transform how we obtain CT scans to achieve low dose, high resolution images for medical diagnosis and monitoring. However, the materials currently used to manufacture these detectors require extremely high purity and are, therefore, economically expensive to achieve, limiting their widespread adoption. This project will employ perovskite composites to considerably reduce production costs and facilitate the scalability of direct X-ray detectors, thus opening avenues to making them universal in CT imaging.

OTROS PROYECTOS / OTHER PROJECTS

Desarrollo de Dispositivos Emisores de Luz basados en Perovskita Nanoestructurada

Código/Code:	201960E090
Periodo/Period:	01-09-2019 / 31-08-2024
Organismo Financiador/Financial source:	CSIC (Intramural)
Importe total/Total amount:	187.789 €
Investigador responsable/Research head:	Hernán Míguez García

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Diseño y realización de filtros dicroicos para aplicaciones en energía solar

Periodo/Period:	01-01-2023 / 31-12-2024
Organismo Financiador/Financial source:	BLUESOLAR FILTERS, SL
Importe total/Total amount:	151.250 €
Investigador responsable/Research head:	Hernán Míguez García

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Inkjet-Printed and Nanopatterned Photonic Phosphor Motifs with Strongly Polarized and Directional Light-Emission

Cabello-Olmo, E; Romero, M; Kainz, M; Bernroitner, A; Kopp, S; Muhlberger, M; Lozano, G; Mïguez, H
Advanced Functional Materials, **33** (2023) 2305907
Agosto, 2023 · DOI: 10.1002/adfm.202305907

Herein a versatile and scalable method to prepare periodically corrugated nanophosphor surface patterns displaying strongly polarized and directional visible light emission is demonstrated. A combination of inkjet printing and soft lithography techniques is employed to obtain arbitrarily shaped light emitting motifs. Such predesigned luminescent drawings, in which the polarization and angular properties of the emitted light are determined and finely tuned through the surface relief, can be used as anti-counterfeiting labels, as these two specific optical features provide additional means to identify any unauthorized or forged copy of the protected item. The potential of this approach is exemplified by processing a self-standing photoluminescent quick response code whose emission is both polarized and directionally beamed. Physical insight of the mechanism behind the directional out-coupled photoluminescence observed is provided by finite-difference time-domain calculations.

Highly Nonstoichiometric YAG Ceramics with Modified Luminescence Properties

Cao, WW; Becerro, AI; Castaing, V; Fang, X; Florian, P; Fayon, F; Zanghi, D; Veron, E; Zandona, A; Genevois, C; Pitcher, MJ; Allix, M
Advanced Functional Materials, **33** (2023) 2213418
Enero, 2023 · DOI: 10.1002/adfm.202213418

$Y_3Al_5O_{12}$ (YAG) is a widely used phosphor host. Its optical properties are controlled by chemical substitution at its YO_8 or AlO_6/AlO_4 sublattices, with emission wavelengths defined by rare-earth and transition-metal dopants that have been explored extensively. Nonstoichiometric compositions $Y_{3+x}Al_{5-x}O_{12}$ (x not equal 0) may offer a route to new emission wavelengths by distributing dopants over two or more sublattices simultaneously, producing new local coordination environments for the activator ions. However, YAG typically behaves as a line phase, and such compositions are therefore challenging to synthesize. Here, a series of highly nonstoichiometric $Y_{3+x}Al_{5-x}O_{12}$ with $0 <= x <= 0.40$ is reported, corresponding to <= 20% of the AlO_6 sublattice substituted by Y^{3+}, synthesized by advanced melt-quenching techniques. This impacts the up-conversion luminescence of Yb^{3+}/Er^{3+}-doped systems, whose yellow-green emission differs from the red-orange emission of their stoichiometric counterparts. In contrast, the YAG:Ce^{3+} system has a different structural response to nonstoichiometry and its down-conversion emission is only weakly affected. Analogous highly nonstoichiometric systems should be obtainable for a range of garnet materials, demonstrated here by the synthesis of $Gd_{3.2}Al_{4.8}O_{12}$ and $Gd_{3.2}Ga_{4.8}O_{12}$. This opens pathways to property tuning by control of host stoichiometry, and the prospect of improved performance or new applications for garnet-type materials.

Non-sticky interactions

Esteso, V
Nature Physics, **19** (2023) 161-162
Febrero, 2023 · DOI: 10.1038/s41567-022-01935-y

Quantum mechanical fluctuations of the electromagnetic field in a vacuum between two close together objects result in an attractive force. Now, it has been experimentally shown that by exploiting a similar repulsive interaction, attraction between objects can be modulated simply by tuning temperature.

Lanthanide vanadate-based trimodal probes for near-infrared luminescent bioimaging, high-field magnetic resonance imaging, and X-ray computed tomography

Gómez-González, E; González-Mancebo, D; Núñez, NO; Caro, C; Garcia-Martin, ML; Becerro, AI; Ocaña, M
Journal of Colloid and Interface Science, **646** (2023) 721-731
Septiembre, 2023 · DOI: 10.1016/j.jcis.2023.05.078

We have developed a trimodal bioimaging probe for near-infrared luminescent imaging, high-field magnetic resonance imaging, and X-ray computed tomography using Dy^{3+} as the paramagnetic component and Nd^{3+} as the luminescent cation, both of them incorporated in a vanadate matrix. Among different essayed architectures (single phase and core-shell nanoparticles) the one showing the best luminescent properties is that consisting of uniform $DyVO_4$ nanoparticles coated with a first uniform layer of $LaVO_4$ and a second layer of Nd^{3+}-doped $LaVO_4$. The magnetic relaxivity (r2) at high field (9.4 T) of these nanoparticles was among the highest values ever reported for this kind of probes and their X-ray attenuation properties, due to the presence of lanthanide cations, were also better than those of a commercial contrast agent (iohexol) commonly used for X-ray computed to-mography. In addition, they were chemically stable in a physiological medium in which they could be easily dispersed owing to their one-pot functionalization with polyacrylic acid, and, finally, they were non-toxic for human fibroblast cells. Such a probe is, therefore, an excellent multimodal contrast agent for near-infrared

Carboxylate functionalized $NaDy(MoO_4)_2$ nanoparticles with tunable size and shape as high magnetic field MRI contrast agents

Gómez-González, E; Nuñez, NO; Caro, C; Garcia-Martin, ML; Ocaña, M
Journal of Colloid and Interface Science, **629** (2023) 310-321
Enero, 2023 · DOI: 10.1016/j.jcis.2022.08.130

Uniform sodium-dysprosium double molybdate ($NaDy(MoO_4)_2$) nanoparticles having different morphologies (spheres and ellipsoids) and tunable size have been synthesized for the first time in literature. The procedure is based on a homogeneous precipitation process at moderated temperatures (≤ 220°C) from solutions containing appropriated precursors dissolved in ethylene glycol-water mixtures, in the absence (spheres) or the presence (ellipsoids) of tartrate anions. The effects of the morphological characteristics (size and shape) of the nanoparticles on the magnetic relaxivity at high field (9.4 T) have been evaluated finding that the latter magnitude was higher for the spheres than for the ellipsoids, indicating their better suitability as contrast agents for high-field magnetic resonance imaging. Such nanoparticles have been successfully coated with polymers bearing carboxylate functional groups through a layer-by-layer process, which improves the colloidal stability of the nanoparticles in physiological media. It has been also found that the coating layer had no significant effects on the nanoparticles relaxivity and that such coated nanoparticles exhibited a high biocompatibility and a high chemical stability. In summary, we have developed $NaDy(MoO_4)_2$ based bioprobes which meet the required criteria for their use as contrast agents for high-field magnetic resonance imaging.

Responsive Optical Materials Based on Ligand-Free Perovskite Quantum Dots Embedded in Mesoporous Scaffolds

Romero-Pérez, C; Zanetta, A; Fernandez-Delgado, N; Herrera-Collado, M; Hernandez-Saz, J; Molina, SI; Calio, L; Calvo, ME; Míguez, H
ACS Applied Materials & Interfaces, **15** (2023) 1808-1816
Enero, 2023 · DOI: 10.1021/acsami.2c16867

Herein we show that dispersing inorganic cesium lead bromide ($CsPbBr_3$) perovskite quantum dots (QDs) in optical quality films, possessing an accessible and controlled pore size distribution, gives rise to fluorescent materials with a controlled and highly sensitive response to ambient changes. A scaffold-based synthesis approach is employed to obtain ligand-free QDs, whose pristine surface endows them with high sensitivity to the presence of different vapors in their vicinity. At the same time, the void network of the host offers a means to gradually expose the embedded QDs to such vapors. Under these conditions, the luminescent response of the QDs is mediated by the mesostructure of the matrix, which determines the rate at which vapor molecules will adsorb onto the pore walls and, eventually, condensate, filling the void space. With luminescence quantum yields as high as 60%, scaffold-supported ligand-free perovskite nanocrystals display intense photoemission signals over the whole process, as well as high photo- and chemical stability, which allows illuminating them for long periods of time and recovering the original response upon desorption of the condensed phase. The results herein presented open a new route to explore the application of perovskite QD-based materials in sensing.

Persistent Luminescence $Zn_2GeO_4:Mn^{2+}$ Nanoparticles Functionalized with Polyacrylic Acid: One-Pot Synthesis and Biosensing Applications

Calderon-Olvera, RM; Arroyo, E; Jankelow, AM; Bashir, R; Valera, E; Ocaña, M; Becerro, AI
ACS Applied Materials & Interfaces, **15** (2023) 20613-20624

Marzo, 2023 · DOI: 10.1021/acsami.2c21735

Zinc germanate doped with Mn^{2+} ($Zn_2GeO_4:Mn^{2+}$) is known to be a persistent luminescence green phosphor with potential applications in biosensing and bioimaging. Such applications demand nanoparticulated phosphors with a uniform shape and size, good dispersibility in aqueous media, high chemical stability, and surfacefunctionalization. These characteristics could be major bottlenecks and hence limit their practical applications. This work describes a one-pot, microwave-assisted hydrothermal method to synthesize highly uniform $Zn_2GeO_4:Mn^{2+}$ nanoparticles (NPs) using polyacrylic acid (PAA) as an additive. A thorough characterization of the NPs showed that the PAA molecules were essential to realizing uniform NPs as they were responsible for the ordered aggregation of their building blocks. In addition, PAA remained attached to the NPs surface, which conferred high colloidal stability to the NPs through electrostatic and steric interactions, and provided carboxylate groups that can act as anchor sites for the eventual conjugation of biomolecules to the surface. In addition, it was demonstrated that the as-synthesized NPs were chemically stable for, at least, 1 week in phosphate buffer saline (pH range = 6.0-7.4). The luminescence properties of Zn_2GeO_4 NPs doped with different contents of Mn^{2+} (0.25-3.00 mol %) were evaluated to find the optimum doping level for the highest photoluminescence (2.50% Mn) and the longest persistent luminescence (0.50% Mn). The NPs with the best persistent luminescence properties were photostable for at least 1 week. Finally, taking advantage of such properties and the presence of surface carboxylate groups, the Zn_2GeO_4:0.50%Mn^{2+} sample was successfully used to develop a persistent luminescence-based sandwich immunoassay for the autofluorescence-free detection of interleukin-6 in undiluted human serum and undiluted human plasma samples. This study demonstrates that our persistent Mn-doped Zn_2GeO_4 nanophosphors are ideal candidates for biosensing applications.

Ultrapure Green High Photoluminescence Quantum Yield from $FAPbBr_3$ Nanocrystals Embedded in Transparent Porous Films

Romero-Pérez, C; Delgado, NF; Herrera-Collado, M; Calvo, ME; Míguez, H
Chemistry of Materials, **35** (2023) 5541-5549
Julio, 2023 · DOI: 10.1021/acs.chemmater.3c00934

Achieving highly transparent and emissive films based on perovskite quantum dots (PQDs) is a challenging task since their photoluminescence quantum yield (PLQY) typically drops abruptly when they are used as building blocks to make a solid. In this work, we obtain highly transparent films containing $FAPbBr_3$ quantum dots that display a narrow green emission (λ = 530 nm, full width at half-maximum (FWHM) = 23 nm) with a PLQY as high as 86%. The method employed makes use of porous matrices that act as arrays of nanoreactors to synthesize the targeted quantum dots within their void space, providing both a means to keep them dispersed and a protective environment. Further infiltration with poly(methyl methacrylate) (PMMA) increases the mechanical and chemical stability of the ensemble and serves to passivate surface defects, boosting the emission of the embedded PQD and significantly reducing the width of the emission peak, which fulfills the requirements established by the Commission Internationale de l'Éclairage (CIE) to be considered an ultrapure green emitter. The versatility of this approach is demonstrated by fabricating a color-converting layer that can be easily transferred onto a light-emitting device surface to modify the spectral properties of the outgoing radiation.

Europium doped-double sodium bismuth molybdate nanoparticles as contrast agents for luminescence bioimaging and X-ray computed tomography

Calderon-Olvera, RM; Núñez, NO; González-Mancebo, D; Monje-Moreno, JM; Muñoz-Rui, MJ; Gómez-González, E; Arroyo, E; Torres-Herrero, B; De la Fuente, JM; Ocaña, M
Inorganic Chemistry Frontiers, **10** (2023) 3202
Febrero, 2023 · DOI: 10.1039/D2QI02664C

A one-pot method for the synthesis of uniform $Eu3^{+}$-doped $NaBi(MoO_4)_2$ nanoparticles with an ellipsoidal shape and tetragonal crystal structure functionalized with polyacrylic acid is reported for the first time in the literature. The method is based on a homogeneous precipitation reaction from solutions in an ethylene glycol/water medium containing appropriate bismuth, sodium, and molybdate precursors and polyacrylic acid. The luminescence properties (excitation and emission spectra and luminescence lifetime) of such nanoparticles are evaluated for different Eu^{3+} doping levels, finding an intense red emission for all synthesized samples. The X-ray attenuation properties of the nanoparticles have been also analyzed, which were found to be better than those of a commercially computed tomography contrast agent (iohexol). The dispersibility of the nanoparticles in a physiological medium was also analyzed, finding that they could be well dispersed in a *2-N*-morpholinoethanesulfonic acid monohydrate medium (pH = 6.5). Finally, the cell viability of such a phosphor has been analyzed using MIA-PaCa-2 cells and its *in vivo* toxicity has been evaluated using the nematode Caenorhabditis elegans model finding no significant toxicity in both cases up to a nanoparticle concentration of 100 μg mL^{-1}, which is within the range required for most in vivo applications. The developed Eu^{3+}-doped $NaBi(MoO_4)_2$ nanoparticles are, therefore, excellent candidates for their use as bimodal probes for luminescence imaging and X-ray computed tomography.

Effect of the effective refractive index on the radiative decay rate in nanoparticle thin films

Romero, M; Sánchez-Valencia, JR; Lozano, G; Míguez, H
Nanoscale, **15** (2023) 15279-15287
Septiembre, 2023 · DOI: 10.1039/d3nr03348a

In this work, we theoretically and experimentally study the influence of the optical environment on the radiative decay rate of rare-earth transitions in luminescent nanoparticles forming a thin film. We use electric dipole sources in finite-difference time-domain simulations to analyze the effect of modifying the effective refractive index of transparent layers made of phosphor nanocrystals doped with rare earth cations, and propose a correction to previously reported analytical models for calculating the radiative decay rate. Our predictions are tested against an experimental realization of such luminescent films, in which we manage to vary the effective refractive index in a gradual and controllable manner. Our model accurately accounts for the measurements attained, allows us to discriminate the radiative and non-radiative contributions to the time-resolved photoluminescence, and provides a way to rationally tune the spontaneous decay rate and hence the photoluminescence quantum yield in an ensemble of luminescent nanoparticles.

Determination of the optical constants of ligand-free organic lead halide perovskite quantum dots

Rubino, A; Lozano, G; Calvo, ME; Mïguez, H
Nanoscale, **15** (2023) 2553-2560
Febrero, 2023 · DOI: 10.1039/d2nr05109e

Precise knowledge of the optical constants of perovskite lead halide quantum dots (QDs) is required to both understand their interaction with light and to rationally design and optimize the devices based on them. However, their determination from colloidal nanocrystal suspensions, or films made out of them, remains elusive, as a result of the difficulty in disentangling the optical constants of the organic capping ligands and those of the semiconductor itself. In this work, we extract the refractive index and extinction coefficient of ligand-free methylammonium lead iodide ($MAPbI_3$) and bromide ($MAPbBr_3$) nanocrystals. In order to prevent the use of organic ligands in the preparation, we follow a scaffold assisted synthetic procedure, which yields a composite film of high optical quality that can be independently and precisely characterized and modelled. In this way, the contribution of the guest nanocrystals can be successfully discriminated from that of the host matrix. Using a Kramers-Kronig consistent dispersion model along with an effective medium approximation, it is possible to derive the optical constants of the QDs by fitting the spectral dependence of light transmitted and reflected at different angles and polarizations. Our results indicate a strong dependence of the optical constants on the QD size. Small nanocrystals show remarkably large values of the extinction coefficient compared to their bulk counterparts. This analysis opens the door to the rigorous modelling of solar cells and light-emitting diodes with active layers based on perovskite QDs.

Surfactant-Dependent Bulk Scale Mechanochemical Synthesis of $CsPbBr_3$ Nanocrystals for Plastic Scintillator-Based X-ray Imaging

Ghosh, J; O'Neill, J; Masteghin, MG; Braddock, I; Crean, C; Dorey, R; Salway, H; Anaya, M; Reiss, J; Wolfe, D; Sellin, P
ACS Applied Nano Materials, **6**(16) (2023) 14980-14990
Agosto, 2023 · DOI: 10.1021/acsanm.3c02531

We report a facile, solvent-free surfactant-dependentmechanochemicalsynthesis of highly luminescent $CsPbBr_3$ nanocrystals (NCs)and study their scintillation properties. A small amount of surfactantoleylamine (OAM) plays an important role in the two-step ball millingmethod to control the size and emission properties of the NCs. Thesolid-state synthesized perovskite NCs exhibit a high photoluminescencequantum yield (PLQY) of up to 88% with excellent stability. $CsPbBr_3$ NCs capped with different amounts of surfactant were dispersedin toluene and mixed with polymethyl methacrylate (PMMA) polymer andcast into scintillator discs. With increasing concentration of OAMduring synthesis, the PL yield of $CsPbBr_3$/PMMA nanocompositewas increased, which is attributed to reduced NC aggregation and PL quenching. We also varied the perovskite loading concentration inthe nanocomposite and studied the resulting emission properties. Themost intense PL emission was observed from the 2% perovskite-loadeddisc, while the 10% loaded disc exhibited the highest radioluminescence(RL) emission from 50 kV X-rays. The strong RL yield may be attributedto the deep penetration of X-rays into the composite, combined withthe large interaction cross-section of the X-rays with the high-Zatoms within the NCs. The nanocomposite disc shows an intense RL emissionpeak centered at 536 nm and a fast RL decay time of 29.4 ns. Further,we have demonstrated the X-ray imaging performance of a 10% $CsPbBr_3$ NC-loaded nanocomposite disc.

Enhancement of upconversion photoluminescence in phosphor nanoparticle thin films using metallic nanoantennas fabricated by colloidal lithography
Ngo, TT; Viaña, JM; Romero, M; Calvo, ME; Lozano, G; Míguez, H
Materials Advances, **4** (2023) 6381-6388
Noviembre, 2023 · DOI: 10.1039/D3MA00775H

Lanthanide-doped upconversion nanoparticles (UCNPs), as multifunctional light sources, are finding utility in diverse applications ranging from biotechnology to light harvesting. However, the main challenge in realizing their full potential lies in achieving bright and efficient photon upconversion (UC). In this study, we present a novel approach to fabricate an array of gold nanoantennas arranged in a hexagonal lattice using a simple and inexpensive colloidal lithography technique, and demonstrate a significant enhancement of UC photoluminescence (UCPL) by up to 35-fold through plasmon-enhanced photoexcitation and emission. To elucidate the underlying physical mechanisms responsible for the observed UCPL enhancement, we provide a comprehensive theoretical and experimental characterization, including a detailed photophysical description and numerical simulations of the spatial electric field distribution. Our results shed light on the fundamental principles governing the enhanced UCNPs and pave the way for their potential applications in photonic devices.

Mn^{2+}-doped $MgGeO_3$ nanophosphors with controlled shape and optimized persistent luminescence
González-Mancebo, D; Arroyo, E; Becerro, AI; Ocaña, M
Ceramics International, **49** (2023) 36791-36799
Noviembre, 2023 · DOI: 10.1016/j.ceramint.2023.09.008

Mn^{2+}-doped $MgGeO_3$ ($MgGeO_3$:Mn^{2+}) is an efficient persistent phosphor that emits red luminescence for long time after stopping excitation with UV light. For optical and biotechnological uses a precise control of particle size and shape is highly desired since these parameters may have a strong influence on the properties and suitability of phosphor materials for the intended applications. To the best of our knowledge, $MgGeO_3$:Mn^{2+} has been synthesized by conventional solid-state-reaction, which yields particles of heterogeneous size and shape. Here, we report for the first time in the literature a salt-assisted method for the synthesis of $MgGeO_3$:Mn^{2+} nanoparticles with uniform shape (nanorods) and a mean size of 350 nm x 99 nm. The rigorous study of the luminescence properties of the $MgGeO_3$:Mn^{2+} nanorods revealed that whereas the optimum doping level for photoluminescence was 2.0 mol% Mn^{2+}, the best persistent luminescence was attained with just 0.5 mol% Mn^{2+}, which is ascribed to the different mechanisms of both luminescence processes. The optimum persistent nano-phosphor showed an intense red emission, which persisted at least 17 h after stopping the excitation. Such excellent properties make the developed nanophosphor an attractive candidate for use in optical and biotech-nological applications.

Collective plasmonic resonances enhance the photoluminescence of rare-earth nanocrystal films processed by ultrafast annealing
Cabello-Olmo, E; Higashino, M; Murai, S; Tanaka, K; Lozano, G; Míguez, H
Chemical Communications, **59** (2023) 1289-1292
Enero, 2023 · DOI: 10.1039/d2cc04779a

Herein, we demonstrate that rapid thermal annealing allows achieving close-to-one photoluminescence quantum yield while preserving the transparency of rare-earth nanocrystal films, which further enables their integration with nanophotonics. The combination with periodic arrays of aluminum nanodisks that support collective plasmonic resonances leads to enhanced directional emission.

Modeling Weakly Scattering Random Media: A Tool to Resolve the Internal Structure of Nanoporous Materials

Jiménez-Solano, A; Miranda-Muñoz, JM; Carretero-Palacios, S; Miguez, H
Advanced Photonics Research, **4** (2023) 5
Mayo, 2023 · DOI: 10.1002/adpr.202200267

Nanoporous media scatter a small fraction of the light propagating through them, even if pore sizes are significantly smaller than the characteristic visible wavelengths. The disordered spatial modulation of the refractive index at the few or few tens of nanometers length scale, resulting from the presence of randomly distributed air bubbles or solid aggregates within a continuous solid background, gives rise to these weak scattering effects. However, standard theoretical approaches to describe this kind of media use effective medium approximations that do not account for diffuse, ballistic, and specular components. Herein, all spectral components and the angular distribution of the scattered light are captured through optical modeling. A Monte Carlo approach, combining scattering Mie theory and Fresnel equations, implemented within a genetic algorithm, allows us to decode the void and aggregate size distribution and hence the internal structure of a nanocrystalline titania (TiO_2) film chosen as a paradigmatic example. The approach allows to generically describe the scattering properties of nanoporous materials which, as shown herein, may be used to decipher their internal structure from the fitting of their far-optical field properties.

Understanding ice and water film formation on soil particles by combining density functional theory and Casimir-Lifshitz forces

Bostrom, M; Kuthe, S; Carretero-Palacios, S; Esteso, V; Li, Y; Brevik, I; Gopidi, HR; Malyi, OI; Glaser, B; Persson, C
Physical Review B, **108** (2023) 125434
Septiembre, 2023 · DOI: 10.1103/PhysRevB.108.125434

Thin films of ice and water on soil particles play crucial roles in environmental and technological processes. Understanding the fundamental physical mechanisms underlying their formation is essential for advancing scientific knowledge and engineering practices. Herein, we focus on the role of the Casimir-Lifshitz force, also referred to as dispersion force, in the formation and behavior of thin films of ice and water on soil particles at 273.16 K, arising from quantum fluctuations of the electromagnetic field and depending on the dielectric properties of interacting materials. We employ the first-principles density functional theory (DFT) to compute the dielectric functions for two model materials, $CaCO_3$ and Al_2O_3, essential constituents in various soils. These dielectric functions are used with the Kramers-Kronig relationship and different extrapolations to calculate the frequency-dependent quantities required for determining forces and free energies. Moreover, we assess the accuracy of the optical data based on the DFT to model dispersion forces effectively, such as those between soil particles. Our findings reveal that moisture can accumulate into almost micron-sized water layers on the surface of calcite (soil) particles, significantly impacting the average dielectric properties of soil particles. This research highlights

the relevance of DFT-based data for understanding thin film formation in soil particles and offers valuable insights for environmental and engineering applications.

Oxidation and coordination states assumed by transition metal dopants in an invert ultrabasic silicate glass

Zandona, A; Castaing, V; Shames, AI; Helsch, G; Deubener, J; Becerro, AI; Allix, M; Goldstein, A
Journal of Non-Crystalline Solids, **603** (2023) 122094
Marzo, 2023 · DOI: 10.1016/j.jnoncrysol.2022.122094

An ultrabasic invert silicate glass ($46SiO_2{\cdot}11Na_2O{\cdot}21CaO{\cdot}22BaO$, optical basicity index equal to 0.71) was synthesized (O_2 atmosphere) and used as host for various transition metal dopants. Optical absorption, emission and electron paramagnetic spectroscopies were used to characterize oxidation and coordination states. Some of the dopants displayed only their maximal oxidation state (Ti^{4+}, V^{5+}, Cr^{6+}, Mo^{6+} and W^{6+}). Others exhibited mixed valences: (i) Mn^{3+} was the dominant species, alongside Mn^{2+} and Mn^{5+}; (ii) stable Fe^{3+} prevailed, although some Fe^{2+} was preliminarily suggested by the absorption spectrum; (iii) Co^{3+} probably accompanied the dominant Co^{2+} tetrahedral oxide complex; (iv) like in "conventional" silicate glasses, only Ni^{2+} was detected, though simultaneously located in tetrahedral and octahedral sites (somewhat distorted); (v) Cu^{+} was surprisingly identified alongside the expected 6-fold coordinated Cu^{2+}. Drastic reduction of the oxygen content in the melting atmosphere led to conversion of Cr^{6+} to Cr^{3+}, despite the extreme basicity of the host.

Measurement principles for quantum spectroscopy of molecular materials with entangled photons

Moretti, L; Rojas-Gatjens, E; Uboldi, L; Tiede, DO; Kumar, EJ; Trovatello, C; Preda, F; Perri, A; Manzoni, C; Cerullo, G; Kandada, ARS
Journal of Chemical Physics, **159** (2023) 084201
Agosto, 2023 · DOI: 10.1063/5.0156598

Nonlinear spectroscopy with quantum entangled photons is an emerging field of research that holds the promise to achieve superior signal-to-noise ratio and effectively isolate many-body interactions. Photon sources used for this purpose, however, lack the frequency tunability and spectral bandwidth demanded by contemporary molecular materials. Here, we present design strategies for efficient spontaneous parametric downconversion to generate biphoton states with adequate spectral bandwidth and at visible wavelengths. Importantly, we demonstrate, by suitable design of the nonlinear optical interaction, the scope to engineer the degree of spectral correlations between the photons of the pair. We also present an experimental methodology to effectively characterize such spectral correlations. Importantly, we believe that such a characterization tool can be effectively adapted as a spectroscopy platform to optically probe system-bath interactions in materials.

Origin of anomalously stabilizing ice layers on methane gas hydrates near rock surface

Li, Y; Corkery, RW; Carretero-Palacios, S; Berland, K; Esteso, V; Fiedler, J; Milton, KA; Brevik, I; Bostrom, M
Physical Chemistry Chemical Physics, **25** (2023) 6636-6652
Marzo, 2023 · DOI: 10.1039/d2cp04883c

Gas hydrates (GHs) in water close to freezing temperatures can be stabilised via the formation of ice layers. In a recent work [Bostrom et al., Astron. Astrophys., A54, 650, 2021], it was found that a surface region with partial gas dilution could be essential for obtaining nano- to micron-sized anomalously stabilizing ice layers. In this paper, it is demonstrated that the Casimir-Lifshitz free energy in multi-layer systems could induce thinner, but more stable, ice layers in cavities than those found for gas hydrates in a large reservoir of cold water. The thickness and stability of such ice layers in a pore filled with cold water could influence the leakage of gas molecules. Additional contributions, e.g. from salt-induced stresses, can also be of importance, and are briefly discussed.

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Síntesis y caracterización de nanopartículas basadas en Eu^{3+}:$NaBi(MoO_4)_2$ con posibles aplicaciones en biomedicina
R.M. Calderón Olvera, S. Ruiz Herrera, M. Ocaña Jurado, N. Núñez
Ciencia en la Universidad, de docentes a estudiantes (Eds: A.M. Beltrán y M. Félix Ángel), (Punto Rojo Libros, SL) pags. 212-235
ISBN: 0979-83-98188-08-0

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

SPIE Photonics West 2023
28 enero – 02 febrero [San Francisco, Estados Unidos de América]

Translucent persistent phosphor films and nanophotonics: beyond limits set by composition. *V. Castaing, G. Lozano, H. Míguez*. CONFERENCIA INVITADA

Materials for Sustainable Development Conference · MATSUS23
06-10 marzo [Valencia, España]

Charge carrier recombination dynamics in perovskite nanocrystal arrays: from connected to isolated nanostructures. *J. Galisteo López*. COMUNICACIÓN ORAL

NanoSpain Conference 2023
25-28 abril [Tarragona, España]

Eu^{3+} doped $NaBi(MoO_4)_2$ nanoparticles as contrast agents for bioimaging. *R.M. Calderón-Olvera, N.O. Núñez, D. González-Mancebo, J.M. Monje Moreno, M.J. Muñoz-Rui, E. Gómez-González, E. Arroyo, B. Torres Herrero, J.M. De la Fuente, M. Ocaña*. PÓSTER

Perovskite Workshop 2023
10-11 mayo [Lund, Suecia]

Iodide Nanodomain formation in mixed halide perovskites: let's discuss on the role of defects. *J.F. Galisteo López*. CONFERENCIA INVITADA

European Materials Research Society 2023 E-MRS Spring Meeting
29 mayo – 02 junio [Estrasburgo, Francia]

Spherical garnet-based persistent nanophosphors suitable for long-lasting optical imaging. *E. Arroyo, B. Torres, J.M. de la Fuente, M. Ocaña, A.I. Becerro*. COMUNICACIÓN ORAL

12th International Colloids Conference
11-14 junio [Mallorca, España]

Effects of the size and shape of carboxylate functionalized $NaD_y(MoO_4)_2$. *E. Gómez-González, N.O. Núñez, C. Caro, M.L. García*-Martín, M. Ocaña. PÓSTER

20th International Conference on Luminiscence · ICL 2023
27 agosto – 01 septiembre [Paris, Francia]

Nanophotonics tunes the emission properties of transparent thin films made of rare-earth nanocrystals. *G. Lozano*. COMUNICACIÓN ORAL

Transparent persistent phosphor films allow optical environment design: beyond limits set by composition. *V. Castaing, M. Romero, G. Lozano, H. Míguez*. COMUNICACIÓN ORAL

Optical environment determines radiative decay rate: the role of refractive index. *M. Romero, G. Lozano, H. Míguez*. PÓSTER

Persistent luminescence nanoparticles for biosensing. *E. Arroyo, R.M. Calderón, A.M. Jankelow, R. Bashir, E. Valera, M. Ocaña, A.I. Becerro*. PÓSTER

European Materials Research Society 2023 E-MRS Fall Meeting
18-21 septiembre [Varsovia, Polonia]

Advanced functionalities of perovskite quantum dots embedded in porous scaffolds. *H. Míguez*. COMUNICACIÓN ORAL

New Inorganic Functional Oxides: Synthesis, Characterisation and Simulations
04-06 octubre [Orleans, Francia]

Wet-deposition of nanophosphor particles: an alternative method to obtain translucent films with original optical properties. *V. Castaing, M. Romero, G. Lozano, H. Míguez*. CONFERENCIA

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESS AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

2nd Conference on Advanced Materials in Spain · AMatS
13-15 noviembre [Zaragoza, España]

Light-matter coupling in optoelectronic materials. *H. Míguez*. CONFERENCIA

INAM Annual Symposium 2023
14 noviembre [Universidad Jaume I, Castellón, España]

Light-matter coupling in optoelectronic materials. H. Míguez. CONFERENCIA PLENARIA

SEMINARIOS / SEMINARS

18 diciembre | **Persistent phosphors: from glow in the dark toys to advanced optical devices**
Dr. Víctor Castaing
Lugar: Instituto de Física de Materia Condensada (PMC) de la "Ecole Polytechnique". Francia

FORMACION / TRAINING

FORMACIÓN DE POSTGRADO / MASTER DEGREE THESIS

Título:	**Síntesis, caracterización y estudio de las propiedades ópticas de materiales con luminiscencia persistente**
Autor:	Aída Rodríguez Rodríguez
Tutores:	Ana Isabel Becerro Nieto, Manuel Ocaña Jurado

Grado: Trabajo Fin de Máster · Máster en Ciencia y Tecnología de Nuevos Materiales
Centro: Universidad de Sevilla
Fecha Defensa: 06 de julio de 2023

DOCENCIA / TEACHING

El personal del ICMS imparte docencia en titulaciones de Grado y doble Grado de la Universidad de Sevilla. La docencia se desarrolla en diversos centros: Facultad de Física, Facultad de Biología, Facultad de Química, Facultad de Farmacia y Escuela Técnica Superior de Ingeniería Informática.

ESTANCIAS DE PERSONAL DEL ICMS EN OTROS CENTROS
PERSONNEL OF THE ICMS IN OTHER LABORATORIES

Instituto de Nanociencia y Materiales de Aragón (INMA)

Zaragoza, España	**Encarnación Arroyo Porriño**	10/07/23 - 14/07/23
		07/02/23 - 07/03/23

PREMIOS Y RECONOCIMIENTOS / PRIZES AND ACKNOWLEDGEMENTS

Award in European Materials Research Conference (EMRS 2023 Spring Meeting)
Encarnación Arroyo Porriño premio "Young Researcher Award in European Materials Research Conference (EMRS 2023 Spring Meeting)", in recognition of an oustanding paper presented in the frame of Symposium H Advanced strategies for smart functional and multifunctional biomaterials and biointerfaces.

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Potenciostato y sistema electroquímico
- Analizador de potencial Z, tamaño de partícula y pesos moleculares (Malvern, ZS90)
- Liofilizador de altas prestaciones Epsilon 2-4 (CHRIST)
- Estufa de desecación de 90 litros (RAYPA)
- Cámara Incubadora Opaq + Orbital Maxi (OVAN)
- pH & Ion-metro GLP 22+ (CRISON A)
- Espectrómetro visible-UV CARY-100. Medidas de coeficiente de absorción con luz normal y polarizada.

- Fluorímetro espectroscópico (HORYBA Jobin Yvon Fluorolog) con accesorio para la determinación de tiempos de vida. Microscopio de fluorescencia (HORYBA Jobin Yvon sigle photon controller: FluoroHub).
- Sistema de medida de porosidades en capas delgadas.
- Vis-NIR FTIR espectrofotómetro Bruker GmbH Fuente de excitación continua normal y angular. Specular Reflectance Attached Microscope.
- Tunable Supercontinuum White Laser Source. Fianium LTD 4W total output 400nm – 2400nm range Acousto-Optic Tunable Filter
- Perfilómetro mecánico DektakXT en su versión automática (platina XY motorizada y giro de 360o motorizado) y que incluye soporte de muestras cerámico para muestras flexibles.
- Fluorímetro Edinburgh FLS1000 con accesorios (esfera integradora y criostato).

Unidad Externa de Investigación: Física de Materiales

External Unit: Physics of Materials

PERSONAL / PERSONNEL

Catedráticos de Universidad	Dr. Javier S. Blázquez Gámez
	Dr. Alberto Criado Vega
	Dr. Luis Esquivias Fedriani
	Dr. Victorino Franco García
	Dra. Ángela María Gallardo López
	Dr. Antonio Muñoz Bernabé
Profesores Titulares de Universidad	Dra. Josefa María Borrego Moro
	Dr. Rafael Caballero Flores
	Dra. M. del Carmen Gallardo Cruz
	Dr. Felipe Gutiérrez Mora
	Dr. Jhon Jairo Ipus Bados
	Dr. José María Martín Olalla
	Dr. Víctor Morales Flórez
	Dra. Ana Morales Rodríguez
	Dra. Rocío Moriche Tirado
	Dr. Francisco Javier Romero Landa
	Dra. Bibi Malmal Moshtaghion Enterazi
Doctores Contratados	Dr. Luis M. Moreno Ramírez
	Dra. Jia Yan Law
Investigadores en Formación	Gdo. Álvaro Díaz García
	Gda. Carmen Muñoz Ferreiro
	Gdo. Pedro Rivero Antúnez
	Gdo. Antonio Vidal Crespo
Profesores Eméritos	Dra. Clara F. Conde Amiano
Investigadores Honorarios	Dr. Jaime del Cerro González
	Dr. Arturo Domínguez Rodríguez
	Dr. Justo Jiménez Fernández

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Multi-property Compositionally Complex Magnets for Advanced Energy Applications · CoCoMag

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
GRANT AGREEMENT NO. 101099736	01-06-2023 31-05-2026	Comisión Europea	365.500 €

Investigador Principal Research Head	Componentes Research Group
Victorino Franco García	Álvaro Díaz García Jia Yan Law Luis Miguel Moreno Ramírez

Development and Validation of a New Magnetocaloric High-Performance Hydrogen Liquefier Prototype · HyLICAL

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
GRANT AGREEMENT NO. 101101461	01-01-2023 31-12-2027	Comisión Europea	358.835 €

Investigador Principal Research Head	Componentes Research Group
Victorino Franco García	Álvaro Díaz García, Aun Nawaz Khan Jia Yan Law, Luis Miguel Moreno Ramírez Jorge Revuelta Losada, Carlos Romero Muñiz

Desarrollo de Nanogeneradores piezoeléctricos flexibles y de alta eficiencia basados en nanocompuestos perovskita/PVDF (NANOGEN)

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
TED2021-132021-131458A-100	01-12-2022 30-11-2024	Ministerio de Ciencia e Innovación	149.500 €

Investigador Principal Research Head	Componentes Research Group
Rocío Moriche Tirado (US)	Francisco J. Gotor Martínez María Jesús Sayagués de Vega Rosalía Poyato Galán Ana Morales Rodríguez Felipe Gutiérrez Mora Ángela Gallardo López

Abordando las Limitaciones de Materiales Magnetocalóricos para su Implementación en Aplicaciones Energéticamente Eficientes

Código Code	Periodo Period	Organismo Financiador Financial Source
PID2019-105720RB-I00	01-06-2020 31-05-2024	Ministerio de Ciencia e Innovación

Investigador Principal Research Head	Componentes Research Group
Victorino Franco García	Josefa María Borrego Moro Jhon Jairo Ipus Bados

Diseño de cerámicas avanzadas con nanomateriales 2D para dispositivos electroquímicos de alta temperatura

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PID2022-140191NB-100	01-09-2023 31-08-2027	Ministerio de Ciencia e Innovación	156.250 €

Investigador Principal Research Head	Componentes Research Group
Ana Morales Rodríguez Rosalía Poyato Galán	Ángela Gallardo López Felipe Gutiérrez Mora Rocío del Carmen Moriche Tirado

A la Búsqueda de Nuevos Cerámicos Ultraduros a Base de Boro para Aplicaciones Estructurales en la Nueva Generación de Aviones y uso Seguro y Eficiente de la Energía

Código Code	Periodo Period	Organismo Financiador Financial Source
PID2019-103847RJ-I00	01-10-2020 30-09-2023	Ministerio de Ciencia e Innovación

Investigador Principal Research Head	Componentes Research Group
Bibi Malmal Moshtaghion Entezari	Francisco Luis Cumbreras Hernández Arturo Domínguez Rodríguez Diego Gómez García

Fundamentos y potencialidades del refuerzo de compuestos de matriz cerámica con alótropos de carbono (FRAC)

Código Code	Periodo Period	Organismo Financiador Financial Source
P20_01121	05-10-2021 30-06-2023	Junta de Andalucía

Investigador Principal Research Head	Componentes Research Group
Víctor Morales Flórez	Arturo Domínguez Rodríguez Luis María Esquivias Fedriani Francisco de Paula Jiménez Morales María del Carmen Lemos Fernández

Desarrollo de cerámicas avanzadas con nanomateriales 2D para su aplicación en sistemas de propulsión y frenado en la industria aeroespacial (AEROCER-2D)

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P20_01024	05-10-2021 31-03-2023	Junta de Andalucía	60.125 €

Investigador Principal Research Head	Componentes Research Group
Ángela Gallardo López	Felipe Gutiérrez Mora Ana Morales Rodríguez Antonio Muñoz Bernabé Rosalía Poyato Galán Rocío Moriche Tirado

Transiciones de fase termo-magnéticas para un uso eficiente de la energía y de los recursos

Código Code	Periodo Period	Organismo Financiador Financial Source
P18-RT-746	01-01-2020 31-03-2023	Junta de Andalucía

Investigador Principal Research Head	Componentes Research Group
Victorino Franco García	Javier S. Blázquez Gámez Josefa M. Borrego Moro Alejandro Conde Amiano Jhon Jairo Ipus Bados Alejandro F. Manchón Gordón Hariharan Srikanth

OTROS PROYECTOS / OTHER PROJECTS

Hysteresis and frequency response as limiting factors for efficient thermomagnetic energy conversion

Código/Code: FA8655-21-1-7044
Periodo/Period: 30-09-2021 / 29-09-2024
Organismo Financiador/Financial source: Air Force Office of Scientific Research
Investigador responsable/Research head: Victorino Franco García
Componentes/Research group: Jia Yan Law, Luis Miguel Moreno Ramírez

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Characterization of Fe-based materials for additive manufacturing
Código/Code: 4728/0665
Periodo/Period: 02-02-2023 / 01-02-2024
Organismo Financiador/Financial source: ARCELORMITAL INNOVACIÓN,

INVESTIGACIÓN E INVERSIÓN SL
Investigador responsable/Research head: Victorino Franco García

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

An overview of polymeric composite scaffolds with piezoelectric properties for improved bone regeneration

Donate, R; Paz, R; Moriche, R; Sayagués, MJ; Alemán-Rodríguez, ME; Monzón, M
Materials & Design, **231** (2023) 112085
Julio, 2023 · DOI: 10.1016/j.matdes.2023.112085

Despite the dramatic change that Tissue Engineering or stem cell therapies have brought to current therapeutic strategies, there is a lack of functionalities in the available biomaterials for manufacturing scaffolds to treat several highly prevalent osseous diseases (osteochondral defects, osteoporosis, etc.). One promising approach to fill this gap involves the development of innovative piezoelectric scaffolds for improved bone regeneration. Scaffolds with the appropriate piezoelectricity can positively influence the proliferation and differentiation of mesenchymal stem cells to regenerate bone tissue, since surface electrical charges play a key role in the mechanotransduction process. In this work, polymeric-based composite scaffolds with piezoelectric properties intended for bone tissue engineering are reviewed. Special attention is paid to biocompatible, piezoelectric polymers that show suitable properties to be pro-cessed by additive manufacturing techniques. Previous works on composite scaffolds based of these poly-meric matrices and containing piezoceramic additives are summarized. The use of piezoelectric nanostructured composite formulations containing lead-free ceramic oxide nanoparticles with per-ovskite structure is highlighted. Also, different commonly applied mechanical stimuli to activate the piezoelectric effect of the developed materials are presented. Finally, other applications of such scaffolds are mentioned, including their capabilities for real-time monitoring.

Using a computationally driven screening to enhance magnetocaloric effect of metal monoborides

Romero-Muñiz, C; Law, JY; Moreno-Ramírez, LM; Díaz-García, A; Franco, V
Journal of Physics-Energy, **5** (2023) 024021
Abril, 2023 · DOI: 10.1088/2515-7655/acce6e

In most cases, substitution studies that aim to optimize magnetic properties are performed at the magnetic atomic site. However, in the case of MnB, magnetic substitutions at the Mn site significantly decrease the once promising magnetocaloric and magnetic properties. This study employs computationally directed search to optimize the magnetocaloric properties of MnB where partial substitutions of boron atoms ($Mn_{50}B_{50-x}Si_x$ and $Mn_{50}B_{50-x}Ge_x$ where x = 3.125, 6.25, and 12.5) reveal new compounds with a greater magnetocaloric effect than pure MnB at the same Curie temperature. These new compounds were obtained by arc melting the pure elements and further characterized. The computationally driven screening process is based on density functional theory calculations that do not require large databases of known compounds. This work demonstrates that using simple computational screening procedures to search for new magnetocaloric materials with improved properties can be done quickly, cost-effectively, and while maintaining reliability.

Excellent cryogenic magnetocaloric properties in heavy rare-earth based $HRENiGa_2$ (HRE = Dy, Ho, or Er) compounds

Guo, D; Moreno-Ramírez, LM; Law, JY; Zhang, YK; Franco, V
Science China-Materials, **66** (2023) 249-256
Enero, 2023 · DOI: 10.1007/s40843-022-2095-6

$RENiX_2$ compounds, where RE = rare-earth element and X = *p*-block element, have been highly regarded for cryogenic magnetocaloric applications. Depending on the elements, they can crystallize in $CeNiSi_2$-type, $NdNiGa_2$-type, or $MgCuAl_2$-type crystal structures, showing different types of magnetic ordering and thus affect their magnetic properties. Regarding the magnetocaloric effect, $MgCuAl_2$-type aluminides show larger values than those of the $CeNiSi_2$-type silicides and the $NdNiGa_2$-type gallides due to the favored ferromagnetic ground state. However, $RENiGa_2$ gallides can crystallize in either $NdNiGa_2$- or $MgCuAl_2$-type structures depending on the RE element. In this work, we select heavy RE (HRE) elements for exploring the microstructure, magnetic ordering and magnetocaloric performance of $HRENiGa_2$ (HRE = Dy, Ho or Er) gallides. They all crystallize in the desired $MgCuAl_2$-type crystal structure which undergoes a second-order transition from ferro- to para-magnetic state with increasing temperature. The maximum isothermal entropy change ($|\Delta S_{iso}^{max}|$) values are 6.2, 10.4, and 11.4 J kg^{-1} K^{-1} (0-5 T) for $DyNiGa_2$, $HoNiGa_2$, and $ErNiGa_2$, respectively, which are comparable to many recently reported cryogenic magnetocaloric materials. Particularly, the excellent magnetocaloric properties of $HoNiGa_2$ and $ErNiGa_2$ compounds, including their composite, fall in the temperature range that enables them for the in-demand hydrogen liquefaction systems.

Large thermal conductivity and robust mechanical properties of Ni-Mn-Ga/Cu magnetocaloric composites prepared by spark plasma sintering

Zhang, YC; Gao, Y; Franco, V; Yin, HBC; Peng, HX; Qin, FX
Science China-Materials, **66** (2023) 3670-3680
Septiembre, 2023 · DOI: 10.1007/s40843-023-2491-6

Magnetic refrigeration technology based on the magnetocaloric effect can better meet the requirements of efficient energy consumption and conversion. From engineering perspective, preparing magnetocaloric composites is an effective and efficient approach to combine desirable magnetocaloric performance, large thermal conductivity and ameliorated mechanical properties. In the present work, Ni-Mn-Ga/Cu magnetocaloric composites were prepared by spark plasma sintering (SPS) and compared with their counterparts fabricated via conventional methods. Magnetic properties were studied in detail and the magnetocaloric effect of Ni-Mn-Ga/Cu composites was characterized to be better than that of their hot-pressed counterparts and that of many micro/nano-sized Ni-Mn-Ga alloys. Besides, the composites exhibited favorable thermal conductivity of 11.2 W mK^{-1}. The Hassel-man-Johnson model was adopted and modified to relate the thermal conductivity to the microstructure of the composites. Compared with arc-melted alloys, these SPS magnetocaloric composites sintered at different temperatures exhibited largely enhanced mechanical performance with minimum fracture stress of 340 MPa and strain of 4%. Furthermore, the failure mechanism of Ni-Mn-Ga/Cu magnetocaloric composite was elucidated by finite element simulation based on an extended linear Drucker-Prager model. The above findings from both experiments and simulation advance the knowledge of magnetocaloric materials and promote the development of magnetic refrigeration technology towards practical applications.

Ultra-low hysteresis in giant magnetocaloric $Mn_{1-x}V_xFe_{0.95}(P,Si,B)$ compounds

Lai, JW; You, XM; Law, J; Franco, V; Huang, BW; Bessas, D; Maschek, M; Zeng, DC; Van Dijk, N; Brück, E

Journal of Alloys and Compounds, **930** (2023) 167336

Enero, 2023 · DOI: 10.1016/j.jallcom.2022.167336

Large thermal hysteresis in the $(Mn,Fe)_2(P,Si)$ system hinders an efficient heat exchange and thus limits the magnetocaloric applications. Substitution of manganese by vanadium in the $Mn_{1-x1}V_{x1}Fe_{0.95}P_{0.593}Si_{0.33}B_{0.077}$ and $Mn_{1-x2}V_{x2}Fe_{0.95}P_{0.563}Si_{0.36}B_{0.077}$ compounds enable a significant reduction in the thermal hysteresis without losing the giant magnetocaloric effect. For the composition closest to the critical one, where first-order crossovers to second-order phase transition in the series of $x_2 = 0.02$, $Mn_{0.98}V_{0.02}Fe_{0.95}P_{0.563}Si_{0.36}B_{0.077}$ exhibits a thermal hysteresis that is reduced from 1.5 to 0.5 K by 67%, yielding an adiabatic temperature change of 2.3 K and magnetic entropy change of 5.6 J/kgK for an applied field of 1 T, which demonstrates its potential for highly efficient magnetic heat pumps utilizing low-cost permanent magnets.

All-d-metal Ni(Co)-Mn(X)-Ti (X = Fe or Cr) Heusler alloys: Enhanced magnetocaloric effect for moderate magnetic fields

Khan, AN; Moreno-Ramírez, LM; Díaz-García, A; Law, JY; Franco V

Journal of Alloys and Compounds, **931** (2023) 167559

Enero, 2023 · DOI: 10.1016/j.jallcom.2022.167559

All-d-metal Ni(Co)-Mn-Ti Heusler alloys show high magnetocaloric/barocaloric effects ascribed to the occurrence of a martensitic transformation together with excellent mechanical properties. However, high magnetic fields are needed to fully drive the transformation and to obtain their maximum responses. To further tune the martensitic transition and the associated magnetocaloric response, we systematically investigate the role of partial Mn substitution by Fe or Cr on the parent composition $Ni_{36}Co_{14}Mn_{35}Ti_{15}$. On the one hand, Cr doping increases the entropy change of the transformation but causes a tighter overlap of both martensitic and Curie transitions. This significantly reduces the magnetization difference between austenite and martensite and, consequently, strongly decreases the magnetocaloric response. On the other hand, Fe doping reduces the entropy change of the transformation and separates both martensitic and Curie transitions while keeping the magnetization difference among both phases. These two combined features reduce the magnetic field needed to completely drive the martensitic transformation and leads to higher and broader isothermal entropy change peaks for moderate magnetic field changes, reaching up to 25% enhancement for 2T when compared to the undoped alloy.

On the order of magnetic transition in $MnCo_{1-x}Fe_xGe$ (x=0.20, 0.06 and 0.03) mechanical alloys

Vidal-Crespo, A; Ipus, JJ; Blázquez, JS; Conde, CF

Journal of Alloys and Compounds, **930** (2023) 167381

Enero, 2023 · DOI: 10.1016/j.jallcom.2022.167381

Mechanically amorphized $MnCo_{1-x}FexGe$ alloys ($x = 0.20$, 0.06 and 0.03) were used as precursors to obtain hexagonal austenite single phase samples. Combining thermomagnetic and magnetocaloric analysis and in situ X-ray diffraction, we observed that the presence of a distribution of transition

temperatures jeopardizes the first order character of the magnetoelastic transition from the ferromagnetic to paramagnetic state. Both magnetothermal and in situ X-ray diffraction identify the presence of such distribution and the first order character of the magnetoelastic transition.

Reversibility and thermal dependence of the martensitic transformation in a melt-spun $Ni_{55}Fe_{17}Ga_{26}Co_2$ Heusler alloy

Manchón-Gordón, AF; Vidal-Crespo, A; Blázquez, JS; Kowalczyk, M; Ipus, JJ; Kulik, T; Conde, CF
Journal of Alloys and Compounds, **946** (2023) 169484
Junio, 2023 · DOI: 10.1016/j.jallcom.2023.169484

An almost single phase 14 M modulated martensite is obtained in melt spun ribbon of $Ni_{55}Fe_{17}Ga_{26}Co_2$ Heusler alloy. The effect of thermal treatments on the stability of the reverse martensitic transformation from 14 M modulated martensite to austenite phase in this system has been investigated by both non-isothermal and isothermal treatments. Heating above martensitic transformation promotes a continuous reduction of the martensitic transformation temperature, which stabilizes the austenite phase at room temperature and induces the precipitation of the gamma phase. However, thermal treatments at temperatures between the austenite start and finish temperatures induce the decoupling of the austenite formation in a subsequent heating. The two successive reverse martensitic transformations could be ascribed to the untransformed martensite in the previous interrupted heating and to the new martensite formed during cooling.

First-order phase transition in high-performance $La(Fe,Mn,Si)_{13}H$ despite negligible hysteresis

Moreno-Ramírez, LM; Law, JY; Borrego, JM; Barcza, A; Greneche, JM; Franco, V
Journal of Alloys and Compounds, **950** (2023) 169883
Julio, 2023 · DOI: 10.1016/j.jallcom.2023.169883

Optimizing the performance of magnetocaloric materials is facilitated by understanding the thermomagnetic transitions they undergo, including the order of these transitions and their strength. Those exhibiting strong first-order phase transitions (FOPT) are accompanied by large heating and cooling responses but with relatively small cyclic responses, while materials with second-order (SOPT) character exhibit moderate heating and cooling responses. However, the lack of hysteresis could partially compensate for the lower magnitudes with a more cyclic response. One way to effectively maximize the cyclic response, combining the advantages of FOPT and SOPT, is to fine tune the transition towards the borderline of FOPT-SOPT, which can minimize hysteresis. For the well-known $La(Fe,Si)_{13}$ family, it is challenging to identify and/or evaluate the critical point where FOPT crossovers to SOPT based on conventional techniques. To address these ambiguities, in this work, we apply the field dependence exponent n criteria to a series of lowly hysteretic and high-performance $La(Fe,Mn,Si)_{13}H$ magnetocaloric materials with compositions close to the critical one. Even if the sample with the lowest hysteresis resembles characteristics of SOPT, it is evidently identified as undergoing FOPT from the n criteria: (1) existence of $n>2$ overshoot and (2) n at the transition temperature, $n_{transition}$, is 0.37. This proximity to the critical composition ($n_{transition}=0.4$) further explains the low hysteresis observed. This FOPT character of the series is confirmed by temperature-dependent ^{57}Fe Mössbauer spectrometry studies, fitting the hyperfine field to the Bean-Rodbell model instead of the usual Brillouin function. As it is a zero-field method, the confirmation by Mössbauer spectrometry gives further strength to the n-criterion.

Sol-gel method and reactive SPS for novel alumina-graphene ceramic composites

Rivero-Antúnez, P; Zamora-Ledezma, C; Sánchez-Bajo, F; Moreno-López, JC; Anglaret, E; Morales-Flórez, V

Journal of the European Ceramic Society, **43** (2023) 1064-1077

Marzo, 2023 · DOI: 10.1016/j.jeurceramsoc.2022.10.043

Reinforced ceramic matrix composites of alumina and graphene oxide have been widely researched, but there are still unresolved issues such as the optimum distribution of the graphene or the presence of efficient bonds between filler and matrix. This work introduces a novel fabrication procedure based on the sol–gel method, using boehmite as an alumina precursor, and graphene oxide nanoplatelets as the reinforcing phase. Full densification of the samples was done through reactive spark plasma sintering under milder conditions than usual. Structural characterization was done by XRD, SEM and micro-Raman among other techniques, and the presence of Al-O-C bonds was studied by XPS. Mechanical characterization was performed by Vickers microindentation and nanoindentation. No significant change was observed concerning the Young's modulus, hardness or fracture toughness, though improvements in the homogeneity of the distribution of the graphene and the chemical bonds between the matrix and the reinforcing phase were confirmed.

Electrical performance of orthotropic and isotropic 3YTZP composites with graphene fillers

López-Pernía, C; Muñoz-Ferreiro, C; Moriche, R; Morales-Rodríguez, A; Gallardo-López, A; Poyato, R

Journal of the European Ceramic Society, **43** (2023) 1605-1612

Abril, 2023 · DOI: 10.1016/j.jeurceramsoc.2022.11.068

3 mol% yttria tetragonal zirconia polycrystal (3YTZP) composites with orthotropic or isotropic microstructures were obtained incorporating few layer graphene (FLG) or exfoliated graphene nanoplatelets (e-GNP) as fillers. Electrical conductivity was studied in a wide range of contents in two configurations: perpendicular ($\sigma_{\perp}$) and parallel ($\sigma_{//}$) to the pressing axis during spark plasma sintering (SPS). Isotropic e-GNP composites presented excellent electrical conductivity for high e-GNP contents ($\sigma_{\perp}$ ~3200 S/m and $\sigma_{//}$ ~1900 S/m for 20 vol% e-GNP), consequence of their misoriented distribution throughout the matrix. Optimum electrical performance was achieved in the highly anisotropic FLG composites, with high electrical conductivity for low contents ($\sigma_{\perp}$ ~680 S/m for 5 vol%), percolation threshold below 2.5 vol% FLG and outstanding electrical conductivity for high contents ($\sigma_{\perp}$ ~4000 S/m for 20 vol%), result of the high aspect ratio and low thickness of FLG.

R-curve evaluation of 3YTZP/graphene composites by indirect compliance method

López-Pernía, C; Muñoz-Ferreiro, C; Moriche, R; Prada-Rodrigo, J; Moreno, P; Reveron, H; Chevalier, J; Morales-Rodríguez, A; Poyato, R; Gallardo-López, A

Journal of the European Ceramic Society, **43** (2023) 3486-3497

Julio, 2023 · DOI: 10.1016/j.jeurceramsoc.2023.02.002

This work addresses the crack growth resistance of 3 mol% Yttria-doped Tetragonal Zirconia Polycrystalline (3YTZP) spark-plasma sintered (SPS) composites containing two types of graphene-based nanomaterials (GBN): exfoliated graphene nanoplatelets (e-GNP) and reduced graphene oxide (rGO). The crack growth resistance of the composites is assessed by means of their R-Curve behavior determined by three-point bending tests on single edge "V" notched beams (SEVNB), in two different

orientations of the samples: with the crack path perpendicular or parallel to the pressure axis during the SPS sintering. The sharp edge notches were machined by ultrashort laser pulsed ablation (UPLA). The compliance and optical-based methods for evaluating the crack length are compared on the basis of the experimental R-Curve results in composites with 2.5 vol% rGO tested in the perpendicular orientation. Moreover, the activation of reinforcement mechanisms is evaluated by both the fracture surface inspection by Scanning Electron Microscopy and a compliance analysis. It is shown that the indirect compliance method is relevant and reliable for calculating the R-Curve of 3YTZP/GBN composites. The effect of the type and content of GBN on the crack growth resistance of the composites is also discussed.

Sustainable Nanomagnetism: Investigating the Influence of Green Synthesis and pH on Iron Oxide Nanoparticles for Enhanced Biomedical Applications

Abdullah, JAA; Díaz-García, Law, JY; Romero, A; Franco, V; Guerrero, A
Polymers, **15** (2023) 3850
Septiembre, 2023 · DOI: 10.3390/polym15183850

This study comprehensively analyzed green nanomagnetic iron oxide particles (GNMIOPs) synthesized using a green method, investigating their size, shape, crystallinity, aggregation, phase portions, stability, and magnetism. The influence of pH and washing solvents on the magnetic properties of the nanoparticles and their incorporation into PCL membranes was examined for biomedical applications. Polyphenols were utilized at different pH values (1.2, 7.5, and 12.5), with washing being performed using either ethanol or water. Characterization techniques, including XRD, SEM, TEM, FTIR, and VSM, were employed, along with evaluations of stability, magnetic properties, and antioxidant activity. The findings indicate that both pH levels and the washing process exert a substantial influence on several properties of NMIOPs. The particle sizes ranged from 6.6 to 23.5 nm, with the smallest size being observed for GNMIOPs prepared at pH 12.5. Higher pH values led to increased crystallinity, cubic Fe_3O_4 fractions, and reduced crystalline anisotropy. SEM and TEM analyses showed pH-dependent morphological variations, with increased aggregation being observed at lower pH values. GNMIOPs displayed exceptional magnetic behavior, with the highest saturation magnetization being observed in GNMIOPs prepared at pH 7.5 and 12.5 and subsequently washed with ethanol. The zeta potential measurements indicated a stability range for GNMIOPs spanning from −31.8 to −41.6 mV, while GNMIOPs synthesized under high-pH conditions demonstrated noteworthy antioxidant activity. Furthermore, it was explored how pH and washing solvent affected the morphology, roughness, and magnetic properties of GNMIOP-infused nanofiber membranes. SEM showed irregularities and roughness due to GNMIOPs, varying with pH and washing solvent. TEM confirmed better dispersion with ethanol washing. The magnetic response was stronger with ethanol-washed GNMIOPs, highlighting the influence of pH and washing solvent on membrane characteristics.

Quantifying the Structure and Properties of Nanomagnetic Iron Oxide Particles for Enhanced Functionality through Chemical Synthesis

Abdullah, JAA; Díaz-García, Law, JY; Romero, A; Franco, V; Guerrero, A
Nanomaterials, **13** (2023) 2242
Agosto, 2023 · DOI: 10.3390/nano13152242

This comprehensive study investigates the properties of chemical nanomagnetic iron oxide particles (CNMIOPs) synthesized through a chemical method. The primary objective is to examine how pH levels

and washing solvents affect the magnetism properties of these nanoparticles. Three different pH levels (1.2, 7.5, and 12.5) using NaOH and two washing solvents (ethanol and water) are employed. The characterization techniques include FTIR, SEM, TEM, XRD, ZSP, and VSM. Furthermore, the study incorporates two specific pH- and solvent-dependent CNMIOPs into PCL electrospun materials to analyze their performance in a targeted application. The results show that pH and the washing process significantly affect the CNMIOPs' properties. Higher pH levels result in smaller particles with higher crystallinity and reduce crystalline anisotropy. SEM and TEM analysis confirm different morphologies, including cubic, spherical, and elongated shapes. Ethanol-washed CNMIOPs exhibit superior magnetic behavior, with the highest magnetization saturation at pH 12.5 (Ms = 58.3 emu/g). The stability of the CNMIOPs ranges from −14.7 to −23.8 mV, and higher pH levels exhibit promising antioxidant activity. Furthermore, the study explores the effects of pH and washing solvents on CNMIOP-infused nanofiber membranes, with better dispersion observed with ethanol washing. Overall, this research provides valuable insights into the properties and behavior of CNMIOPs under varying pH and washing conditions.

Experimental study of the structural, magnetic, electrical, and mechanical properties of possible half-metallic $Co_{2-x}V_xFeGe$ Heusler alloys

Mahat, R; Karki, U; Shambhu, KC; Law, JY; Franco, V; Gupta, A; LeClair, P
Journal of Physics and Chemistry of Solids, **172** (2023) 110988
Enero, 2023 · DOI: 10.1016/j.jpcs.2022.110988

In this study, we experimentally investigated quaternary Heusler alloys $Co_{2-x}V_xFeGe$ with $0 \leq x \leq 1$ prepared by arc melting and annealing, and showed that they are promising candidates for spintronics applications. Single phase microstructures were observed for V compositions from $x=0.25$ to $x=0.625$. Other V concentrations were multi-phased. All single phase samples had a face centered cubic crystal structure with a lattice constant that increased linearly with the V concentration. The low-temperature saturation magnetic moments were shown to obey the Slater–Pauling rule of thumb for half-metals, which is a prerequisite for half metallicity. All alloys had high Curie temperatures, which scaled linearly with the saturation magnetic moment, thereby facilitating applications at room temperature and above. Electrical transport measurements were performed to elucidate the electronic structures of the alloys. The temperature dependence of the electrical resistivity was analyzed and discussed in the framework of the two-current conduction model by considering the existence of an energy gap in the electronic spectrum around the Fermi level of the spin down sub-band. High mechanical hardness values were also observed.

Touch-free reactive flash sintering of dense strontium hexaferrite permanent magnet

Jalali, SIA; Manchón-Gordón, AF; Chacartegui, R; Sánchez-Jiménez, PE; Blázquez, JS; Perejón, A; Raj, R; Pérez-Maqueda, LA
Journal of the American Ceramic Society, **106** (2023) 7202-4208
Diciembre, 2023 · DOI: 10.1111/jace.19389

This work presents an extension of the touch-free flash sintering technique. In the proposed technique, chemical reaction and sintering occur in a single step, without the use of electrodes, in the presence of electric and magnetic fields. We show that a dense, single-phase strontium hexaferrite magnet can be produced from a mixture of commercial carbonate and oxide powders in a single step in a little more

than a minute. This new technique implies significant reduction in energy and time consumption (primarily because of ultrafast processing) relative to conventional sintering.

Effect of thermal treatments below devitrification temperature on the magnetic and magnetocaloric properties in mechanically alloyed $Fe_{70}Zr_{30}$ powders

Manchón-Gordón, A.F.; Blázquez, JS; Kowalczyk, M; Ipus, JJ; Kulik, T; Conde, CF
Journal of Non-Crystalline Solids, **609** (2023) 122267
Junio, 2023 · DOI: 10.1016/j.jnoncrysol.2023.122267

In this work, the relaxation of the amorphous structure of mechanically alloyed $Fe_{70}Zr_{30}$ powders has been analyzed through interrupted heating ramps below the devitrification temperature. As a result of such thermal treatment, Curie temperature and temperature at maximum magnetic entropy change curves shift to higher temperatures as the temperature of heating treatment increases. This effect can be attributed to both the release of the stress accumulated in the amorphous powder during the milling process and to the initiation of nucleation of alpha-Fe crystallites, as it has been shown by Mössbauer spectroscopy.

A practical analysis for decelerated growth processes to get physically meaningful kinetic parameters from classical nucleation and growth theory despite of over-growth

Blázquez, JS; Caballero-Flores, R; Manchón-Gordón, AF; Borrego, JM; Conde, CF
Journal of Non-Crystalline Solids, **610** (2023) 122305
Junio, 2023 · DOI: 10.1016/j.jnoncrysol.2023.122305

We have analyzed the overgrowth problem arising in decelerated growth processes of spherical crystals in the frame of classical nucleation and growth theory developed by Kolmogorov, Johnson and Mehl, and Avrami (KJMA). To do that, simulations of decelerated growth transformations with a constant nucleation rate have been performed, changing the linear growth rate of spherically shaped nuclei from null (instantaneous growth rate) to constant (characteristic of interface controlled growth processes). We propose the determination of the actual kinetic parameters through the analysis of the inflection point of time evolution of transformed fraction. The correlations found between the effective kinetic parameters from direct KJMA analysis and the actual ones make it possible obtaining physically meaningful parameters. The proposed analysis has been applied to the nanocrystallization of amorphous FINEMET-type compositions.

Structural, Vibrational, and Magnetic Characterization of Orthoferrite $LaFeO_3$ Ceramic Prepared by Reaction Flash Sintering

Manchón-Gordón, AF; Sánchez-Jiménez, PE; Blázquez, JS; Perejón, A; Pérez-Maqueda, LA
Materials, **16** (2023) 1019
Febrero, 2023 · DOI: 10.3390/ma16031019

$LaFeO_3$ perovskite ceramics have been prepared via reaction flash technique using Fe_2O_3 and La_2O_3 as precursors. The obtained pellets have been investigated using several techniques. The formation of $LaFeO_3$ has been clearly confirmed by X-ray diffraction. The scanning electron microscopy micrographs have shown the microporous character of the obtained pellets due to the low temperature and dwell

time used in the synthesis process (10 min at 1173 K). The orthorhombic-rhombohedral phase transition has been observed at approximately 1273 K in differential thermal analysis measurements, which also allows us to determine the Néel temperature at 742 K. The fitted Mössbauer spectra exposed the presence of a single sextet ascribed to the Fe^{+3} ions in the tetrahedral site. Finally, magnetic measurements at room temperature indicate the antiferromagnetic character of the sample.

A simple phenomenological model to describe stability of homogeneous solid solutions in high entropy alloys from metallic bonding potential

Blázquez, JS; García-Pînto, N; Conde, CF
Materialia, **28** (2023) 101744
Mayo, 2023 · DOI: 10.1016/j.mtla.2023.101744

A simple model based on the potential parameters used to describe metallic bonding is extended to solid solu-tions. A figure of merit (an effective temperature, T_{eff}) is proposed using a simple average over the potential coefficients to discern whether a homogeneous solid solution is expected to be stable or not in high entropy alloy compositions. Teff is calculated as the ratio between the solid solution excess in bonding energy over the average mixture divided by the configurational entropy. Application to the sexinary AlCrCuFeNiCo system stablishes a stability threshold for $T_{eff} < 500$ K. The model can successfully describe both the deviations from Vegard's law observed in binary alloys and the differences in this parameter between B2 ordered and bcc disordered phases considering average potential coefficients over the different possible atomic couples.

Thermal arrest analysis of the reverse martensitic transformation in a $Ni_{55}Fe_{19}Ga_{26}$ Heusler alloy obtained by melt-spinning

Vidal-Crespo, A; Manchón-Gordón, AF; Blázquez, JS; Ipus, JJ; Svec, P; Conde, CF
Journal of Thermal Analysis and Calorimetry, **148** (2023) 2367-2375
Marzo, 2023 · DOI: 10.1007/s10973-022-11889-1

$Ni_{55}Fe_{19}Ga_{26}$ ribbons obtained by melt-spinning technique exhibit a martensitic transformation from L21 cubic austenite phase to 14 M martensite phase above room temperature. We have taken advantage of the existence of thermal hysteresis of the martensitic phase transition (~11 K) to analyze the effect of isothermal treatments on the reverse martensitic transformation, which has been analyzed by means of interrupted heating using differential scanning calorimetry. The experimental findings clearly indicate a time-depending effect in the martensitic transformation at temperatures between the austenite start and finish temperatures. Moreover, it has been observed that two successive martensitic transformations take place after the isothermal arrest was performed.

Kinetic analysis of non-isothermal volume melting processes by differential scanning calorimetry

Blázquez, JS; Borrego, JM; Conde, CF
Journal of Thermal Analysis and Calorimetry, **148** (2023) 4307-4315
Mayo, 2023 · DOI: 10.1007/s10973-023-12006-6

The onset of melting of standard samples, ascribed to surface melting, is generally used for calibration of calorimeters. However, in non-isothermal conditions, nucleation-driven volume melting, which is

thermally activated, takes place. In this work, we propose an approximation in the frame of the classical nucleation and growth transformation kinetics to extend to non-isothermal regimes the analysis of processes governed by constant nucleation and interface controlled growth. The approximation allows both to observe the temperature dependence of nucleation activation energy with the overheating and to obtain the surface energy between the liquid nucleus and the surrounding solid phase for pure indium and lead (~10 mJ m^{-2}) and for a $Fe_{70}B_5C_5Si_3Al_5Ga_2P_{10}$ bulk metallic glass eutectic composition (~ 50 mJ m^{-2}). These values are about 50% lower than the theoretical ones for homogeneous nucleation, which can be ascribed to the random heterogeneous nucleation occurring at the crystals boundaries.

The dispersion of carbon nanotubes in composite materials studied by computer simulation of Small Angle Scattering

Garrido-Regife, L; Rivero-Antúnez, P; Morales-Flórez, V
Physica B-Condensed Matter, **649** (2023) 414450
Enero, 2023 · DOI: 10.1016/j.physb.2022.414450

Although numerous efforts have been made to reinforce ceramic materials by adding a nanostructured phase like carbon nanotubes (CNT), the appearance of aggregates during the manufacturing processes continues to be a problem. Given the size of the CNT (nm-μm), techniques such as Small Angle Scattering (SAS) can be a useful tool to study the formation of the aggregates and to quantify the degree of homogenization of the nanophase in the matrix. In this work, systems with different concentrations of CNT have been simulated in different states of aggregation, starting from a perfectly homogeneous dispersion of individualized CNT, and progressively aggregated. A Guinier regime appears in the scattering signal in the range of low values of the modulus of the scattering vector, q, as the aggregation occurs. Two parameters from the intensity curve are proposed to quantify the quality of the dispersion of the nanophase in the ceramic matrix.

Current perspective in magnetocaloric materials research

Law, JY; Moreno-Ramírez, LM; Díaz-García, A; Franco, V
Journal of Applied Physics, **133** (2023) 040903
Enero, 2023 · DOI: 10.1063/5.0130035

Magnetocaloric refrigeration has remained a promising alternative to conventional refrigeration for the last few decades. The delay in reaching the market is significantly based on materials' related issues, such as hysteresis/reversibility, mechanical stability, or formability. This perspective paper shows the current trends in magnetocaloric materials research, highlighting the families of alloys and compounds that are gaining attention in the recent years. It also includes an overview of novel approaches that can be used to analyze these properties that could improve the applicability of magnetocaloric materials.

Review on magnetocaloric high-entropy alloys: Design and analysis methods

Law, JY; Franco, V
Journal of Materials Research, **38** (2023) 37-51
Enero, 2023 · DOI: 10.1557/s43578-022-00712-0

The search for high-performance functional alloys with improved service life and reliability entails the optimization of their mechanical properties. Recently, the high-entropy alloy (HEA) design concept has

found new alloys with excellent mechanical properties. It utilizes multiprincipal elements to yield high configurational entropy of mixing, entailing a large compositional freedom with wide window of opportunities for property exploration. Their functional properties are usually modest when compared to conventional materials. The discovery of HEAs with optimal combination of mechanical and functional properties would be a leap forward in the reliability of functional devices. This review article focuses on magnetocaloric HEAs, the design approaches, and the appropriate analysis methods for their performance. We will highlight the efficient strategic search within the vast HEA space, which has been instrumental for significantly enhancing MCE performance, closing the pre-existing gap between magnetocaloric HEAs and high-performance conventional magnetocaloric materials.

Selective and rapid detection of acetone using aluminum-doped ZnO-based sensors

Benamara, M; Rivero-Antúnez, P; Dahman, H; Essid, M; Bouzidi, S; Debliquy, M; Lahem, D; Morales-Florez, V; Esquivias, L; Silva, JPB; El Mir, L

Journal of Sol-Gel Science and Technology, **108** (2023) 13-27
Enero, 2023 · DOI: 10.1007/s10971-023-06197-5

We report the preparation and characterization of pure and doped ZnO nanoparticles with 1%, 3%, and 5% aluminum (AZO) using a sol-gel method followed by annealing at 400 °C for 2 h. The structural and morphological properties of the AZO nanoparticles were analyzed using X-ray Diffraction (XRD), Transmission Electron Microscopy (TEM) techniques, and Scanning Electron Microscopy (SEM) equipped with Energy Dispersive Spectrometry (EDS). Optical and specific area properties were investigated by photoluminescence (PL) and N_2 physisorption measurements. The results showed that pure and doped AZO nanoparticles crystallize under a hexagonal wurtzite structure and exhibit spherical shapes with nanometric dimensions. TEM and SEM images revealed that the pure and Al-doped ZnO were round nanoparticles with a size smaller that 100 nm. FTIR measurements were conducted to investigate the presence of Al-O stretching vibrations, which served as an indication of aluminum incorporation into the ZnO lattice. The results confirmed the successful integration of aluminum into the ZnO structure. Additionally, XPS measurements were performed to examine the elemental composition of the AZO samples. The presence of Zn 2p peaks in all AZO samples, along with the presence of Al 2p peaks in the Al-doped ZnO structures, provided further evidence for the successful incorporation of Al ions into the ZnO lattice. The PL spectra revealed the presence of various defects (oxygen vacancies, interstitials) in the structure of pure and doped ZnO. Moreover, we fabricated gas sensors by spray-coating the AZO nanoparticles on alumina substrates equipped with interdigitated gold electrodes. The sensors demonstrated linear responses to gas concentration in the range of 5 to 50 ppm, with high sensitivity and good reproducibility, particularly for A1ZO (1% Al-doped ZnO), which exhibited the highest response (∼12) at 300 °C under 10 ppm of acetone. Furthermore, A1ZO demonstrated excellent selectivity to acetone compared to other volatile organic compounds (VOCs) gases. Our findings highlight the potential of aluminum-doped ZnO nanoparticles as a promising material for enhancing the sensing properties of acetone gas sensors.

Congresos y Reuniones Internacionales / International Congress and Meetings

Comunicaciones / Communications

Jornada ACerS Materiales vítreos y cerámicos para aplicaciones de alta tecnología
26 octubre [Sevilla, España]

Fabricación y bioactivación de alúmina porosa para aplicaciones biomédicas. *M. González-Sánchez, C. Zamora-Ledezma, J. Elango, F.L. Cumbrera-Hernández, P. Rivero-Antúnez, V. Morales-Flórez*. Comunicación Oral

Docencia / Teaching

Máster en Ciencia y Tecnología de Nuevos Materiales

Aplicaciones Tecnológicas de Materiales Funcionales Dr. Victorino Franco
Física del Estado Sólido Dra. Ángela Gallardo López, Dr. Rocío Moriche, Dr. Víctor Morales Florez
Procesado de Materiales Estructurales Dr. Bibi Malmal Moshtaghion Enterazi
Técnicas de Caracterización de Materiales Dra. Ana Morales Rodríguez, Dr. Jhon Jairo Ipus Bados, Dra. Rocío Moriche Tirado

El personal del ICMS imparte docencia en titulaciones de Grado y doble Grado de la Universidad de Sevilla. La docencia se desarrolla en diversos centros: Facultad de Física, Facultad de Biología, Facultad de Química, Facultad de Farmacia y Escuela Técnica Superior de Ingeniería Informática.

Cooperación Internacional y Otros International Cooperation and Others

- Colaboración con grupo de Jerôme Chevalier y Helen Reveron, INSA Lyon, Mateis. Carmen Muñoz Ferreiro (tesis en cotutela). Financiación: Ayuda de la Univ. De Lyon.
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- Colaboración con Katalin Balazsi, Head of Thin Film Physics Department, Hungarian Academy of Sciences, Centre for Energy Research, Budapest, Hungría

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Calorímetro de barrido diferencial (Perkin-Elmer DSC7)
- Criostato para espectrómetro Mössbauer
- Balanza termogravimétrica (Perkin-Elmer TGA-7)
- Espectrómetro Mössbauer (Wissel MB-500) con horno y criostato.
- Coercímetro (desarrollado en el laboratorio)
- Magnetómetro de muestra vibrante (LakeShore 7000) con horno y criostato.
- Equipo de medida directa de temperatura adiabática (Advanced Magnetic Technologies).
- Molino Planetario (Fritszch Pulverisette Vario 4)
- Equipo de solidificación por enfriamiento ultrarrápido (melt spinning, Bühler)
- Equipo de fusión por arco (MAM1, Bühler)
- Calorímetro de conducción, resolución en la medida del flujo de calor mejor que 0,1 W, fluctuaciones en temperatura del orden de 10-6 K, velocidad de barrido menor de 0,01K/h, rango 80-320K, es posible aplicar tensión uniaxial hasta 30 kg/cm2 y campo eléctrico hasta 800V/cm
- Calorímetro de conducción, rango 80-400K, campo eléctrico 2000V/cm
- Medida de constante dieléctrica, en los mismos calorímetros,
- Medida de ciclo de histéresis en Ferroeléctricos.
- Analizador de Impedancia
- Adelgazador iónico Gatan. Model 691. Precision ion polishing system.
- Autoclave SanoClav
- Balanzas de precisión: GR.-200; AND EK-300i.
- Centrifugadora Rotofix 32A
- 4 Cortadoras Isomet Low Speed Saw (Buehler)
- Cortadora mediana Isomet 1000. Precision saw.
- Cortadora Isomet 4000. Linear Precision Saw. Buehler.
- Embutidora Pneumet II. Mounting Press. Buehler/Metaserv.
- Embutidora Simplimet 1000. Automatic Mounting Press. Buehler
- Estufa
- 2 Discoplan TS Struers
- 2 Dimple Grinder. Model 656. Gatan.
- Durómetro Wilson VH1150
- Durómetro Duramin Struers
- Hornillo/agitador magnético SBS, Heat-stir “Stuart” , CB302
- Horno de tubo de argón. Termolab, Hornos eléctricos TH1700
- Horno de aire Lenton Furnaces
- Horno mufla
- Limpiadores ultrasonidos Bandelin, Sonorex Digitec; Branson 3510
- Máquina de ensayos de deformación Zwick / Roell Zmart. Pro 1185
- Máquina de ensayos de deformación Instron 5982
- Máquina de fluencia con flujo de gases.
- Máquina de fluencia estanca de argón.
- Microscopio Óptico Confocal Leica DCM3D
- Microscopio Óptico Leica DMRD / Leica DMRE / Leica DFC420
- Molino de agitación PM100 Retsch
- Molino de bolas Molino mezclador MM200, Retsch
- Multímetro Keithley 2000 multimeter.
- Plasma etching Emitech k1050X

- Pulidoras Buehler. Beta. Grinder-Polisher y Motopol 8. Buehler Metaserv
- Prensa Manual Astur Sinter
- Prensa Fluxana, Vaneox, Pressing Technology
- 2 Refrigeradoras. (P. Castro Ibérica)
- Registro Tesatronic (Tesa TT60)
- Registro gráfico (Servogor 122 DC/kipp & Zonen)
- Reómetro Reactor Controller Controller 4836
- Rotavapor R-100. Buehi
- 4 Sondas de Ultrasonidos
- Tribómetro Microtest MT/30/SCM/T
- 2 Ultrasonic Disc Cutter Model 601 Gatan.

Servicios Generales
General Services

SERVICIO DE ESPECTROSCOPÍAS VIBRACIONALES / VIBRATIONAL SPECTROSCOPY SERVICE

El Servicio de Espectroscopias vibracionales incluye las Unidades de Espectroscopía Raman y Espectroscopía Infrarroja. Este servicio está dedicado a la determinación de la estructura molecular de los compuestos químicos y la caracterización de materiales.

This Service consists of two different spectroscopies: Raman Spectroscopy and Infrared Spectroscopy. It is devoted to the determination of molecular structure of chemical compounds and materials.

ESPECTROSCOPÍA MICRO-RAMAN / MICRO-RAMAN SPECTROSCOPY

La espectroscopía Raman se basa en un proceso fotónico en el que la radiación incidente es dispersada por la muestra, produciéndose transiciones de tipo vibracional y rotacional. En general, el espectro Raman se interpreta como un espectro vibracional que ofrece información muy similar al espectro de infrarrojo, aunque las vibraciones que se ven reflejadas en el espectro Raman no son siempre las mismas que en aquél. Para que un modo vibracional sea activo en espectroscopía Raman es necesario que se produzcan cambios en la polarizabilidad de los enlaces químicos o la molécula considerada, lo que conlleva la producción de momentos dipolares inducidos. Su campo de aplicación es muy extenso: semiconductores, compuestos del carbono (grafito, diamante, nanotubos, fibras…), catalizadores, pigmentos, etc.

Raman spectroscopy is based on a photonic process in which the incident radiation is dispersed by the sample. This latter is perturbed leading to vibrational and rotational transitions. In general, the Raman spectrum is interpreted like a vibrational one, providing information very similar to the infrared spectroscopy, although the Raman active vibrations are not always the same as those excited with infrared radiation. A Raman vibration mode is active if there is a change of polarizability of the chemical bonds or the considered molecule, which in turn results in the generation of induced dipolar momentum. Its application fields are very broad: semiconductors, carbon compounds (graphite, diamond, nanotubes, fibers…), catalysts, pigments, etc.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- LabRAM Horiba Jobin Yvon dotado de un microscopio confocal y 3 longitudes de excitación (785 cm^{-1} rojo, 532 cm^{-1} verde, y 325 cm^{-1} UV)
  LabRAM Horiba Jobin Yvon equipped with a confocal microscope and 3 excitation lasers (785 cm^{-1} red, 532 cm^{-1} green, and 325 cm^{-1} UV)

Responsables Científicos/ Scientific Responsibles: Dr.Miguel Ángel Centeno Gallego y Dr. Mauricio Calvo Roggiani
Personal Técnico/ Technical Assistant: Dr. Miguel Ángel Avilés Escaño

Espectroscopía Infrarroja / Infrared Spectroscopies

La espectroscopía de Infrarrojos (FT-IR) se basa en la absorción de radiación infrarroja por parte de los materiales. Esta absorción supone un cambio en la energía vibracional de los enlaces, siempre que se produzca un cambio en la polarización de dicho enlace. El resultado obtenido es un espectro en el que se representa la radiación absorbida o transmitida en función del número de onda de la radiación, lo cual permite identificar el enlace correspondiente.
El equipo en el ICMS cubre un rango de número de ondas que va desde 5000 a 250 cm^{-1} (óptica de CsI) y se puede trabajar con purga o en vacío. Se halla equipado con accesorios para trabajar en los modos de Reflectancia Difusa (DRIFT), Reflectancia Total Atenuada (ATR) y Reflexión Especular. Dispone de un microscopio de Infrarrojos que tiene una resolución lateral de 10 μm.

Infrared spectroscopy (FT-IR) is based on the selective absorption of the infrared radiation by the materials. This absorption means a change in the vibrational energy of the chemical bonds, whenever it occurs a change in the polarization. The result is a spectrum showing the absorbed or transmitted radiation as a function of the wavenumber of the radiation, which can be assigned to the corresponding chemical bound.
The equipment at the ICMS works in a wavenumber range from 5000 to 250 cm^{-1} (CsI optic), and can operate with a gas purge or in vacuum. It is equipped with several accessories to do Diffuse Reflectance (DRIFT), Attenuated Total Reflectance (ATR) or Specular Reflectance. It has got an Infrared Microscope with a lateral resolution of 10 μm.

Instrumental Disponible / Available Equipment

- JASCO FT/IR-6200 IRT-5000
  JASCO FT/IR-6200 IRT-5000

Responsables Científicos/ Scientific Responsibles: Dr.Miguel Ángel Centeno Gallego y Dr. Mauricio Calvo Roggiani
Personal Técnico/ Technical Assistant: Dr. Miguel Ángel Avilés Escaño

Espectroscopía de Electroluminiscencia / Electroluminescence Spectroscopy

El servicio de espectroscopía de electroluminiscencia del ICMS permite caracterizar íntegramente la fotoemisión activada por corriente de un dispositivo emisor de luz (LED). El servicio cuenta con una esfera integradora con un puerto que aloja al dispositivo electroluminiscente conectada a un detector CCD. También se dispone de un módulo para la caracterización angular del dispositivo electroluminiscente.
Las medidas permiten obtener las curvas de luminancia vs densidad corriente o vs potencial y la eficiencia cuántica de electroluminiscencia

The ICMS electroluminescence spectroscopy service allows full characterization of current-activated photoemission from an emitting device. The service has an integrating sphere with a port that houses the electroluminescent device connected to a CCD detector. A module for angular characterization of

the electroluminescent device is also available. The measurements allow to obtain the luminance vs current density curves or vs potential and the quantum efficiency of electroluminescence.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Sistema de medida EQE: C9920-12
  Measuring EQE System: C9920-12

- Distribución del brillo de luz: C9920-11
  Light Brightness Distribution: C9920-11

Responsables Científicos/ Scientific Responsibles: Dr. Mauricio Calvo Roggiani y Dr. Hernán Míguez García

ESPECTROSCOPÍA ULTRAVIOLETA, VISIBLE E INFRARROJO CERCANO / ULTRAVIOLET-VISIBLE-NEAR INFRARED SPECTROSCOPIES

La técnica de espectroscopía en el rango ultravioleta, visible e infrarrojo cercano (UV-Vis-NIR) nos permite conocer como materiales de distinta morfología (principalmente polvos, láminas y partículas o moléculas en suspensión) reflejan y transmiten la luz incidente en el rango comprendido entre 190 nm y 3000 nm. De esta forma, es posible extraer información sobre su eficiencia como filtros ópticos, ya sean especulares o difusores, y/o sobre la luz absorbida por ellos, lo que indirectamente nos permite estimar su gap electrónico (en el caso de dieléctricos), las transiciones electrónicas que tienen lugar (en el caso de moléculas o sistemas dopados con átomos de otra especie), o las resonancias plasmónicas (en el caso de metales).

The Ultraviolet-Visible-Near Infrared Spectroscopy (UV-Vis-NIR) reports on the existing energy differences between the more external occupied electronic levels and the nearer unoccupied ones.
The equipment in the laboratory, which works in the wavelength range of 190 nm to 900 nm can operate in the Transmission mode or in Diffuse Reflectance Modes.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Cary 5000 + UMA (Universal Measurement Accesory)
  Cary 5000 + UMA (Universal Measurement Accesory)

- Cary 300
  Cary 300

Responsables Científicos/ Scientific Responsibles: Dr. Gabriel Lozano Barbero, Dr. Hernán Míguez García
Personal Técnico/ Technical Assistant: Dr. Miguel Ángel Avilés Escaño

Laboratorio de Espectroscopía Ultra-Rápida / Ultrafast emission and absorption spectroscopy

El laboratorio de espectroscopía ultra-rápida permite realizar medidas de absorción y emisión resueltas en el tiempo con una resolución temporal de 190 femtosegundos (fs) y un amplio rango temporal que va de los 190 fs a 1 milisegundo (ms). Las medidas pueden realizarse en el rango espectral 350-850 nm.

The ultra-fast spectroscopy laboratory allows performing time-resolved absorption and emission measurements with a time resolution of 190 femtoseconds (fs) over a broad temporal range (190 fs - 1 millisecond). Measurements can be carried out in the 350-850 nm spectral range.

Instrumental Disponible / Available Equipment

- Sistema de excitación láser ultra-rápido formado por un láser pulsado PHAROS (Light Conversion) (longitud de onda de emisión 1030nm, tasa de repetición 1kHz y duración de pulso 190fs) y un amplificador paramétrico (OPA) ORPHEUS (Light Conversion) que produce pulsos de duración y tasa de repetición iguales al PHAROS pero con una longitud de onda sintonizable en el rango 350-2500nm.

- Espectrómetros de absorción para el rango temporal 190fs-8ns (HELIOS, Ultrafast Systems) y 2ns-1ms (EOS, Ultrafast Systems). Ambos sistemas permiten realizar medidas en el rango espectral 350-1100nm con una resolución de 2nm.

- Espectrómetro de emisión para el rango temporal 190fs-5ns (HALCYONE, Ultrafast Systems) operativo en el rango espectral 350-1100nm.

- Sistema de time-correlated single-photon counting (TCSPC) para realizar medidas de emisión resuelta en el tiempo en el rango temporal 1ns-1ms y en el rango espectral 200-850nm.

Responsables Científicos/ Scientific Responsibles: Dr. Hernán Míguez García, Dr. Juan F. Galisteo López

Servicio de Espectrometría de Emisión Atómica / Atomic Emission Spectrometry Service

La espectrometría de emisión atómica de plasma acoplado inductivamente (ICP-OES) es una técnica analítica que permite la cuantificación de elementos hasta nivel traza en muestras en solución. La muestra a analizar es nebulizada y conducida a un plasma de argón, en donde se produce la desolvatación, vaporización, atomización e ionización de los elementos a analizar. Los átomos e iones excitados por la elevada energía térmica suministrada por el plasma emiten durante el proceso de relajación radiación electromagnética de longitudes de onda características de cada elemento. La intensidad de las distintas

líneas de emisión es proporcional a la concentración del analito y con la correspondiente curva de calibración es posible realizar su cuantificación. Esta técnica presenta elevada sensibilidad, excelente límite de detección (en el rango ppb, μg/L), buena precisión, alto rendimiento y capacidad multi-elemental, aunque en determinadas ocasiones se pueden producir interferencias espectrales debido a un alto número de líneas de emisión.
Se pueden suministrar muestras sólidas, realizándose la digestión por parte del servicio, o líquidas en solución acuosa ligeramente ácida. No se admiten muestras en HF. Las muestras líquidas no deben presentar precipitados ni coloides en suspensión y deberán poseer un volumen mínimo de 10 ml. Las muestras se entregarán al técnico encargado del servicio, junto con la solicitud de análisis debidamente cumplimentada que se encuentra disponible en la web del ICMS.

Inductively coupled plasma atomic emission spectrometry (ICP-OES) is an analytical technique that allows the quantification of elements up to the trace level in samples in solution. The sample to be analyzed is nebulized and conducted to an argon plasma, where desolvation, vaporization, atomization and ionization of the elements take place. The atoms and ions reach an excited state by the high thermal energy supplied by the plasma and during the relaxation process electromagnetic radiation is emitted with wavelengths characteristic of each element. The intensity of the different emission lines is proportional to the concentration of the elements, which can be quantified by using appropriate calibration curves. This technique has high detection limits (in the ppb range, µg / L), good reliability, high throughput and multi-elemental capacity, although in some cases spectral interferences can occur due to a high number of emission lines.
Solid samples (digestion will be carried out by the service) or liquid samples in slightly acidic aqueous solution can be supplied. Samples in HF medium are not allowed. Liquid samples must not present precipitates or colloids in suspension and must have a minimum volume of 10 ml. The samples will be delivered to the technician in charge of the service, together with the duly completed analysis request that is available on the ICMS website.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- iCAP 7200 ICP-OES Duo (ThermoFisher Scientific)
  iCAP 7200 ICP-OES Duo (ThermoFisher Scientific)

- Digestor por microondas ETHOS EASY (Milestone)
  Microwave Digestion System ETHOS EASY (Milestone)

Responsables Científicos/ Scientific Responsibles: Dr. Francisco José Gotor Martínez
Personal Técnico/ Technical Assistant: Lda. Belinda Sigüenza Carballo

SERVICIO DE ANÁLISIS TEXTURAL Y TÉRMICO / TEXTURAL AND THERMAL ANALYSIS SERVICE

Este servicio incluye las siguientes Unidades: Análisis Térmico, Fisi-quimisorción, Análisis de Tamaño de Partícula y Potencial Z. Está dedicado a la determinación de la textura, estructura y comportamiento térmico de los materiales.

This Service includes the following units: Thermal Analysis, Physisorption and Chemisorption, Particle Size and Z-potential determination. It is devoted to the characterization of texture, microstructure and thermal behavior of advanced materials.

FISI-QUIMISORCIÓN / PHYSISORPTION-CHEMISORPTION

Este servicio constituye una herramienta básica para la caracterización microestructural de sólidos pulverulentos de distinta naturaleza, en cuanto a porosidad, superficie específica y superficie químicamente activa.
En el servicio se dispone de un analizador de adsorción de gases (Micromeritics, ASAP 2020) que proporciona isotermas de adsorción y desorción, a partir de las cuales se obtienen de ellas la superficie específica y distribución del tamaño de poro y de microporo de estos materiales, incorporando también los accesorios necesarios para medidas de quimisorción.

This service constitutes a basic tool for the microstructural characterization of powdered solids of different natures, regarding to their porosity, specific surface area and chemically active surface.
This service is composed by a physisorption analyser (Micromeritics, ASAP 2020) which provides the complete adsorption/desorption isotherms, from which the specific surface area, pore and micropore size distribution and concentration of reactive sites are obtained. The instrument is also equipped for carrying out chemisorption of different reactive molecules, as O_2, H_2, CO, etc.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Analizador científico de fisisorción ASAP2010 (Micromeritics)
  Physisorption analyser ASAP 2010 (Micromeritics)

- Analizador de quimisorción ASAP2010 (Micromeritics)
  Chemisorption analyser ASAP 2010 (Micromeritics)

- Analizador de fisisorción multimuestra TRISTAR II (Micromeritics)
  Multisample physisorption analyser TRISTAR II (Micromeritics)

- Analizador de fisisorción multimuestra TRISTAR II-Kr (Micromeritics)
  Multisample physisorption analyser TRISTAR II-Kr (Micromeritics)

Responsables Científicos/ Scientific Responsibles: Dr. Gerardo Colón Ibáñez y Dr. Alfonso Caballero Martínez
Personal Técnico/ Technical Assistant: Dª Cristina Gallardo López

ANÁLISIS TÉRMICO / THERMAL ANALYSIS

Las técnicas de análisis térmico permiten estudiar aquellos cambios físicos o químicos que ocurren en los sólidos en función de la temperatura y que conlleven modificaciones en su masa o intercambios de calor con su entorno.
En el servicio se pueden realizar experimentos desde temperatura ambiente hasta 1500 °C, tanto en atmósfera inerte (N_2) como reactiva (aire, O_2,…).
Se dispone de dos técnicas: Análisis Termogravimétrico (TG) y Análisis Térmico Diferencial (ATD).

Thermal analysis techniques allow to studying physical or chemical changes occurring in solid in samples as a function of the temperature. Those changes should involve either a mass change or a heat flow.
The experiments can be performed in the range from room temperature to 1500 °C, both under inert (N_2), or reactive (air, O_2,…) atmospheres.
Two different techniques are available: Thermogravimetry (TG) and Differential Thermal Analysis (DTA)

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Equipo termogravimétrico simultáneo TG/DTA/DSC STA449 F5 Jupiter (NETZSCH)
  STA449 F5 Jupiter (NETZSCH) Simultaneous TG/DTA/DSC Instrument

- Dilatómetro mecánico horizontal DIL 402 Expedis Select (NETZSCH)
  DIL 402 Expedis Select (NETZSCH) Horizontal Dilatometer

- Equipo de análisis térmico simultáneo TG/ATD/CDB TA Instruments Q600
  TA Instruments Q600 Simultaneous TG/DTA/DSC instrument

- Equipo termogravimétrico TG, TA Instruments Q5000
  Thermogravimetric instrument TG, TA Instruments Q5000

- Equipo de calorimetría Calvet, Setaram Sensys
  Calvet Calorimetry Equipment, Setaram Sensys

Responsable Científico/ Scientific Responsible: Dr. Luis A. Pérez Maqueda
Personal Técnico/ Technical Assistant: Dª Cristina Gallardo López

Servicio de Microscopía Electrónica / Electron Microscopy Service

El servicio está dedicado a la caracterización química y estructural de muestras sólidas mediante técnicas de microscopía electrónica. Las técnicas de caracterización disponibles en el servicio son la Microscopía Electrónica de Transmisión (TEM) y la Microscopía Electrónica de Barrido (SEM), con el equipamiento anexo de preparación de muestras para TEM y SEM.

This Service is devoted to the chemical and structural characterization of solid samples by means of electron microscopies. The characterization techniques available at ICMS are Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM), with additional equipment for TEM and SEM sample preparation.

Microscopía Electrónica de Barrido / Scanning Electron Microscopy

La microscopía electrónica de barrido proporciona información microestructural, morfológica y de composición química en escala microscópica. Se puede aplicar a todo tipo de materiales y problemáticas de estudio en ciencia de materiales: cerámicas, plásticos, metales, minerales, catalizadores, muestras de patrimonio histórico, capas finas, recubrimientos, interfases, nanopartículas, etc. El equipo SEM es un microscopio de emisión de campo de cátodo frío que permite realizar imágenes de la morfología y textura superficial de las muestras con una resolución de 1 nm a 15kV. También permite trabajar a bajo voltaje en muestras sin metalizar y en modo transmisión (STEM-in-SEM) en muestras electrón-transparentes. Acoplado al detector de rayos-X (EDX) permite análisis elementales y mapas composicionales.

The scanning electron microscopy provides information about the microstructure, morphology and chemical composition at the microscopic scale of solid samples. It can be applied to all type of materials including ceramics, polymers, metals, minerals, catalysts, samples from cultural heritage, thin films, coatings, interfaces, nanoparticles, etc. The SEM microscope is a field emission cold cathode equipment which enables images of the surface morphology and texture of samples with a resolution of 1 nm at 15kV. It also allows working at low voltages with non-metalized samples and in transmission mode for electron-transparent samples (STEM-in-SEM). Coupled to the X-ray detector (EDX) enables compositional analysis and elemental mapping.

Instrumental Disponible / Available Equipment

- Microscopio SEM, modelo Hitachi S4800 SEM-FEG: cañón de emisión de campo de cátodo frío y voltaje de 0.5-30 kV, resolución de 1 nm a 15kV. Dotado de analizador EDX Bruker-X Flash-4010 con una resolución de 133 eV (en la línea MnKα) y detector con portamuestras para trabajar en modo transmisión (STEM-in-SEM).
  Hitachi S4800 SEM-FEG microscope: cold cathode field emission gun with voltage from 0.5 to 30 kV, resolution of 1nm at 15 kV. Equipped with a Bruker-X Flash-4010 EDX detector with a resolution of 133 eV (at the MnKα line), and a detector with sample holder to work in transmission mode (STEM-in- SEM).
- Equipamiento adicional en el "laboratorio de preparación de muestras para microscopía electrónica"
  Additional equipment in the "electron microscopy samples preparation laboratory"

Responsable Científico/ Scientific Responsible: Dra. Asunción Fernández Camacho, Dra. Cristina T. Rojas Ruiz
Personal Técnico/ Technical Assistant: Dra. M. Carmen Jiménez de Haro

MICROSCOPÍA ELECTRÓNICA DE TRANSMISIÓN / TRANSMISSION ELECTRON MICROSCOPY

La microscopía electrónica de transmisión es una técnica ampliamente utilizada para la caracterización estructural y química de materiales a escala microscópica y nanoscópica, proporcionando imágenes bidimensionales de la textura de la muestra, forma y tamaño de grano y/o de partícula, grado de homogeneidad a escala microscópica, grado de cristalinidad de la muestra, identificación de fases cristalinas, e imágenes de alta resolución que identifican dominios cristalinos. El equipo está dotado de un analizador EDX para el análisis composicional. Puede aplicarse a todo tipo de materiales y campos de estudio en ciencia y tecnología de materiales trabajando sobre muestras electrón-transparentes preparadas en su caso ad-hoc para este fin. El servicio realiza microscopía en modo transmisión: Imágenes en campo claro y campo oscuro, difracción de electrones de área seleccionada y microscopía electrónica de alta resolución así como análisis elemental de área seleccionada. No se dispone de modo STEM.

The transmission electron microscopy is a widely used technique for the microstructural and chemical characterization at micro and nanoscales, providing two-dimensional images of the sample texture and shape as well as grain and/or particle size, degree of homogeneity at the microscopic scale, degree of crystallinity of the sample, identification of crystalline phases, and high resolution images to identify the crystalline domains. The microscope is equipped with an EDX analyzer for compositional analysis. It can be applied to all type of materials and research topics in materials science and technology working with electron-transparent samples prepared ad-hoc for this end. The service performs transmission electron microscopy: Imaging in bright and dark field, selected area electron diffraction and high resolution electron microscopy, as well as elemental analysis of selected areas. It does not provide STEM mode.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Microscopio JEOL 2100Plus (200kV) con filamento de LaB6. Resolución estructural de 0.14 nm entre líneas y 0.23 nm entre puntos, portamuestras de uno y dos giros. Acoplados al equipo se dispone de un sistema de análisis por Energías Dispersivas de Rayos X (EDX X-Max 80T, Oxford Instruments) y una cámara CCD (Gatan) para registro de imágenes. JEOL 2100Plus microscope (200kV) with LaB6 filament. Structural resolution of 0.14 nm between lines and 0.23 nm between points. Sample holders with one and two angles. An X-ray Energy Dispersive Analyzer (EDX X-Max 80T, Oxford Instruments) and a CCD camera (Gatan) for image registration are attached to the equipment.

- Equipamiento adicional en el "laboratorio de preparación de muestras para microscopía electrónica"
  Additional equipment in the "electron microscopy samples preparation laboratory"

Responsable Científico/ Scientific Responsible: Dra. Asunción Fernández Camacho, Dra. T. Cristina Rojas Ruiz

Personal Técnico/ Technical Assistant: Lda. Olga Montes Amorín, Dª María Inmaculada Rosa Cejudo

LABORATORIO DE NANOSCOPÍAS Y ESPECTROSCOPÍAS-LANE / ELECTRON MICROSCOPY SAMPLES PREPARATION LABORATORY

El laboratorio LANE cuenta con un microscopio TEM de emisión de campo Tecnai F30, dotado con modo STEM, detectores HAADF y EDX y filtro de energía (GIF). Las técnicas disponibles incluyen: medidas TEM en campo claro y campo oscuro; TEM de alta resolución; difracción de electrones; análisis STEM-HAADF; análisis EDX y STEM-EDX así como EELS y STEM-EELS, incluyendo medidas puntuales, en línea y mapas composicionales; imágenes EFTEM; análisis espectro-imagen y tomografía electrónica.

The LANE laboratory includes a Tecnai F30 field emission TEM microscope, equipped with STEM mode, HAADF and EDX detectors and an energy filter (GIF). Available techniques include: TEM measurements in bright and dark field; high resolution TEM; electron diffraction; STEM-HAADF analysis; EDX and STEM-EDX analysis as well as EELS and STEM-EELS, including point and in-line measurements and compositional maps; EFTEM images; spectrum-image analysis and electronic tomography.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Microscopio Tecnai G2 F30 S-TWIN de 300KV con cañón de emisión de campo. Resolución estructural de 0.2 nm entre puntos, portamuestras de uno y dos giros. Acoplados al equipo se dispone de un detector EDX Silicon Drift Detector X-Max 80T (Oxford Instruments) y un filtro de energías Gatan (GIF Quantum SE)
  Tecnai G2 F30 S-TWIN 300KV microscope with field emission gun. Structural resolution of 0.2 nm between points, sample holders with one and two angles. Attached to the equipment are an EDX Silicon Drift Detector X-Max 80T Detector (Oxford Instruments) and a Gatan energy filter (GIF Quantum SE)

- Equipamiento adicional en el "laboratorio de preparación de muestras para microscopía electrónica"
  Additional equipment in the "electron microscopy samples preparation laboratory"

Responsable Científico/ Scientific Responsible: Dra. Asunción Fernández Camacho, Dra. T. Cristina Rojas Ruiz

Personal Técnico/ Technical Assistant: Lda. Olga Montes Amorín, Dª María Inmaculada Rosa Cejudo

LABORATORIO DE PREPARACIÓN DE MUESTRAS PARA MICROSCOPÍA ELECTRÓNICA
ELECTRON MICROSCOPY SAMPLES PREPARATION LABORATORY

El laboratorio de preparación de muestras para TEM y SEM dispone de metalizador de oro, evaporador de carbón, metalizador de Cr y carbón, cortadora de disco, pulidora, "disc-grinder", cortadora ultrasónica, pulidora cóncava (dimple) y adelgazador iónico (Fischione 1010).

The laboratory for TEM and SEM samples preparation has a gold coater, a carbon evaporator, a metallization system for Cr and carbon, a diamond wheel cutter, a grinder with disc-grinder device, an ultrasonic cutter, a concave polishing (dimple) and ion thinning (Fischione 1010).

Responsable Científico/ Scientific Responsible: Dra. Asunción Fernández Camacho, Dra. T. Cristina Rojas
Personal Técnico/ Technical Assistants: Dª María Inmaculada Roja Cejudo, Lda. Olga Montes Amorín y Dra. M. Carmen Jiménez de Haro

PREPARACIÓN Y CARACTERIZACIÓN DE SISTEMAS CATALÍTICOS HETEROGÉNEOS / PREPARATION AND CHARACTERIZATION OF HETEROGENEOUS CATALYTIC SYSTEMS

Este Servicio puede suministrar todo tipo de muestras sólidas con actividad catalítica en diversos procesos de interés industrial, energético y medioambiental.
Las muestras se suministran en cualquier etapa de preparación, con o sin pretratamiento o incluso listas para ser utilizadas. Puede incluir su caracterización por diversas técnicas físicas y químicas.

This Service can supply all types of solid samples with catalytic activity in various processes of industrial, energy and environmental interest.
Samples are supplied at any stage of preparation, with or without pretreatment or even ready to use. It can include their characterization by various physical and chemical techniques.

PRESTACIONES DEL SERVICIO / SERVICES PROVIDED

- Preparación de muestras
  Sample preparation
- Tratamientos térmicos y químicos
  Thermal and chemical treatments
- Evaluación de las prestaciones catalíticas
  Evaluation of catalytic performance

Responsables Científicos/ Scientific Responsibles: Dr. Alfonso Caballero Martínez

SERVICIO DE DIFRACCIÓN DE RAYOS X / X-RAY DIFFRACTION LABORATORY SERVICE

La difracción de rayos-X permite la identificación cualitativa y cuantitativa de sustancias cristalinas y su caracterización microestructural y textural.
El servicio dispone en la actualidad de cuatro difractómetros independientes, configurados específicamente para abordar el análisis de muestras policristalinas de muy distinta naturaleza, en lo referente a su composición, estabilidad química, cristalinidad, etc.
Asimismo, con alguno de ellos se pueden llevar a cabo, además de los análisis rutinarios (θ-2θ), otros varios más avanzados, como pueden ser:

- Seguir las transformaciones de fase "in situ" provocadas por calentamientos en atmósfera inerte (vacío, Ar) o reactiva (H_2, O_2,..).
- Caracterizar materiales en la nanoescala (1-100 nm) mediante el estudio de la dispersión de rayos-X a ángulos bajos (SAXS).
- Determinar el grosor, densidad y rugosidad de películas delgadas, mediante Reflectometría de rayos-X.
- Obtener la estructura cristalina de materiales inestables a la atmósfera o muy transparentes a los rayos-X, mediante el empleo de capilares.

X-ray diffraction allows the qualitative and quantitative identification of crystalline substances and their microstructural and textural characterization.
At present, four independent diffractometers are available in this service, specifically configured to analyze the composition, chemical stability, crystallinity and many other properties in polycrystalline samples of a varied nature. Besides ordinary analyses (θ-2θ), part of the equipment can perform some advanced studies as:

- Direct monitoring of transformations undergone in materials under heating, such as phase changes, under inert o reactive atmosphere.
- To characterize materials at the nanoscale (1-100 nm) through X-ray scattering at low angles, using the SAXS technique.
- To measure some physical parameters of layers such as density, thickness and surface roughness with the reflectometry setup.
- To obtain the diffraction patterns of samples either sensitive to the atmosphere or highly transparent to X-rays (organic compounds) employing the capillary configuration.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Difractómetro Panalytical X'PERT PRO con cargador automático de muestras
  Diffractometer PANALYTICAL X'PERT PRO with automatic sample charger

- Difractómetro PHILIPS X'PERT PRO con cámara de alta temperatura (1200 °C) ANTON PAAR HTK 1200
  Diffractometer PHILIPS X'PERT PRO with high temperature chamber (1200 °C) ANTON PAAR HTK 1200

- Difractómetro Panalytical X'PERT PRO (reflectometría, SAXS, ángulo rasante y capilares)
  Diffractometer PANALYTICAL X'PERT PRO (reflectometry, SAXS, low angle scattering and capillary)

- Difractómetro de polvo SIEMENS D5000 DUAL (reflexión y transmisión)
  Diffractometer SIEMENS D5000 DUAL (reflection and transmission)

Responsable Científico/ Scientific Responsible: Dra. Concepción Real Pérez
Personal Técnico/Technical Assistant: Dr. José María Martínez Blanes y Gdo. Angel Arias Pérez

SERVICIO DE ANÁLISIS DE SUPERFICIE/ SURFACE ANALYSIS SERVICE

El Servicio de Análisis de superficie consta de un espectrómetro de Espectroscopía de Fotoelectrones de Rayos X (XPS). Este servicio está dedicado al análisis químico y electrónico de superficies sólidas. También permiten conocer la composición en profundidad (desde la superficie hacia el interior) de los sólidos.

The surface analysis service consists of an X-ray Photoelectron Spectrometer (XPS). This service is devoted to the electronic and chemical analysis of solid surfaces. It also provides information about the compositional depth profile of solids (from their surface toward their bulk).

ANÁLISIS QUÍMICO DE SUPERFICIES POR FOTOEMISIÓN / CHEMICAL SURFACE ANALYSIS BY ELECTRON PHOTOEMISION

Las "Espectroscopías de Fotoelectrones" (XPS/ESCA y AES) son unas poderosas técnicas de análisis cuantitativo no destructivo, sensibles exclusivamente a las primeras capas de la superficie de los sólidos (20-30 Å), lo que permite obtener información sobre las propiedades químicas, físicas y electrónicas de las mismas.
El interés técnico de esta información es enorme en campos tales como corrosión, catálisis, tratamientos de superficies, fenómenos de flotación y adherencia, segregación de fases, etc.
La característica más importante de la Espectroscopía de Fotoelectrones (XPS/ESCA) es que permitir diferenciar distintos estados de oxidación y/o situaciones del entorno (coordinación) de los átomos en las muestras sólidas analizadas. El límite de detección es del 0.5% para cada especie química. El servicio dispone actualmente de dos instrumentos independientes.

Typically, "photoelectron spectroscopies" are a powerful set of non-destructive analysis techniques, exclusively sensitive to the more superficial few atomic layers (20-30 Å), allowing to obtain valuable information about their chemical, physical and electronic properties.
The technical interest of the resulting information is huge in fields such as catalysis, corrosion, surface treatments, floating and adhesion phenomena, or segregation processes, among others. The most remarkable characteristic of X-Ray Photoelectron Spectroscopy (XPS/ESCA) is that it allows to discriminate, for a given element, between different oxidation states or chemical surroundings (coordination).

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

Espectrómetro de Fotoelectrones PHOIBOS 100-DLD, compuesto de:
Photoelectron Spectrometer PHOIBOS 100-DLD, consisting on:

- Cámara de análisis, analizador hemiesférico multicanal PHOIBOS 100-DLD, manipulador de cuatro ejes, y fuentes de excitación de rayos X (dual, AlKα y MgKα, acromático), de luz ultravioleta y de haces de electrones, lo que permite realizar análisis superficiales mediante técnicas de XPS, UPS, ISS y REELS, así como estudios angulares.
  Analysis Chamber, equipped with a hemispheric multichannel analyser PHOIBOS 100-DLD, a four axis manipulator, a dual X-ray source (achromatic AlKα, Mg Kα), a UV lamp, and a electron gun, allowing to perform surface analysis by XPS, UPS. ISS and REELS, including angular resolved studies.

- Dos Precámaras de tratamientos, con vacío residual de 10^{-8} y 10^{-9} mbar respectivamente, en las que es posible someter a las muestras a tratamientos diversos como: calentamientos a alta temperatura (T<800 °C) bajo atmósfera controlada, desbastado iónico con gases inertes o reactivos, exposición a plasmas, iluminación con laser, deposición de metales, óxidos y compuestos sencillos, exfoliación in situ, etc.
  Two prechambers for different treatments, with ultimate vacuum levels of 10^{-8} and 10^{-9} mbar respectively, where samples can be subjected to diverse treatments and transferred to the analysis chamber without exposure to the atmosphere. The possible treatments include heating at high temperature (< 800 °C) under controlled atmosphere, ion sputtering with inert or reactive gases, exposure to plasma, laser treatments, deposition of metals, oxides or simple compounds, exfoliation, etc.

Espectrómetro de Fotoelectrones SPECS, compuesto de:
Photoelectron Spectrometer SPECS, consisting on:

- Cámara de análisis, dotada de analizador hemiesférico multicanal PHOIBOS 100, manipulador de tres ejes, y fuentes de excitación de rayos X (dual, Alkα y MgKα).
  Analysis Chamber, equipped with a hemispheric multichannel analyser PHOIBOS 100, three axis manipulator and dual X-ray source (achromatic Al Kα, Mg Kα).

- Precámara de tratamiento de alta presión y alta temperatura (HPHT Cell). En esta Cámara es posible someter a las muestras a tratamientos térmicos en presencia de gases hasta una presión de 20 atm y 800 °C, tanto en estático como en dinámico (simultáneamente).
  Pre-chamber for High Pressure/High Temperature treatments (HPHT Cell).Samples can be subjected to treatments in the presence of gases up to 20 bar and 800 °C (simultaneously). These treatments can be performed either under static or flowing gas conditions. After treatments, samples can be transferred to the analysis chamber without exposure to the atmosphere.

- Una cámara de inserción rápida dotada de sistema de aparcamiento/ desgasificado, que permite evacuar las muestras a temperatura reducida (T < 150 °C). También es posible la realización de tratamientos de desbatado iónico o la incorporación de otros sistemas (iluminación con luz UV-Vis, evaporación de metales, u otros compuestos, etc.)

A Fast entry chamber, equipped with a parking and degassing system, allowing the samples to be evacuated at moderate temperature (T < 150 °C). It is also possible to sputter the samples under an accelerated ion beam (0.5- 5.0 kV) using inert or reactive gases. Incorporation of some other equipment (Visible light illumination, metal evaporators) is also contemplated.

Responsables Científicos/ Scientific Responsibles: Dr. Juan Pedro Espinós Manzorro y Dr. Juan Pedro Holgado Vázquez
Personal Técnico/Technical Assistant: Dra. Florencia Vattier Lagarrigue, Lda. Verónica Rodríguez Bravo

DETERMINACIÓN DEL MOJADO EN SUPERFICIES/ CONTACT ANGLE AND SURFACE TENSION DETERMINATION SERVICE

La caracterización avanzada del mojado mediante un goniómetro para la determinación del ángulo de contacto de gotas de líquido depositadas sobre una superficie es una técnica de análisis cuantitativo y no destructivo en general, dependiendo de la reactividad que presente el material con el líquido de mojado. La combinación de varios líquidos permite determinar la tensión superficial del material que se moja y realizar estimaciones del trabajo de adhesión en ambientes controlados. El control de la mojabilidad de materiales y superficies inteligentes, bajo la acción de estímulos externos como la aplicación de luz, gradientes de temperatura y/o humedad, cambio de pH o campos eléctricos, son de vital interés en aplicaciones avanzadas de la industria aeronáutica, líneas de comunicación, transporte, protección, patrimonio, energía solar y eólica o biomedicina, entre otras.
La determinación del ángulo de contacto se realiza mediante la aplicación de la ecuación de Young para el equilibrio de tensiones interfaciales, con sensibilidad a escala nanométrica. Los ensayos se pueden realizar en modo estático o en modo dinámico para la obtención de histéresis (ángulo de avance y retroceso) de superficies y valores críticos de deslizamiento de gotas. En cuanto a la tensión superficial del material, los modelos teóricos implementados son los de Owens, Wendt, Rabel and Kaelble, Extended Fowkes, Schultz y Van Oss&Good y Neumann, basados en la existencia de componentes polares y dispersivas. Además, el seguimiento temporal del ángulo de contacto de una superficie da cuenta del envejecimiento y estabilidad en determinados ambientes de uso. Finalmente, la asistencia de una cámara de temperatura y humedad controlada permite la realización de estudios de condensación/evaporación y congelación / descongelación de agua en superficies.
El equipo de medida de ángulo de contacto y tensión superficial, ha sido subvencionado por la Junta de Andalucía (Ayudas a Infraestructuras y equipamientos de I+D+i 2019-PAIDI2020 Fondo Europeo de Desarrollo Regional.

Advanced characterization of wetting using a goniometer to determine the contact angle of liquid droplets deposited on a surface is a quantitative and non-destructive analysis technique in general, depending on the surface reactivity with the wetting liquid. The combination of several liquids allows to determine the surface tension of the wet solid and to estimate the work of adhesion in simulated environments. The control of the wettability of smart surfaces under the action of external stimuli such as the application of light, temperature and/or humidity gradients, changes in pH or electric fields, are of great interest in advanced applications for the aeronautical industry, lines of communication, transportation, protection, heritage, solar and wind energy or biomedicine, among others.

Determination of the contact angle is carried out by applying Young's equation for interfacial tension balance, with sensitivity at the nanometric scale. The tests can be carried out in static or in dynamic modes to obtain hysteresis (advanced and receding angle values) of surfaces and critical values of droplet sliding. Regarding the surface tension of the solid surface, implemented theoretical models are those of Owens, Wendt, Rabel and Kaelble, Extended Fowkes, Schultz and Van Oss&Good and Neumann, based on the existence of polar and dispersive components. In addition, the temporal tracking of the surface contact angle accounts for aging and stability in certain environments. Finally, the assistance of a controlled temperature and humidity chamber allows studies of condensation/evaporation and freezing/thawing of water on surfaces.
The contact angle and surface tension measurement equipment has been supported by the Junta de Andalucía (Aid for R&D infrastructure and equipment 2019-PAIDI2020 European Regional Development Fund)

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

Goniómetro de ángulo de contacto óptico OCA 25 de DataPhysics, compuesto de:
DataPhysics OCA 25 Optical Contact Angle Goniometer, consisting of:

- Sistema de inyección doble con volumen de gota líquida, entre los nanolitros (cercano al estado del arte de la técnica) a las decenas de microlitros, controlado por una válvula magnética para su dispensación.
  Double injection system with liquid drop volume, between nanoliters (close to the state of the art) to tens of microliters, controlled by a magnetic valve for dispensing

- Plataforma de giro TBU100 para estudios de deslizamiento de gotas sobre la superficie (-5° - 95°)
  TBU100 tilting platform for studies of droplet sliding on the surface (-5° - 95°)

- Base portamuestras orientable en las 3 direcciones espaciales
  TBU100 tilting platform for studies of droplet sliding on the surface (-5° - 95°)

- Módulo termoeléctrico TPC160 para el control de la temperatura (de -30°C a 150°C)
  TPC160 thermoelectric module for temperature control (from -30°C to 150°C)

- Módulo para la aplicación de campo eléctrico EWP100 en estudios de estimulación del mojado por campos eléctricos (0-64kV DC/AC, distancia electrodos 3-10mm)
  Module for the application of electric field EWP100 in studies of wetting electrostimulation (0-64kV DC/AC, 3-10mm electrode distance)

- Cámara de electrohumedecimiento HGC30 para el control de la humedad de la atmósfera ambiental (de 5% a 90%)
  HGC30 electro-humidification chamber to control the humidity of the environment (from 5% to 90%)

- Software SCA 21 con rutina integrada para la estimación de tensiones superficiales (0.01-2000 mN/m)
  SCA 21 software with routine for surface tension estimation (0.01-2000 mN/m)

- Sistemas de visualización frontal (3250 f/s) y vertical (2450 f/s)
  Front (3250 f/s) and vertical (2450 f/s) optical systems

Responsable Científico/ Scientific Responsible: Dra. Carmen López Santos

CARACTERIZACIÓN TRIBOLÓGICA Y MECÁNICA DE SUPERFICIES / TRIBOLOGICAL AND MECHANICAL SURFACE CHARACTERIZATION SERVICE

El nanoindentador KLA G200x permite la evaluación de las propiedades mecánicas en la nanoescala (dureza, módulo de Young) lo cual resulta fundamental para recubrimientos y tratamiento superficiales, obviando la contribución del sustrato. La técnica CSM (Continuous Stiffness Measurement) permite una medida continua de la rigidez en función de la penetración o frecuencia. Se trata de una herramienta muy útil no sólo para materiales rígidos como los metales, cerámicas o aleaciones sino también para materiales con comportamiento dependiente del tiempo como polímeros, compuestos o biomédicos.
El equipo cuenta con dos cabezales (baja carga y alta carga) que permite barrer rangos de cargas de hasta 50 y 500 mN, respectivamente.
El servicio incluye la posibilidad de realizar una caracterización superficial por microscopía óptica confocal e interferométrica para conocer la topografía 3D y rugosidad iniciales y después de haber sido sometidas a ensayos mecánicos o tribológicos.

The KLA G200x nanoindenter enables the evaluation of the mechanical properties in the nanoscale (hardness, Young's modulus) which results crucial for thin films and surface treatments, discarding the substrate influence. The CSM (Continuous Stiffness Measurement) option allows a continuous measurement of the stiffness as a function of the frequency or penetration. This operational mode results very useful not only for rigid materials as metals, ceramic or alloys, but also for materials with mechanical response dependent on time, like polymers, composites or biomedical.
The equipment disposes of two actuators (low and high load) that cover forces range up to 50 and 500 mN, respectively.
Additionally, the service includes the possibility of recording the 3D-surface properties by optical and interpherometric microscopy to evaluate the topography and roughness of the initial state of specimens and after being submitted to mechanical and tribological essays.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

- Nanoindentador KLA G200x
  Nanoindenter KLA G200x

- Perfilómetro óptico-3D confocal e interferométrico SENSOFAR S-Neox
  3D-optical profiler confocal and interferometric SENSOFAR S-Neox

Responsable Científico/ Scientific Responsible: Dr. Juan Carlos Sánchez López
Personal Técnico/Technical Assistant: Lda. Belinda Sigüenza Carballo

SERVICIO DE MECANIZADO/ MACHINING WORKSHOP

Se trata de un servicio horizontal fundamental para el Instituto y unidades externas adscritas al mismo, ya que permite mejorar, modificar y adecuar el material y equipamiento científico a las necesidades de cada investigador y/o investigación en curso, incluso llegando a su fabricación partiendo de una necesidad concreta. Ofrece asesoramiento técnico, diseño y fabricación de todos los elementos anteriormente descritos. Además brinda la posibilidad de realizar pequeñas reparaciones y parte del mantenimiento general del equipamiento científico y de laboratorio.

This is a service essential for the Institute and external drives attached to the same. Because it allows you to improve, modify and adapt the material and scientific equipment to the needs of each researcher and/or research in progress. Even going to the extent of their manufacture on the basis of a specific need. Offering technical advice, design and manufacture of all elements described above.

INSTRUMENTAL DISPONIBLE / AVAILABLE EQUIPMENT

El servicio dispone de herramientas manuales y herramientas eléctricas para la conformación de una amplia gama de materiales, contando con la posibilidad de unión de diversos materiales mediante procesos de soldeo.

The service has manual tools and electric tools for the shaping of a wide range of materials, with the possibility of joining different materials by welding processes:

- Soldadura fuerte con diferentes aportes
  Brazing with different contributions

- Soldadura por arco eléctrico
  Electric arc welding

- Soldadura TIG sobre aceros
  TIG welding on steel

Para los procesos de mecanizado por arranque de viruta se cuenta con las siguientes máquinas-herramientas:
The following machine tools are available for chip removal machining processes:

- Centro de mecanizado,HAAS TM 1P
  HAAS CNC milling machine,TM 1P

- Taladro vertical, ERLO TSAR32
  Vertical drill, ERLO TSAR32

- Torno paralelo convencional PINACHO SC200
  Conventional lathe PINACHO SC200

- Torno paralelo semiautomático PINACHO SMART TURN180
  Semi-automatic lathePINACHO SMART TURN180

- Fresadora de torreta Fortex FTX-4-FC VARIO
  Fortex FTX-4-FC VARIO Milling Machine

Personal Técnico/Technical Assistant: D. Juan Carlos Sánchez Martín, D. Adrián Gómez Castaño

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Ruthenium nanoparticles stabilized by 1,2,3-triazolylidene ligands in the hydrogen isotope exchange of E–H bonds (E = B, Si, Ge, Sn) using deuterium gas

Molinillo, P; Puyo, M.; Vattier, F; Lacroix, B; Rendón, N.; Lara, P; Suárez, A
Nanoscale, **904** (2023) 14488-14495
Agosto, 2023 · DOI: 10.1039/D3NR02637J

A series of ruthenium nanoparticles (Ru·MIC) stabilized with different mesoionic 1,2,3-triazolylidene (MIC) ligands were prepared by decomposition of the Ru(COD)(COT) (COD = 1,5-cyclooctadiene; COT = 1,3,5-cyclooctatriene) precursor with H_2 (3 bar) in the presence of substoichiometric amounts of the stabilizer (0.1–0.2 equiv.). Small and monodisperse nanoparticles exhibiting mean sizes between 1.1 and 1.2 nm were obtained, whose characterization was carried out by means of transmission electron microscopy (TEM), including high resolution TEM (HRTEM), inductively coupled plasma (ICP) analysis and X-ray photoelectron spectroscopy (XPS). In particular, XPS measurements confirmed the presence of MIC ligands on the surfaces of the nanoparticles. The Ru·MIC nanoparticles were used in the isotopic H/D exchange of different hydrosilanes, hydroboranes, hydrogermananes and hydrostannanes using deuterium gas under mild conditions (1.0 mol% Ru, 1 bar D_2, 55 °C). Selective labelling of the E–H (E = B, Si, Ge, Sn) bond in these derivatives, with high levels of deuterium incorporation, was observed.

Threads of memory: Reviving the ornament of a dead child at the Neolithic village of Ba`ja (Jordan)

Alarashi, H; Benz, M; Gresky, J; Burkhardt, A; Fischer, A; Gourichon, L; Gerlitzki, M; Manfred, M; Sakalauskaite, J; Demarchi, B; Mackie, M; Colins, M; Odriozola, CP; Garrido Cordero, JA; Avilés, MA; Vigorelli, L; Re, A; Gebel HGK
Plos One, **18** (2023)
Agosto, 2023 · DOI: 10.1371/journal.pone.0288075

In 2018, a well-constructed cist-type grave was discovered at Ba`ja, a Neolithic village (7,400-6,800 BCE) in Southern Jordan. Underneath multiple grave layers, an 8-year-old child was buried in a fetal position. Over 2,500 beads were found on the chest and neck, along with a double perforated stone pendant and a delicately engraved mother-of-pearl ring discovered among the concentration of beads. The first was found behind the neck, and the second on the chest. The meticulous documentation of the bead distribution indicated that the assemblage was a composite ornament that had gradually collapsed, partly due to the burying position. Our aim was to challenge time degradation and to reimagine the initial composition in order to best explore the significance of this symbolic category of material culture, not as mere group of beads, but as an ornamental creation with further aesthetic, artisanal and socioeconomic implications. The reconstruction results exceeded our expectations as it revealed an

imposing multi-row necklace of complex structure and attractive design. Through multiple lines of evidence, we suggest that the necklace was created at Ba`ja, although significant parts of beads were made from exotic shells and stones, including fossil amber, an unprecedented material never attested before for this period. The retrieval of such an ornament from life and its attribution to a young dead child highlights the significant social status of this individual. Beyond the symbolic functions related to identity, the necklace is believed to have played a key role in performing the inhumation rituals, understood as a public event gathering families, relatives, and people from other villages. In this sense, the necklace is not seen as belonging completely to the realm of death but rather to the world of the living, materializing a collective memory and shared moments of emotions and social cohesion.

Actividades Divulgativas
Outreach Activities

CONFERENCIAS INVITADAS IMPARTIDAS POR PERSONAL DEL ICMS
INVITED CONFERENCES BY PERSONNEL OF THE ICMS

04 Abril | **Tuning the nanocolumnar film morphology for industrial applications by magnetron sputtering: perspectives and challenges**
Dr. Alberto Palmero Acebedo
Lugar: Conferencia on-line, MDPI Sciforum

12 Abril | **Thermal treatments of biomass**
Dra. Francisca Romero Sarria
Lugar: École Doctorale. Université de Caen-Normandie (Francia)

CONFERENCIAS Y SEMINARIOS IMPARTIDOS EN EL ICMS
CONFERENCES AND SEMINAR IN THE ICMS

29 junio 2023 · **Dried whole blood as a material for the detection of pathogens**
Prof. Enrique Valera
Universidad de Illinois Urbana-Champaign (EEUU)

We introduce a new approach to blood-based diagnostics where large blood volumes can be rapidly dried, resulting in inactivation of the inhibitory components in blood. In this approach thermal treatments generate a physical microscale and nanoscale fluidic network inside the dried matrix to allow access to target nucleic acid. High heme background is confined to the solid phase, while amplicons are enriched in the clear supernatant (liquid phase), giving fluorescence change comparable to purified DNA reactions. We demonstrate single-molecule sensitivity using a LAMP reaction in our platform and detect a broad spectrum of pathogens, including MRSA, MSSA, E.Coli and Candida albicans from whole blood with a limit of detection of 1.2 CFU/mL in <2.5 h

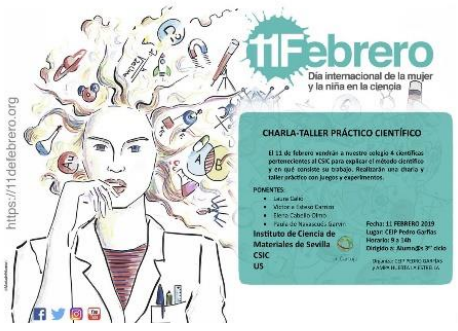
14 septiembre 2023 · **Nanomaterials at the frontline of the energy challenge**
Prof. Valeria Nicolosi
Trinity College Dublin, School of Chemistry, CRANN, AMBER and IForm Centres, Dublin 2, Ireland

Liquid phase exfoliation has been proved to be a cheap, scalable method for the mass production of 2D sheets. This talk will first discuss the galaxy of existent layered materials, with emphasis on synthesis, liquid-phase exfoliation, and characterization, focusing on some key applications recently developed in our laboratories, ranging from energy storage to printed electronics. We will for example discuss how two-dimensional nanomaterials can be formulated in aqueous and organic viscous inks for extrusion printing, inkjet printing, and aerosol jet 3D printing, and demonstrate direct printing on various substrates. The additive- and binary solvent-free inks do not show coffee ring effect, enabling high-resolution printing without substrate pre-treatment. The resulting printed micro-supercapacitors showcase excellent charge storage performance, including areal capacitance up to 100 mF/cm^2 and volumetric capacitance up to 800 F/cm^3 in protic gel electrolyte, coupled with long lifetime and good flexibility. The versatile direct-ink-printing technique highlights the promise of 2D nanomaterials functional inks for scalable fabrication of easy-to-integrate components of printable electronics. In this talk we will also

demonstrate how such inks can be used to develop novel nanomaterials-based battery solutions. Increasing the energy storage capability of batteries necessitates maximization of their areal capacity. This requires thick electrodes performing at near-theoretical specific capacity. However, achievable electrode thicknesses are restricted by mechanical instabilities, with high-thickness performance limited by the attainable electrode conductivity. Here we show that forming a segregated network composite of carbon nanotubes with a range of lithium storage materials (for example, silicon, graphite, and metal oxide particles) suppresses mechanical instabilities by toughening the composite, allowing the fabrication of high-performance electrodes with thicknesses of up to 800 μm. Such composite electrodes display conductivities up to 1 × 104 S m^{-1} and low charge-transfer resistances, allowing fast charge-delivery and enabling near-theoretical specific capacities, even for thick electrodes. The combination of high thickness and specific capacity leads to areal capacities of up to 45 and 30 mAh cm^{-2} for anodes and cathodes, respectively. Combining optimized composite anodes and cathodes yields full cells with state-of-the-art areal capacities (29 mAh cm^{-2}) and specific/volumetric energies (480 Wh kg^{-1} and 1,600 Wh l−1).Andrey Nazarov, Boris Knyazer, Tova Lifshitz, Mark Schvartzman, Ibrahim Abdulhalim, Assessment of intraocular pressure sensing using an implanted reflective flexible membrane, J. Biomed. Opt., 22(4), 047001 (2017).

DIVULGACIÓN / DISSEMINATION

PARTICIPACION EN EL DÍA INTERNACIONAL DE LA MUJER Y LA NIÑA EN LA CIENCIA/ INTERNATIONAL WOMEN AND GIRL'S DAY IN SCIENCE



La ciencia y la igualdad de género son vitales para alcanzar los Objetivos de Desarrollo Sostenible (ODS). Por ello y con el fin de lograr el acceso y la participación plena y equitativa en la ciencia para las mujeres y las niñas, y además para lograr la igualdad de género, la Asamblea General de las Naciones Unidas decidió proclamar en 2016 el 11 de febrero como el Día Internacional de la Mujer y la Niña en la Ciencia. Para la celebración de este día y con el objetivo de dar a conocer el papel de la mujer en la ciencia y fomentar las vocaciones científicas en las niñas, se organizan en España, a través de la plataforma 11F, muchas actividades donde han participado científicos/as y becarios/as del ICMS.

Charlas:

- Científicas ilustres: de la piedra al grafeno. Rosalía Poyato Galan. IES Cavaleri (Mairena del Aljarafe). 10 de febrero. Alumnos de 3º de la ESO
- Un paseo por la investigación científica. Ana Isabel Becerro Nieto. IES Salvador Távora. 11 de febrero. Alumnos de 4º de la ESO y 1º y 2º de Bachillerato.
- "Plasma...¿el cuarto estado de la materia?" Ana María Gómez Ramírez y Manuel Oliva Ramírez. 14 de febrero. IES María Galiana, Montequinto..
- Una científica en tu cole andaluz: ¿Qué sabes de los materiales? Rosalía Poyato Galán. 17 de febrero. Colegio Esclavas SCJ Jerez.. Alumnos de 4º y 5º de Primaria.

Charlas-Talleres

- ¡Seamos científic@s por un día!. Ana Isabel Borrás Martos, Fernando Núñez Gálvez, José Manuel Obrero Pérez, Juan Delgado Álvarez, Ángel Barranco Quero, Víctor López Flores, Víctor Rico Gavira, Vanda Cristina Fortio Godinho, Juan Ramón Sánchez Valencia, Xabier García Casas, Noel Orozco Corrales, Darío Jumilla Núñez, Nerea de Tena Álvarez, Melania Sánchez Villa. 7 de febrero. Colegio Mª Auxiliadora Salesianas (Sevilla). 750 alumnos de Infantil, Primaria y Ciclos Formativos
- ¿Qué hacen los científic@s? +Talleres "Triboeléctricas". Dario Jumilla Nuñez, Pedro Javier Lloreda Jurado, Ana Isabel Borras Martos, Iru Nerea de Tena Alvarez, Lidia Contreras Bernal, Juan Delgado Alvarez, Melania Sanchez Villa, Noel Orozco Corrales, Triana Czermak Alvarez. 8 de febrero. IES Antonio Machado (Sevilla). 150 alumnos de 3º de la ESO
- Mujeres, Luz y Matería. Thi Tuyen Ngo. 9 de febrero. CEIP Pablo Ruiz Picasso, Pino Montano (Sevilla). Alumnos de 3º y 4º de primaria.
- ¿Cómo almacenaremos la energía del futuro?. 9 de febrero. IES Antonio de Ulloa, San José de la Rinconada (Sevilla). Alumnos de 1º y 2º de Bachillerato y 4º de la ESO.
- ¿Qué hacen los científic@s? +Talleres "Triboeléctricas". Victor López Flores, Dario Jumilla Núñez, Ana Isabel Borrás Martos, Nerea de Tena Álvarez, Jorge Budagosky Marcilla, Francisco J. Aparicio Rebollo, Laura Montes Montañez, Fernando Núñez Gálvez, Jaime del Moral Jalón, Juan Delgado Álvarez, Triana Czermak Álvarez, Carmen López Santos. 9 de febrero. IES Margarita Salas (Sevilla). 150 alumnos de 4º ESO, 1º y 2º Bachillerato y Ciclo Formativo de Farmacia
- Las chicas de ciencia también molamos. Marta Romero, Maribel Domínguez, Débora Álvarez, Marcela Martínez. 10 de febrero. Colegio Salesianos de San Juan Bosco, Morón de la Frontera (Sevilla). Alumnos de la ESO
- ¿Qué hacen los científic@s? +Talleres "Triboeléctricas". Ana Isabel Borrás Martos, Iru Nerea de Tena Álvarez, Darío Jumilla Núñez, Jaime del Moral Jalón, Gloria Patricia Moreno Martínez, Victor López Flores, Javier Castillo Seoane, Lidia Contreras Bernal, José Manuel Obrero Pérez. 10 de febrero. IES Gerena (Gerena, Sevilla). 60 alumnos de 4º de la ESO y Bachillerato
- Viaje al mundo de los materiales. Laura Caliò, Ngo Thi Tuyen, Beatriz De Sola Báez, María Morán Pedroso, Clara Bujalance Aguilera. 10 de febrero. CEIP Pedro Garfias (Sevilla). Alumnos de 3º y 4º de la ESO.
- ¿"Cómo almacenaremos la energía del futuro"? Gisela Mariana Arzac. Charla y demostración sobre el hidrógeno y celdas de combustible. 11 de febrero. IES Antonio de Ulloa (la Rinconada). Alumnos de 1º y 2º de Bachillerato y 4º de la ESO.
- Científicas y Energías Renovables. Andrea Vañes Vallejo, Beatriz de Sola Baéz, María Morán Pedroso. 13 de febrero. CEIP El Llanete (Morón de la Frontera). Alumnos de 3º-6º de primaria.
- ¿Qué hacen los científic@s? +Talleres "Triboeléctricas". Ana Isabel Borrás; Ángel Barranco; Nerea de Tena Álvarez; Xabier García; Elisa Guisado; Francisco Javier Martínez. 13 de febrero. IES Llanes (Sevilla). 30 alumnos (ESO)
- "Plasmanía - Ciencia XX 2023; mujeres de CienciAFicción". Ana María Gómez Ramírez. 10 de febrero. Colegio de Educación Infantil "La Raza". Alumnos de primaria.
- Nanotecnología para energía limpia. Gloria Patricia Moreno Martínez, Laura Montes, Javier Castillo, Lidia Contreras. 15 de febrero. IES Pino Rueda (Umbrete). Alumnos de 4º de la ESO y en el IES Tartessos (Camas). Alumnos de 4º de la ESO y 1º de Bachillerato

- ¿Qué hacen los científic@s?+Talleres. Ana Isabel Borrás Martos, Jaime del Moral Jalón, Dario Jumilla Núñez, Javier Lloreda, Jorge Budagosky, Juan Ramón Sanchez Valencia, Angel Barranco Quero, Mikel Martinez Olaizola, Xabier Garcia Casas, Melania Sanchez, Triana Czemark, Nerea de Tena Álvarez, Víctor López Flores. 21 de febrero. Attendis (Espartinas, Sevilla). 250 alumnos de Infantil y Primaria
- La ciencia también es cosa de chicas. María Isabel Domínguez; Débora Álvarez; Estela Ruiz López; Juan Luis Martín Espejo; Ligia Amelia Luque Álvarez; Guillermo Sempere; Angel Bochs Cruz; Sergio Carrasco; Melania Serrano; Marcela Martínez Tejada; Victor López Flores; Ana Isabel Borrás Martos; Iru Nerea de Tena Álvarez; Dario Jumilla; Gloria Patricia Moreno Martínez; Laura Montes Montañez; Fernando Núñez; Juan Delgado Álvarez; Triana Czermak; Jaime del Moral Jalón. CEIP Joaquín Turina, 13 de marzo. Alumnos de Infantil y Primaria

FESTIVAL DE NANOCIENCÍA Y NANOTECNOLOGÍA 10 A LA MENOS 9 / NANOSCIENCE AND NANOTECHNOLOGY 10 A LA MENOS 9

El VII Festival de Nanociencia, es un festival organizado a nivel nacional, que pretende, de una forma amena, acercar a todos los públicos la escala nanométrica, sus efectos y cómo este conocimiento va a cambiar nuestras vidas a través de innumerables aplicaciones y productos.

Días 13 y 19 de abril

Visita al ICMS de Los alumnos del colegio "Las Salesianas de Sevilla" y IES Juan de Mairena

Charla: Bienvenidos al mundo de los nanomateriales: Dr. Juan Ramón Sánchez-Valencia

Visita guiada a los laboratorios: Como preparamos y vemos los nanomateriales

Laboratorio de solidos coloidales: Ana Isabel Becerro, Elizabet Gómez, Nuria Núñez
Laboratorio de técnicas de plasma y tecnología de vacío: Victor Rico y Cristina Rojas
Laboratorio de catálisis: Celda de Hidrogeno: Gisela Arzac
Laboratorio de materiales ópticos MOM: Manuel Romero y Clara Bujalance
Microscopio Electrónico de Transmisión: T. Cristina Rojas y Gisela Arzac

Día 21 de abril

Taller fabricación de celda solar de colorante. IES Antonio de Ulloa (La Rinconada), Mauricio Calvo y Gisela Arzac

Días 11 y 24 de mayo

Intercambiando energía con la nanotecnología: CEIP Juan Ramon Jiménez-Los Viveros, y CEIP Rico Cejudo. Actividades realizadas por el Grupo de Nanotecnología en superficies y plasma

CONCURSO DE NANORELATOS

Este concurso, a nivel de Andalucía, está organizado por el Instituto de Ciencia de Materiales de Sevilla, dentro del marco del VII Festival de la Nanociencia y la Nanotecnología 10alamenos9. El objetivo de este concurso es fomentar en la comunidad educativa el interés por el mundo a escala nanométrica, el denominado nanomundo, que a pesar de su diminuto tamaño es muy diverso e interesante. Hay dos categorías, una para estudiantes de 14-15 años (A) y otra para 16-17 años (B), dotadas con premios de 200€ y diploma.

Ganadores: Categoría A: "Ratón de biblioteca", que en verdad es Cristina Hernández Utrilla (4º ESO, Colegio San Juan Bosco de Sevilla), con su relato titulado "Una última esperanza".
Accésit: IodineVictorIV que en verdad es Victor Hernando Saucedo (3º ESO, Colegio San Juan Bosco de Sevilla), con su relato titulado "Viaje al centro de la sangre".
Categoría B: "Gerardo Raya", que en verdad es Mª de las Mercedes Rodríguez Gálvez (1º bachillerato de las Escuelas Profesionales de la Sagrada Familia de Sevilla), con su relato titulado "Soluciones extraordinarias para diagnósticos extraordinarios"

FERIA DE LA CIENCIA / FAIR OF SCIENCE

La 21 Feria de la Ciencia de Sevilla del 2023, 4ª Feria Virtual (del 10 al 12 de mayo de 2023), constituye un punto de encuentro donde se desarrollan actividades de divulgación de la Ciencia y la Tecnología, realizando demostraciones y experimentos para facilitar la comprensión de contenidos científicos.
La exposición del ICMS se centra en tres de los ejes temáticos de la Feria de la Ciencia: Ciencias para el Desarrollo Sostenible, Acción por el clima y STEM, y ha sido organizada por los miembros de la comisión de divulgación del Instituto, realizando actividades y demostraciones enmarcadas en distintas temáticas:

Produciendo energía de forma sostenible: Celda de combustible, Fabricación de una celda solar de colorante o celda de Graetzel, triboelectricidad. **Generando superficies autolimpiables.** Y para los más peques: Aprendemos sobre materiales de forma divertida con juegos de cartas, viendo materiales con microscopios USB.
Exposición de carteles sobre los Materiales que nos rodean.

Participantes: Gisela Arzac, Rosalía Poyato Galan, Juan Ramon Sanchez-Valencia, Juan Pedro Holgado, T. Cristina Rojas, Maria del Carmen Hidalgo,Francisco Javier Coto Ruiz, Beatriz de Sola Báez, Mauricio Calvo, Manuel Romero, Gabriel Lozano Barbero, Clara Bujalance, Maria Morán, Ngo Thi Tuyen, Encarnación Arroyo, Alvaro Carmo de Can, Gerardo Colon, Víctor Rico Gavira, Nuria Núñez, Mª Hiedra Acosta, Ana de la Cruz Blanco, Darío Jumilla, Mikel Martinez, Juan Delgado, Nerea de Tena Alvarez , Fernando Núñez, Triana Czermark Alvarez, Laura Montes Martinez, Gloria Patricia Moreno, Florencia Vattier Lagarrigue, Carlos Martinez Garcia, Angel Arias Perez, Antonio Moreno Gonzalez, Andrea Vañes Vallejo, Nabil Mohamed Amghar

The Fair of Science (10 to 12 May 2023, in Seville) constitutes a meeting point where many activities for spreading of science and technology were carried out. Demonstrations and experiments where presented to facilitate the understanding of scientific aspects.

PARTICIPACION EN LA NOCHE EUROPEA / EUROPEAN RESEARCHERS' NIGHT

La Noche Europea de los Investigadores (#NIGHTs-pain. www.lanochedelosinvestigadores.es) celebrada el 29 septiembre de 2023 en Sevilla, es un proyecto de divulgación científica enmarcado en Horizonte 2020, bajo las acciones Marie Skłodowska-Curie. Su principal objetivo es acercar los investigadores a los ciudadanos para que conozcan su trabajo, los beneficios que aportan a la sociedad y su repercusión en la vida cotidiana. Se celebra simultáneamente en 371 ciudades europeas desde 2005.

El ICMS ha participado con las siguientes actividades:

Talleres:

- Color estructural. Ngo Thi Tuyen, María Morán Pedroso
- Grafeno+ Cerámica = Biomaterial para prótesis más duraderas. Rosalía Poyato Galán
- La magia de los materiales. Ángela Gallardo López, Rocío Moriche Tirado, Carmen Muñoz Ferreiro, Felipe Gutiérrez Mora, Ana Morales Rodríguez, Ana de la Cruz Blanco

SEMANA DE LA CIENCIA Y LA TECNOLOGÍA / SCIENCE AND TECHNOLOGY WEEK

La semana de la Ciencia, celebrada en el ICMS y cicCartuja los días 9 y 10 de noviembre con visitas de escolares , café con ciencia y las jornadas de jóvenes científicos, es un evento de carácter europeo diseñado para demostrar cómo la ciencia y la tecnología nos afectan y cómo éstas pueden ser utilizadas para mejorar nuestras vidas y el mundo que nos rodea.

Café con Ciencia

El café con Ciencia acerca de forma original y atractiva la ciencia y sus protagonistas. Esta actividad de divulgación genera un punto de contacto entre profesionales de la ciencia y alumnos de secundaria, promoviendo la reflexión sobre diversos asuntos en un entorno cercano y participativo.
En esta edición se compartió un desayuno virtual con estudiantes de bachillerato para dialogar sobre temas concretos de sus estudios y sobre sus respectivas trayectorias profesionales. Esta actividad cumple el triple objetivo de comunicar la ciencia a través de sus propios protagonistas, promover la cultura científica y fomentar vocaciones investigadoras.
Las mesas de encuentro tienen una hora de duración, y se desarrollan con grupos reducidos de quince alumnos.

Mesa. *Revoluciones Tecnológicas del Siglo XXI: de la Nanomedicina a la Inteligencia Artificial*. Dr. Alberto Palmero Acebedo

PROGRAMA CULTURAL de la Red Municipal de Bibliotecas de Sevilla

Charla dirigida a Centros Educativos de ESO, Bachillerato, organizadas por el Instituto de las Cultura y las Artes de Sevilla."Energía Solar de Concentración: cuando los rayos del sol se cosechan". Dr. Juan Carlos Sánchez López. 14 de noviembre. Biblioteca de San Jerónimo.

CIENCIA EN EL BARRIO

Ciencia en el barrio es una iniciativa del CSIC de divulgación científica por la igualdad que acerca la ciencia a barrios de Madrid, Sevilla y Barcelona que no contaban con esta oferta cultural.
Taller de "Luminiscencia y Nanociencia". Ana Isabel Becerro Nieto.IES Santa Aurelia (Sevilla) Alumnos de 4º ESO

MATERIAL DE DIVULGACIÓN

- **Análisis de los estereotipos de género y de la percepción que tiene el alumnado de primaria sobre la actividad científica y el papel de la ciencia en la sociedad. Un estudio a través del dibujo infantil**
  Gisela M. Arzac, Cristina Rojas
  Material-ES 2023:7(4);78-80
  LITERATURA DE DIVULGACIÓN

- **ColaboRaciones: Premios Manuel Losada Villasante en su XI Edición**
  Luis Pérez-Villarejo, Pedro J. Sánchez Soto
  Revista Químicos del Sur. Número 115, pgs. 56-59 (2023)
  ARTÍCULOS EN REVISTA

- **Entregados los Premios de Investigación cicCartuja-Ebro Foods**
  Concepción Real Pérez, Pedro J. Sánchez Soto
  Revista Químicos del Sur. Número 115, pgs. 60-61 (2023)
  ARTÍCULOS EN REVISTA

- **Premios de Investigación de la Real Maestranza de Caballería de Sevilla y de la Real Academia Sevillana de Ciencias**
  Pedro J. Sánchez Soto
  Revista Químicos del Sur. Número 115, pgs. 53-55 (2023)
  ARTÍCULOS EN REVISTA

- **Un buen lanzamiento…de altos vuelos**
  Pedro J. Sánchez Soto
  Revista Químicos del Sur. Número 115, pgs. 3-6 (2023)
  EDITORIAL

- **Investigadores de Jaén patentan un cemento menos contaminante fabricado con cenizas de cáscar de arroz**
  MD Eliche Quesada, Pedro J. Sánchez Soto
  Europa Press. Octubre (2023)
  NOTICIAS

- **Químicos del Sur. Una profesión al servicio de la sociedad**
  Pedro J. Sánchez Soto
  Revista Químicos del Sur. Número 115, pgs. 92-93 (2023)
  RESEÑA BIBLIOGRÁFICA

- **CSIC Cicerón. Fabricación sostenible de nanomateriales para energías limpias**
  Ana Isabel Borrás Martos, Ángel Barranco Quero
  Gabinete de Comunicación CSIC
  https://www.youtube.com/watch?v=eqvFxTBY4fM
  MATERIAL AUDIOVISUAL

- **CSIC Cicerón. La nanotecnología de fabricación de películas delgadas al auxilio de la electrolisis para la producción de hidrógeno**
  Francisco Yubero Valencia
  Delegación del CSIC en Asturias
  https://delegacion.asturias.csic.es/wp-content/uploads/2023/09/CICERON_Francsico-Yubero_ICMS1.mov
  MATERIAL AUDIOVISUAL

- **Científicas y tecnólogas del futuro**
  Cristina Rojas, Encarnación Arroyo, Gisela Arzac
  Red Municipal de Bibliotecas
  https://www.rmbs.es/blog/biblioteca-san-jeronimo/cientificas-y-tecnologas-del-futuro/
  MATERIAL AUDIOVISUAL

- **Los Ma-tch-teriales**
  Rosalía Poyato
  El canal de Lola la Científica
  https://www.youtube.com/watch?v=jafrWrO4jlo
  MATERIAL AUDIOVISUAL

- **Lecciones de la naturaleza para domar el hielo y recolectar energía**
  Raúl Limón, Ángel Barranco Quero, Ana Isabel Borrás Martos
  El País. 4 diciembre 2023
  http://elpais.com/ciencia/2023-12-04/lecciones-de-la-naturaleza-para-domar-el-hielo-y-recolectar-energia.html
  PRENSA

- **Un científico utrerano colabora en la patente de un cemento más ligero y menos contaminante**
  Pedro J. Sánchez Soto
  El Periódico de Utrera. Noviembre 2023
  PRENSA

- **Tarjetas de contacto del proyecto "Sound of Ice" destinada a público industrial en ferias, congresos y encuentros**
  Nerea de Tena Álvarez, Ana Isabel Borrás Martos
  MATERIAL DOCENTE

- **Fichas didácticas para la celebración de talleres destinados a Primaria sobre hidrofobicidad, fluidos no newtoniano, el experimento de Newton, cromatografía en papel**
  Vanda Fortio
  MATERIAL DOCENTE

- **Concurso mediante la aplicación 'Plickers' sobre el 11F, el ámbito de las energías limpias y su relación con el plasma y el objetivo de los dos proyectos europeos 3DScavenegrs y Sound of Ice**
  Lidia Contreras Bernal, Javier Castillo Seoane, Laura Montes Montañez
  JUEGOS DIDÁCTICOS INTERACTIVOS

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