ICMS

Instituto de Ciencia de Materiales de Sevilla

Memoria de Actividades
Annual Report

Consejo Superior de Investigaciones Científicas

Universidad de Sevilla

Junta de Andalucía

2022

Consejo Superior de Investigaciones Científicas
Universidad de Sevilla
Junta de Andalucía

Instituto de Ciencia de Materiales de Sevilla

Memoria de Actividades
Annual Report
2022

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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

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Presentación

A través de esta Memoria 2022, 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 2022, contaba con 148 empleados, de los cuales 60 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 2022, 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 148 people, 60 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 et cetera.

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.

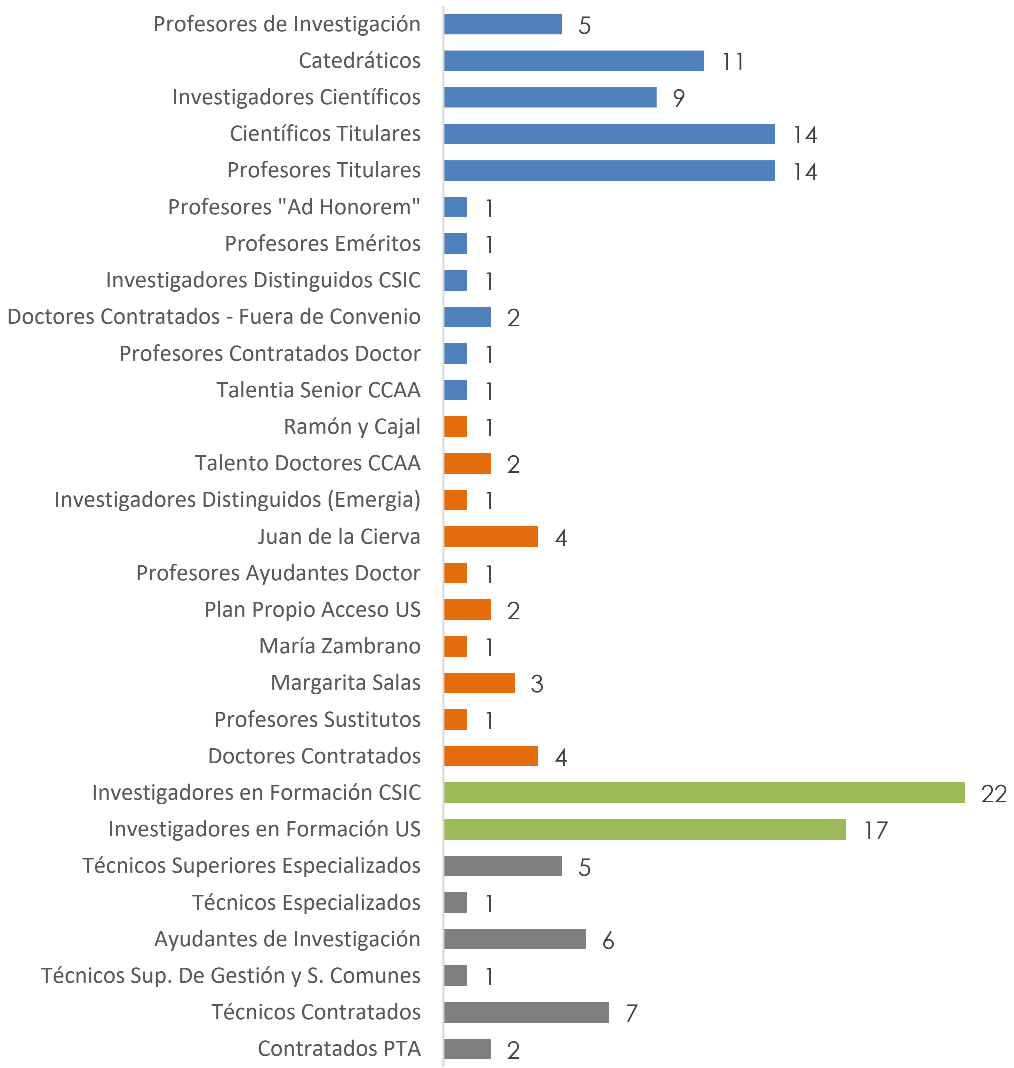
Dr. Juan Pedro Espinós Manzorro
Director of the Institute of Materials Science of Seville

El ICMS en 2022
ICMS in 2022

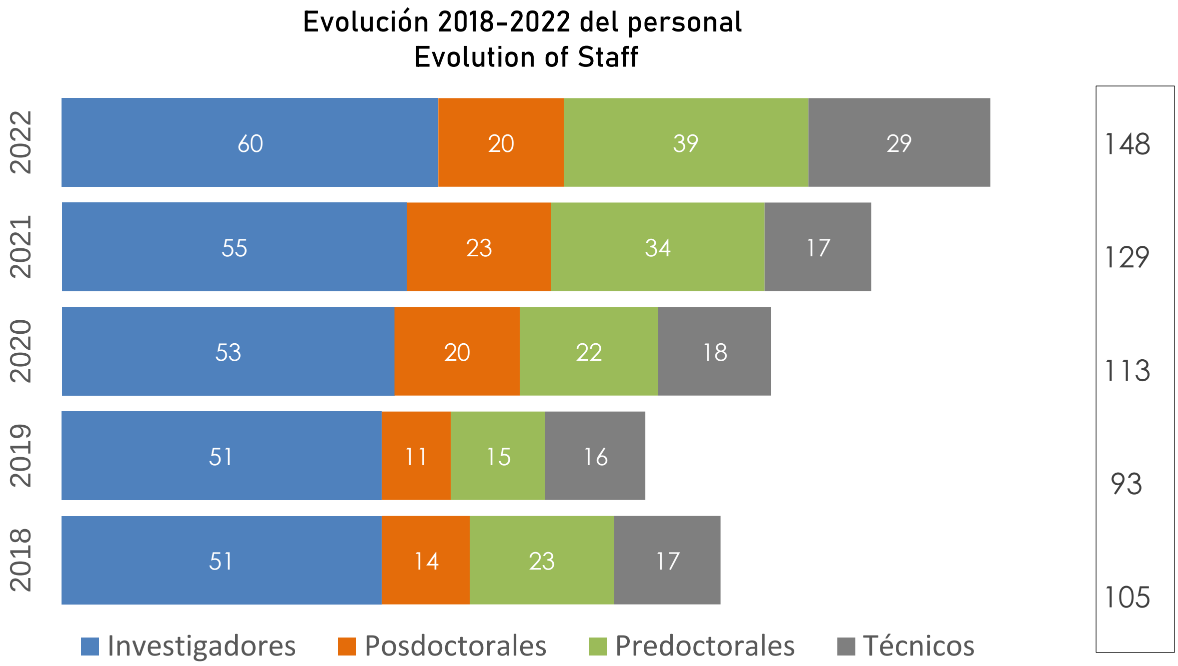
Datos Estadísticos del ICMS
Statistical Data of ICMS

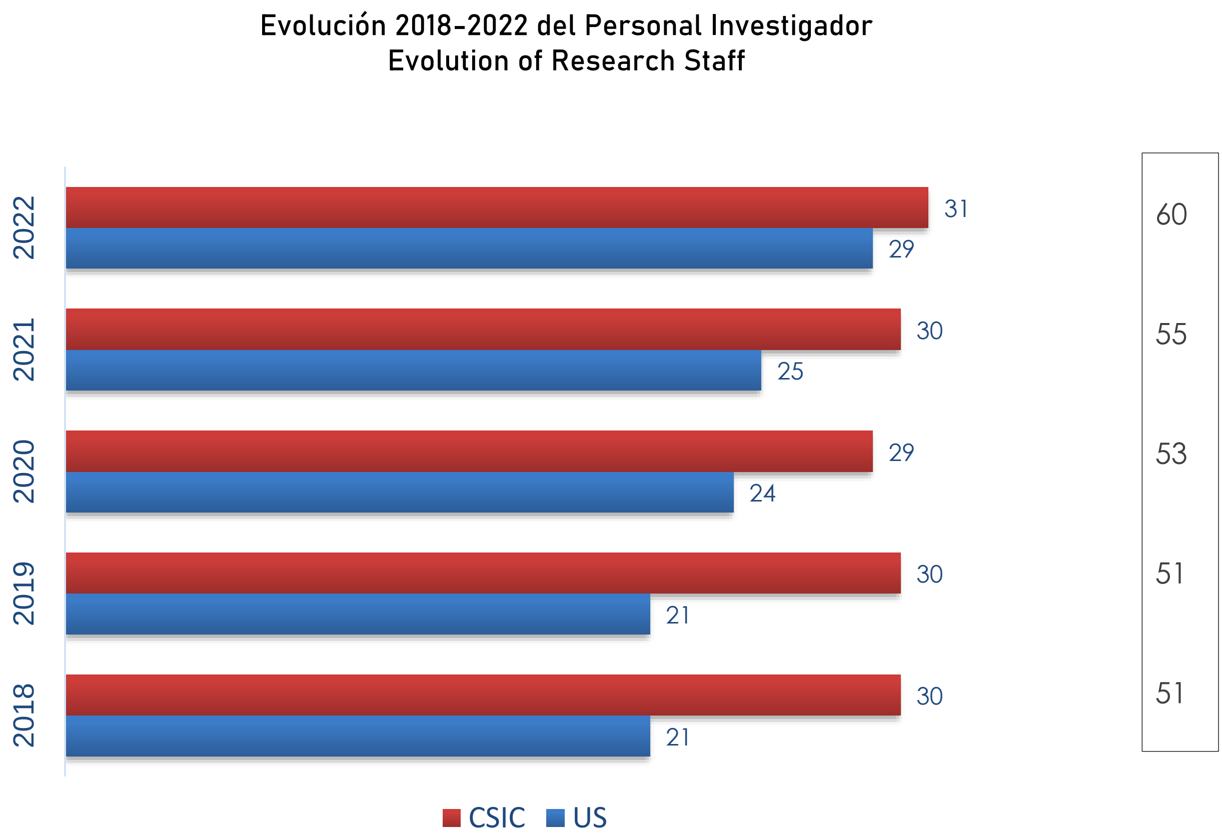
RECURSOS HUMANOS / HUMAN RESOURCES

Distribución del personal por categorías
Distribution by professional category

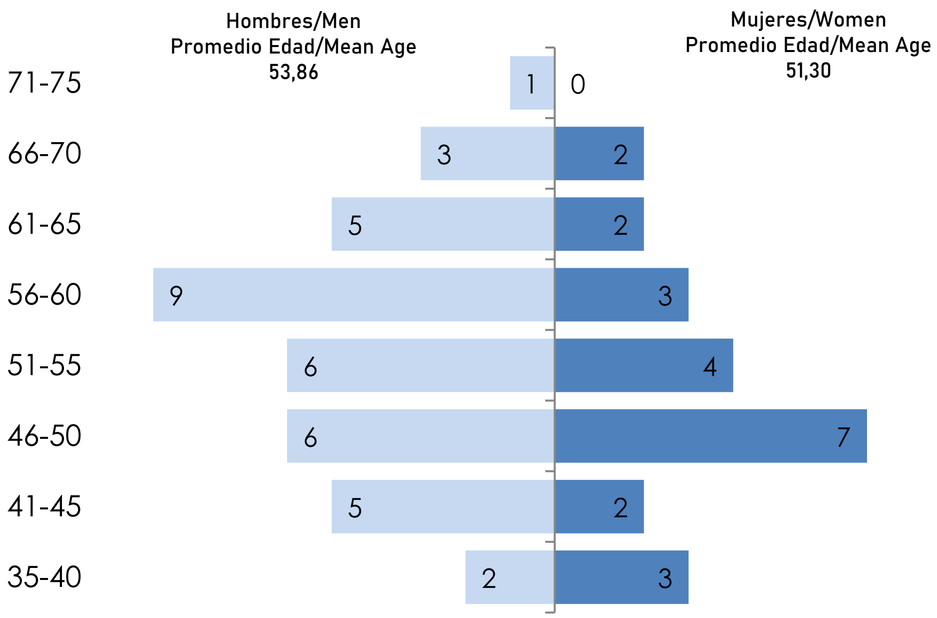


*Datos a 31 de Diciembre de 2022


Evolución 2018-2022 del personal
Evolution of Staff
2022
60
20
39
29
148
2021
55
23
34
17
129
2020
53
20
22
18
113
2019
51
11
15
16
93
2018
51
14
23
17
105
Investigadores
Posdoctorales
Predoctorales
Técnicos


Evolución 2018-2022 del Personal Investigador
Evolution of Research Staff
2022
31
29
60
2021
30
25
55
2020
29
24
53
2019
30
21
51
2018
30
21
51
CSIC
US

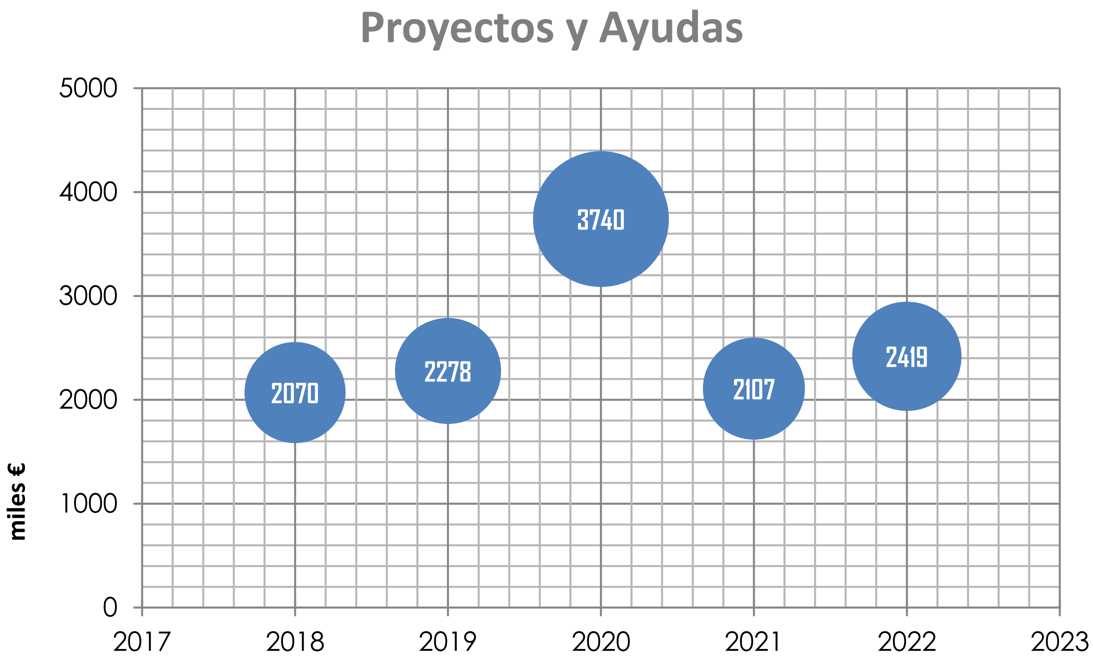
Distribución del personal Investigador (sexo y edad)
Distribution by Scientific staff (gender and age)



Promedio Edad/Mean Age
52,88

FINANCIACIÓN / FUNDING

Financiación conseguida por año (miles€)(PCO)
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
Number of Scientific Papers published in a Specific Journal Arranged by Their Impact Factor (SCI)

Revista Journal	Artículos Papers	Factor De Impacto Impact Factor (*)	Mejor Pct	
Progress in Energy and Combustion Science	1	29,5	D1	Q1
Advanced Materials	1	29,4	D1	Q1
Advanced Energy Materials	1	27,8	D1	Q1
Applied Catalysis B: Environmental	3	22,1	D1	Q1
Nano Energy	1	17,6	D1	Q1
Renewable & Sustainable Energy Reviews	1	15,9	D1	Q1
Chemical Engineering Journal	4	15,1	D1	Q1
Journal of the American Chemical Society	1	15	D1	Q1
Critical Reviews in Environmental Science and Technology	1	12,6	D1	Q1
Journal of Materials Chemistry A	1	11,9	D1	Q1
Journal of Cleaner Production	1	11,1	D1	Q1
Food Hydrocolloids	1	10,7	D1	Q1
Energy Conversion and Management	2	10,4	D1	Q1
Science of the Total Environment	1	9,8	D1	Q1
Journal of Energy Storage	2	9,4		Q1
Current Opinion in Green and Sustainable Chemistry	1	9,3		Q1
Advanced Optical Materials	2	9	D1	Q1
Energy	2	9	D1	Q1
Chemosphere	1	8,8		Q1
Journal of Environmental Chemical Engineering	1	8,7	D1	Q1
Renewable Energy	1	8,7		Q1
ACS Sustanaible Chemistry & Engineering	1	8,4	D1	Q1
Applied Materials Today	2	8,3		Q1
International Journal of Biological Macromolecules	1	8,2	D1	Q1
Food Research International	1	8,1	D1	Q1
Solar RRL	1	7,9		Q1
Materials Today Sustainability	2	7,8		Q1

Revista Journal	Artículos Papers	Factor De Impacto Impact Factor (*)	Mejor Pct	
Journal of CO2 Utilization	1	7,7		Q1
Journal of Environmental Chemical Engineering	1	7,7		Q1
Fuel	6	7,4		Q1
Inorganic Chemistry Frontiers	1	7	D1	Q1
Solar Energy Materials and Solar Cells	1	6,9		Q1
Alexandria Engineering Journal	1	6,8	D1	Q1
Applied Surface Science	2	6,7	D1	Q1
Nanoscale	2	6,7		Q1
Journal of Materials Chemistry C	1	6,4		Q1
Journal of Alloys and Compounds	3	6,2	D1	Q1
Biomass & Bioenergy	1	6		Q1
Sustainable Chemistry and Pharmacy	1	6		Q1
ACS Applied Nano Materials	2	5,9		Q2
Journal of Physical Chemistry Letters	1	5,7		Q1
Journal of the European Ceramic Society	2	5,7	D1	Q1
Frontiers in Plant Science	1	5,6	D1	Q1
International Journal of Molecular Sciences	2	5,6		Q1
Applied Catalysis A: General	2	5,5		Q2
Frontiers in Chemistry	2	5,5		Q2
Surface & Coatings Technology	1	5,4		Q1
Catalysis Today	6	5,3		Q1
Energy & Fuels	2	5,3		Q1
Nanomaterials	2	5,3		Q1
Ceramics International	2	5,2		Q1
Materials Advances	1	5		Q2
Polymers	1	5		Q1
Results in Engineering	1	5		Q1
Chemical Communications	1	4,9		Q2
Molecular Catalysis	1	4,6		Q2
Archives of Civil and Mechanical Engineering	1	4,4		Q1
Journal of Central South University	1	4,4		Q1
Journal of Thermal Analysis and Calorimetry	2	4,4		Q1
Photochemical & Photobiological Sciences	1	4,33		Q2

Revista Journal	Artículos Papers	Factor De Impacto Impact Factor (*)	Mejor Pct	
Journal of Photochemistry and Photobiology A-Chemistry	1	4,3		Q2
Chemosensors	1	4,2		Q2
Biomass Conversionand Biorefinery	1	4		Q2
Chemelectrochem	1	4		Q2
Catalysts	1	3,9		Q2
Chemical Engineering Research and Design	1	3,9		Q2
Journal of Clinical Medicine	1	3,9		Q1
Materials Today Communications	1	3,8		Q2
Advanced Photonics Research	1	3,7		Q2
International Journal of Refractory Metals & Materials	1	3,6		Q1
Materials Science and Engineering: B	1	3,6		Q2
Plasma Processes and Polymers	3	3,5		Q1
Royal Society Open Science	1	3,5		Q1
Boletin de la Sociedad Española de Ceramica y Vidrio	3	3,4		Q1
European Physical Journal Plus	1	3,4		Q1
Materials	7	3,4		Q2
Journal of Solid State Chemistry	1	3,3		Q2
Materials Letters	1	3		Q2
Journal of the Iranian Chemical Society	1	2,4		Q3
Chemistry	1	2,1		Q3
International Journal of Applied Ceramic Technology	1	2,1		Q2
Reaction Kinetics Mechanisms and Catalysis	2	1,8		Q4
Surface and Interface Analysis	1	1,7		Q4
Total	**128**	**7,23**		

Mejor PCT									
D1		Q1		Q2		Q3		Q4	
38	29,69 %	94	73,44 %	29	22,83 %	2	1,57 %	3	2,36 %

(*) Factor de Impacto correspondiente al año 2022
Journal Citation Reports of 2022

Composición y Estructura

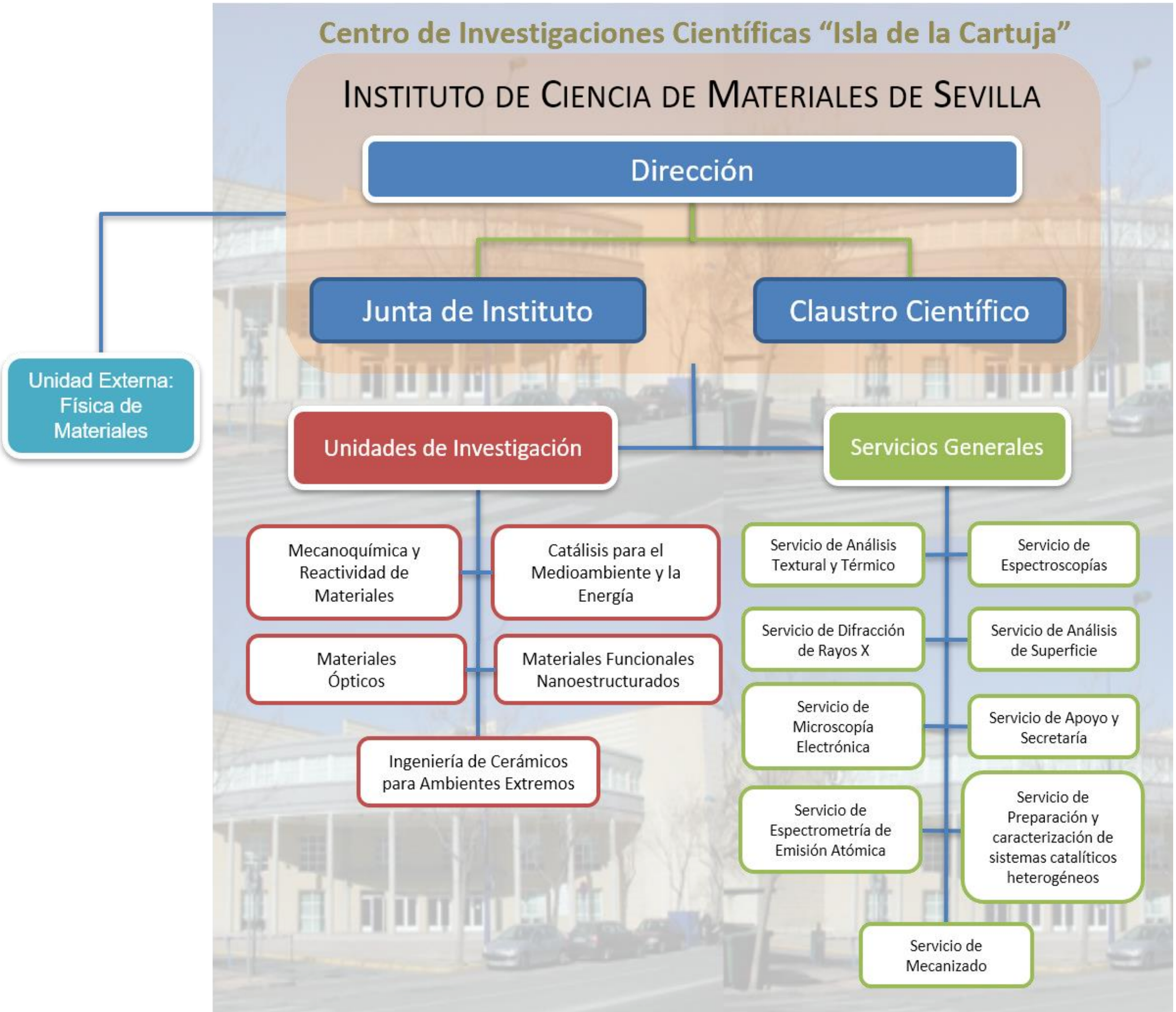
Structure and Organisation

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 (Junta de Andalucía - Consejo Superior de Investigaciones Científicas - Universidad de Sevilla). 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 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 (Junta de Andalucía - Consejo Superior de Investigaciones Científicas - Universidad de Sevilla). 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 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



DIRECCIÓN / DIRECTORATE

Director / Director:	Dr. **Juan Pedro Espinós Manzorro**
Vicedirectora / Vicedirector:	Dra. **Anna Dimitrova Penkova**

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Dra. **Svetlana Lyubomirova Ivanova**
Representante del Personal Científico de plantilla del CSIC
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Representante del Personal No Científico y No Profesorado de plantilla
D. **Juan Carlos Martín Sánchez**

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Alcalá González, María Dolores
Álvarez Molina, Rafael
Aparicio Rebollo, Francisco J.
Arcenegui Troya, Juan Jesús
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
Budagosky Marcilla, Jorge A.
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.
Contreras Bernal, Lidia
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 de los Reyes, Daniel
Fortio Godinho, Vanda
Franco García, Víctorino
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 Castaño, Miriam
González Mancebo, Daniel
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
L
López Flores, Víctor
López Santos, Carmen
Lozano Barbero, Gabriel
M
Malet Maenner, Pilar
Manchón Gordón, Alejandro F.
Martín Olalla, José María
Martínez Blanes, José María
Martínez Fernández, Julián
Martínez Martínez, Sergio
Martínez Tejada, Leidy Marcela
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
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
Pérez Maqueda, Luis Allan
Poyato Galán, Rosalía
R
Ramírez de Arellano-López, Antonio
Ramírez Rico, Joaquín
Ramírez Reina, Tomás
Real Pérez, Concepción
Regodón Harkness,Guillermo
Rico Gavira, J. Víctor
Rguez. González-Elipe, Agustín
Rojas Ruiz, T. Cristina
Romero Landa, Francisco Javier
Romero Sarria, Francisca
Ruiz López, Estela
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
Y
Yubero Valencia, Francisco

Directorio / Directory

Unidades de Investigación / Research Units

Catálisis para el medioambiente y la Energía
Catalysis for Enviroment and energy

Catedráticos	Dr. Alfonso Caballero Martínez
	Dra. Svetlana Ivanova
	Dr. José Antonio Odriozola Gordón
Investigadores Científicos	Dr. Miguel Ángel Centeno Gallego
	Dr. Gerardo Colón Ibáñez
Científicos Titulares	Dra. M. Carmen Hidalgo López
	Dr. Juan Pedro Holgado Vázquez
Profesores Titulares	Dr. Luis F. Bobadilla Baladrón
	Dr. José Manuel Córdoba Gallego
	Dra. María Isabel Domínguez Leal
	Dra. Leidy Marcela Martínez Tejada
	Dra. Anna Dimitrova Penkova
	Dra. Rosa María Pereñíguez Rodríguez
	Dr. Tomás Ramírez Reina
	Dra. Francisca Romero Sarria
Profesores Eméritos	Dr. José Antonio Navío Santos
Doctores Contratados	Dra. Miriam González Castaño
	Dr. Muhammad Asif Nawaz
	Dra. Laura Pastor Pérez
	Dra. Estela Ruiz López
Investigadores en Formación	Gda. Débora Álvarez Hernández
	Gdo. José Rubén Blay Roger
	Gdo. Sergio Carrasco Ruiz
	Gda. Ligia Amelia Luque Álvarez
	Gdo. Juan Luis Martín Espejo
	Gda. María Ribota Peláez
	Lda. María Saif
Técnicos Contratados	Gdo. Marcos González Tejero
Garantía Juvenil	Gdo. Ángel Bochs Cruz
	Gdo. Álvaro Grijuela Gaciño

INGENIERÍA DE CERÁMICAS PARA MEDIOAMBIENTES AGRESIVOS
ENGINEERED CERAMICS FOR EXTREME ENVIRONMENTS

Catedráticos	Dr. Miguel Ángel Castro Arroyo
	Dr. Manuel Jiménez Melendo
	Dra. Pilar Malet Maenner
	Dr. Julián Martínez Fernández
	Dr. Antonio Ramírez de Arellano-López
	Dr. Joaquín Ramírez Rico
Investigadores Científicos	Dra. María Dolores Alba Carranza
Científicos Titulares	Dr. José Jesús Benítez Jiménez
Profesores Titulares	Dr. Alfonso Bravo León
Doctores Contratados	Dra. Esperanza Pavón González
Investigadores en Formación	Lda. Ana Castro Chincho
	Gda. Sol Fernández Muñoz
	Gda. Irene Lamata Bermejo
	Gdo. Marcos Vázquez González

MECANOQUÍMICA Y REACTIVIDAD DE MATERIALES
MECHANOCHEMISTRY AND REACTIVITY OF MATERIALS

Profesores de Investigación	Dr. Luis Allan Pérez Maqueda
Catedráticos	Dr. Diego Gómez García
Investigadores Científicos	Dr. Francisco José Gotor Martínez
	Dra. Concepción Real Pérez
	Dr. Pedro José Sánchez Soto
Científicos Titulares	Dra. Rosalía Poyato Galán
	Dra. María Jesús Sayagués de Vega
Profesores Titulares	Dra. María Dolores Alcalá González
	Dra. María Regla Ayala Espinar
	Dr. Antonio Perejón Pazo
Talentia Senior CCAA	Dr. Pedro E. Sánchez Jiménez
Doctores Contratados	Dr. Juan Jesús Arcenegui Troya
	Dra. Eva Gil González
	Dr. Alejandro F. Manchón Gordón
	Dr. Sergio Martínez Martínez
Investigadores en Formación	Ldo. Nabil Mohamed Amghar
	Gda. Sandra Molina Molina
Garantía Juvenil	Gda. Andrea Vañes Vallejo

MATERIALES FUNCIONALES NANOESTRUCTURADOS
NANOSTRUCTURED FUNCTIONAL MATERIALS

Profesores de Investigación	Dr. Juan Pedro Espinós Manzorro
	Dra. Asunción Fernández Camacho
Catedráticos	Dr. José Cotrino Bautista
Investigadores Científicos	Dr. Ángel Barranco Quero
	Dr. Juan Carlos Sánchez López
	Dr. Francisco Yubero Valencia
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	Dra. María Aránzazu Díaz Cuenca
	Dr. Alberto Palmero Acebedo
	Dra. T. Cristina Rojas Ruiz
	Dr. Juan Ramón Sánchez Valencia
Profesores Titulares	Dr. Rafael Álvarez Molina
	Dra. Ana María Gómez Ramírez
Profesores "Ad Honorem"	Dr. Agustín Rodríguez González-Elipe
Doctores (Laboral Fijo)	Dra. Vanda Cristina Fortio Godinho
	Dr. Jorge Gil Rostra
Doctores Contratados	Dr. Francisco J. Aparicio Rebollo
	Dr. Jorge A. Budagosky Marcilla
	Dra. Lidia Contreras Bernal
	Dr. Daniel Fernández de los Reyes
	Dr. Víctor López Flores
	Dra. Carmen López Santos
	Dr. Manuel Oliva Ramírez
	Dr. Guillermo F. Regodón Harkness
Investigadores en Formación	Ldo. Javier Castillo Seoane
	Gda. Triana Czermak Álvarez
	Gdo. Jaime Del Moral Jalón
	Gdo. Juan Delgado Álvarez
	Ldo. Xabier García Casas
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Research Units

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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

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PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Reactores estructurados no convencionales para el craqueo catalítico de metano libre de CO_2

Structured unconventional reactors for CO_2-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)

MINISTERIO DE CIENCIA E INNOVACIÓN
Financiado por la Unión Europea NextGenerationEU
Plan de Recuperación, Transformación y Resiliencia
AGENCIA ESTATAL DE INVESTIGACIÓN

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)

MINISTERIO DE CIENCIA E INNOVACIÓN
UNIÓN EUROPEA
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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 bad-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)

MINISTERIO DE CIENCIA E INNOVACIÓN
UNIÓN EUROPEA
FONDO EUROPEO DE DESARROLLO REGIONAL
"Una manera de hacer Europa"
AGENCIA ESTATAL DE INVESTIGACIÓN

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.

Valorización de CO_2: obtención de hidrocarburos mediante procesos catalíticos de hidrogenación

CO_2 valorization: obtaining hydrocarbons through catalytic hydrogenation processes

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-1263455	01-02-2020 31-01-2022	Junta de Andalucía	80.000 €

Investigador Principal Research Head	Componentes Research Group
Alfonso Caballero Martínez Juan Pedro Holgado Vázquez	Gerardo Colón Ibáñez Rosa María Pereñíguez Rodríguez Andrew M. Beale (UCL) Ángeles M. López Martín Francisco Jesús Platero Moreno

RESUMEN / ABSTRACT

En el presente proyecto se llevarán a cabo diversos estudios y desarrollos relacionados con la reducción de CO_2 a productos de alto valor añadido, como metano, olefinas ligeras, gasolinas y otros hidrocarburos funcionalizados, de gran interés económico, energético y medioambiental. El uso de hidrógeno como agente reductor, obtenido éste a su vez de fuentes renovables supone, además de la reducción de las emisiones de gases de efecto invernadero, una vía para el almacenamiento de la energía procedente de fuentes renovables, muchas de ellas de carácter intermitente y por tanto difícilmente acoplable a las necesidades de consumo.

Con todo ello en este proyecto se propone el desarrollo de nuevos sistemas catalíticos heterogéneos basados en Ni, Fe, Co, Ru e In, entre otros metales, los cuales han mostrado en los últimos años un gran potencial para esta reacción de hidrogenación. Dado el carácter bifuncional de los mecanismos de reacción involucrados en estas reacciones, se seleccionarán soportes micro y mesoporosos de composición variable (zeolitas, SBA-15, etc.), así como otros basados en estructura perovskita ABO_3. Para ello se emplearán una serie de técnicas de preparación recientemente descritas (Cristalización por Microondas, Proceso de Autocombustión, Mesoestructuración por Nanocasting y Porosidad Jerarquizada) 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 perovskita, que actúen tanto como agentes promotores de los sistemas catalíticos como de precursores de aleaciones metálicas en los sistemas catalíticos reducidos, permitirá obtener materiales con propiedades catalíticas modulables, muy variadas y versátiles.

This project will carry out several studies and developments related to the reduction of CO_2 to valuable products, such as methane, light olefins, gasolines and other functionalized hydrocarbons, of economic, energetic and environmental interest. The use of hydrogen as a reducing agent, obtained from renewable sources, in addition to the reduction of greenhouse gas emissions, is a way to store energy from renewable sources, many of which are intermittent and therefore difficult to match with consumption needs.

Therefore, this project proposes the development of new heterogeneous catalytic systems based on Ni, Fe, Co, Ru and In, among other metals, which have shown in recent years a great potential for this hydrogenation reaction. Given the bifunctional character of the reaction mechanisms involved in these reactions, micro and mesoporous supports of variable composition (zeolites, SBA-15, etc.) will be selected, as well as others based on ABO_3 perovskite structure. For this purpose, a series of recently described preparation techniques (Microwave Crystallization, Self-Combustion Process, Mesostructuring by Nanocasting and Hierarchical Porosity) will be used to obtain systems with high specific surface area and controlled nanostructure. The combination of different elements in the A and B positions of the perovskite structure, acting both as promoting agents of the catalytic systems and as precursors of metallic alloys in the reduced catalytic systems, will allow obtaining materials with modular, varied and versatile catalytic properties.

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

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
P20-00156	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 H_2-free hydrodeoxygenation - a rEVolutionary approach Enabling pRactical BIOmass upgrading: CLEVER-BIO

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)

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
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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.

Ácido fórmico como vector energético: viabilidad de los ciclos de carga y descarga de hidrógeno

Formic acid as energy vector: feasability of hydrogen charge/discharge cycles

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P18-RT-3405	01-01-2020 31-12-2022	Junta de Andalucía	102.268 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El presente proyecto se encuadra en la actual tendencia a nivel mundial de búsqueda de tecnologías para la captura y uso del dióxido de carbono (Carbon dioxide Capture and Utilization CCU). Su interés radica en la utilización directa del CO_2 atmosférico para almacenar hidrógeno verde, esto es, producido con la ayuda de energías renovables, en forma de ácido fórmico, usado como vector energético. Desde el punto de vista medioambiental, el desarrollo de esta tecnología permitiría preservar la huella de CO_2 durante el ciclo completo de generación, almacenamiento y liberación de energía, sin generar más gases de efecto invernadero. La posibilidad de almacenar hidrógeno de esta forma facilitaría su transporte y su uso en aplicaciones deslocalizadas diversas, tanto móviles como estacionarias. Indirectamente, esta tecnología racionalizaría el almacenamiento de las energías renovables, haciéndolas independientes de las condiciones climáticas. Este proyecto pretende estudiar la viabilidad de la tecnología basándose en el desarrollo de un único catalizador, estable y selectivo para los ciclos de carga y descarga de hidrógeno (CO_2/HCOOH).

This project is part of the current trend for future technologies of Carbon dioxide Capture and Utilization (CCU). His interest lies in a direct use of atmospheric CO_2 to store green hydrogen (produced with the help of renewable energies) as formic acid directly used as an energy vector. From an environmental point of view, the development of this technology would make possible the preservation of the CO_2 footprint during the complete cycle of energy generation, storage and release, without generating more greenhouse gases. The possibility of storing hydrogen in this way would facilitate its transport and its use in diverse applications, both mobile and stationary. Indirectly, this technology would rationalize the storage of renewable energies, making them independent of climatic conditions. This project aims to study the feasibility of the technology based on the development of one unique stable and selective catalyst for both, hydrogen charge and discharge cycles (CO_2 / HCOOH).

CO_2 como fuente de carbono para la producción de compuestos químicos de alto valor añadido

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-1263288	01-02-2020 31-01-2022	Junta de Andalucía	100.000 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El principal reto científico de este proyecto es el diseño de un dispositivo catalítico activo y selectivo en la reducción catalítica de CO_2 a CO. El proyecto pretende resolver dos problemas interrelacionados, el diseño del catalizador, que pasa por una comprensión a nivel molecular de la reacción estudiada, y el diseño de un reactor de microcanales que permita realizar la reacción en régimen isotermo y tiempos de residencia muy cortos. Para ello se propone la síntesis de catalizadores constituidos por metales nobles o de transición soportados en óxidos reducibles para llevar a cabo el proceso catalítico analizando los factores determinantes de la reacción: tamaño de partícula de la fase metálica, reducibilidad del soporte, interacciones metal-soporte y resistencia de la desactivación. Las características de la reacción exigen el desarrollo de reactores de microcanales que permitan disminuir las pérdidas de carga y los tiempos de residencia manteniéndose isotermos. El estudio, por tanto, busca diseñar un dispositivo catalítico activo, selectivo y estable que trabaje en régimen isotermo y permita tiempos de residencia inferiores a 100 ms.

The main scientific challenge of this project is active and selective catalytic device design for the catalytic reduction of CO_2 to CO. The project aims to solve two related problems, the design of the catalyst, which requires a deep understanding at the molecular level, and the design of a microchannel reactor that allows reaction in isothermal regime and with very short residence times. For this, the use of noble and/or transition metals supported on reducible oxides catalysts are proposed in this project to carry out the indicated process analyzing some reaction determining factors: metal phase particle size, support reducibility, metal-support interactions, and deactivation behavior. The characteristics of the reaction require the development of microchannel reactors that allow the reduction of the charge loss and residence time while maintaining the reaction isothermal. This project, therefore, is dedicated to design an active, selective and stable catalytic device that works in an isothermal regime and allows residence times of less than 100 ms.

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

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

Verificación de la composición química de una muestra

Periodo/Period:	27-06-2022 / 26-07-2022
Organismo Financiador/Financial source:	Fruit Tech Natural
Investigador responsable/Research head:	Alfonso Caballero Martínez

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

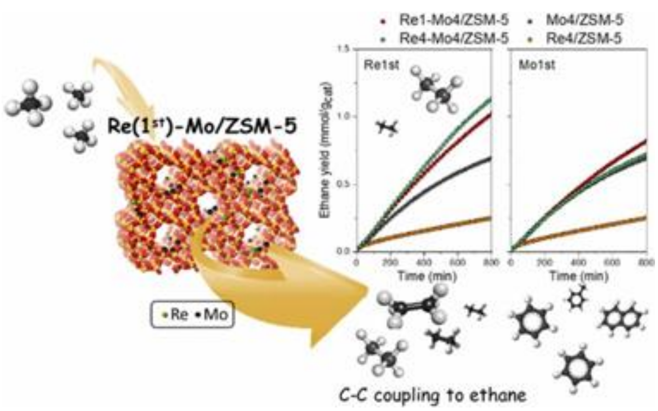
Analysis of Dry Reforming as direct route for gas phase CO_2 conversion. The past, the present and future of catalytic DRM technologies

le Sache, E; Reina, TR
Progress in Energy and Combustion Science, **89** (2022) 100970
Marzo, 2022 | **DOI:** 10.1016/j.pecs.2021.100970

Transition to low carbon societies requires advanced catalysis and reaction engineering to pursue green routes for fuels and chemicals production as well as CO_2 conversion. This comprehensive review provides a fresh perspective on the dry reforming of methane reaction (DRM) which constitutes a straightforward approach for effective CO_2 conversion to added value syngas. The bottleneck for the implementation of this process at industrial scale is the development of highly active and robust heterogeneous catalysts able to overcome the CO_2 activation barrier and deliver sufficient amount of the upgrading products at the desired operation conditions. Also, its high energy demand due to the endothermic nature of the reaction imposes extra difficulties. This review critically discusses the recent progresses on catalysts design ranging from traditional metal-supported catalysts to advanced structured and nanostructured systems with promising performance. The main advantages and culprits of the different catalytic systems are introduced aiming to inspire the catalysis community to further refine these formulations towards the development of "supercatalysts" for DRM. Besides the design of increasingly complex catalyst morphologies as well as other promising alternatives aiming at reducing the energy consumption of the process or tackle deactivation through reactor design are introduced.

Characterization of Re-Mo/ZSM-5 catalysts: How Re improves the performance of Mo in the methane dehydroaromatization reaction

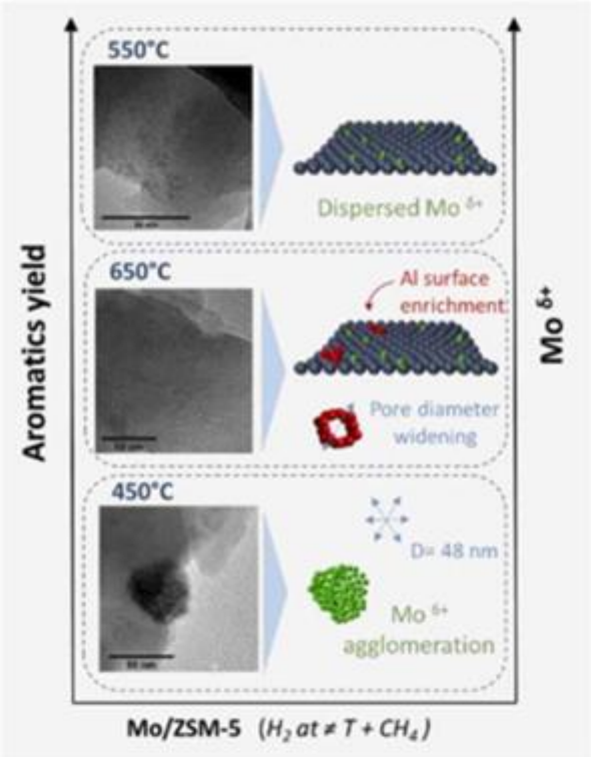
López-Martín, A; Sini, MF; Cutrufello, MG; Caballero, A; Colón, G
Applied Catalysis B-Environmental, **304** (2022) 120960
Mayo, 2022 | **DOI:** 10.1016/j.apcatb.2021.120960



In this study, the promoting effect of rhenium addition as a co-dopant on Mo/ZSM-5 catalysts system has been analysed. Hence, bimetallic (Re-Mo/ZSM-5) catalysts have been synthesized using a sequential impregnation methodology. The catalytic performance for direct aromatization of methane reaction has been determined and correlated with their physical and chemical state combining multiple characterization techniques. An important synergy between Mo and Re, affected by the sequential impregnation, has been observed. Thus, Re1-Mo4/ZSM-5 in which Re has been incorporated first shows notably higher aromatic yields and stability against deactivation. Characterization results suggest that catalytic enhancement is due to the important effect of Re presence in close interaction with Mo. Improved evolution of ethane through C-C coupling would be correlated to this catalytic performance. As we discuss, Mo nature and location in the bimetallic systems are strongly conditioned by Re and the impregnation sequence and favours such intermediate step.

Unraveling the Mo/HZSM-5 reduction pre-treatment effect on methane dehydroaromatization reaction

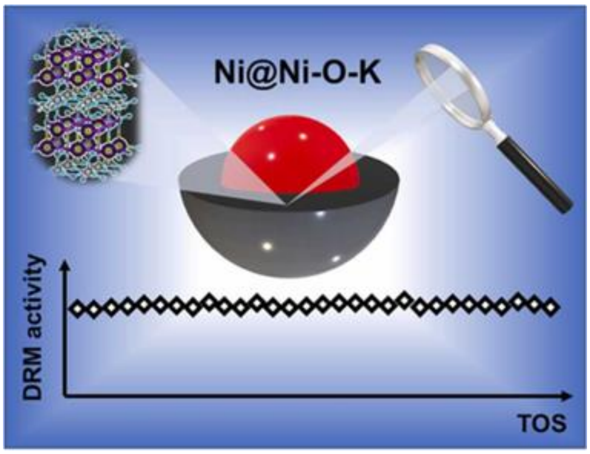
López-Martín, A; Caballero, A; Colón, G
Applied Catalysis B-Environmental, **312** (2022) 121382
Septiembre, 2022 | **DOI:** 10.1016/j.apcatb.2022.121382



Reduction pre-treatment at different temperatures were performed over Mo/HZSM-5 system before methane dehydroaromatiztion reaction. We have shown the crucial effect of reduction temperature on the final catalytic performance. Outstanding improvement in the aromatics conversion has been attained. Thus, H_2 formation form methane cracking reaction seems to be hindered for pre-treated catalysts. As a consequence, the deposition of coke in these samples appeared also notably suppressed. The optimum performance has been achieved for reduction pre-treatment at 550 °C. For this temperature, we have observed that the fraction of reduced Mo species is higher.

Evidence of new Ni-O-K catalytic sites with superior stability for methane dry reforming

Azancot, L; Blay, V; Blay-Roger, R; Bobadilla, LF; Penkova, A; Centeno, MA; Odriozola, JA
Applied Catalysis B-Environmental, **307** (2022) 121148
Junio, 2022 | **DOI:** 10.1016/j.apcatb.2022.121148



Liquid fuels produced via Fischer-Tropsch synthesis from biomass-derived syngas constitute an attractive and sustainable energy vector for the transportation sector. This study focuses on the role of potassium as a promoter in Ni-based catalysts for reducing coke deposition during catalytic dry reforming. The study provides a new structural link between catalytic performance and physicochemical properties. We identify new Ni-O-K chemical states associated with high stability in the reforming process, evidenced by different characterization techniques. The nickel particles form a core surrounded by a Ni-O-K phase layer (Ni@Ni-O-K) during the reduction of the catalyst. This phase likely presents an alkali-nickelate-type structure, in which nickel is stabilized in oxidation state + 3. The Ni-O-K formation induces essential changes in the electronic, physical, structural, and morphological properties of the catalysts, notably enhancing their long-term stability in dry reforming. This work thus provides new directions for designing more efficient catalysts for sustainable gas-to-liquids processes.

Electrocatalytic CO_2 conversion to C_2 products: Catalysts design, market perspectives and techno-economic aspects

Ruiz-López, E; Gandara-Loe, J; Baena-Moreno, F; Reina, TR; Odriozola, JA
Renewable & Sustainable Energy Reviews, **161** (2022) 112329
Junio, 2022 | **DOI:** 10.1016/j.rser.2022.112329

The energy crisis caused by the incessant growth in global energy demand joint to its associated greenhouse emissions motivates the urgent need to control and mitigate atmospheric CO_2 levels. Leveraging CO_2 as carbon pool to produce value-added products represents a cornerstone of the circular economy. Among the CO_2 utilization strategies, electrochemical reduction of CO_2 conversion to produce fuels and chemicals is booming due to its versatility and end-product flexibility. Herein most of the studies focused on C_1 products although C_2 and C_{2+} compounds are chemically and economically more appealing targets requiring advanced catalytic materials. Still, despite the complex pathways for C_{2+} products formation, their multiple and assorted applications have motivated the search of suitable electrocatalysts. In this review, we gather and analyse in a comprehensive manner the progress made regarding C_{2+} products considering not only the catalyst design and the electrochemistry features but also techno-economic aspects in order to envisage the most profitable scenarios. This state-of-the-art analysis showcases that electrochemical reduction of CO_2 to C_2 products will play a key role in the decarbonisation of the chemical industry paving the way towards a low-carbon future.

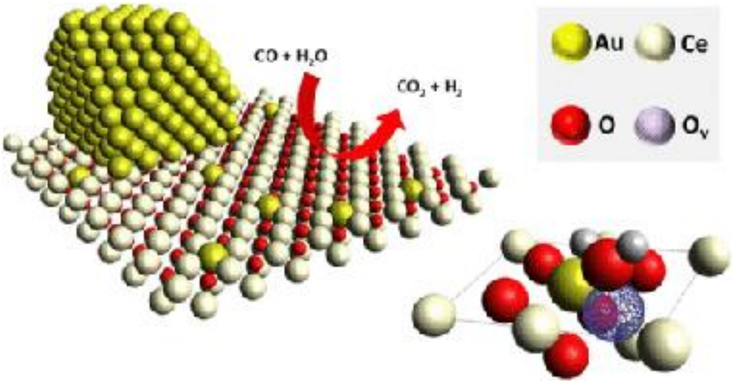
Shepherding reaction intermediates to optimize H_2 yield using composite-doped TiO_2-based photocatalysts

Barba-Nieto, I.; Colón, G; Fernández-García, M; Kubacka, A
Chemical Engineering Journal, **442** (2022) 136333
Agosto, 2022 | **DOI:** 10.1016/j.cej.2022.136333

Optimization of Pt-promoted TiO_2-based is key to promote the photocatalytic production of hydrogen using sacrificial alcohol molecules. Combination of doping and surface decoration of the mentioned base photoactive material is here exploited to maximize hydrogen yield. Using the quantum efficiency parameter, it is shown that the resulting composite system can boost activity up to 7.3 times within the whole methanol:water mixture ratio, yielding quantum efficiencies in the ca. 13-16 % range. The key role of the different components in generating charge carrier species and their use to trigger the sacrificial molecule evolution and control reaction kinetics are examined through an in-situ spectroscopic study. The study unveils the complex reaction mechanism, with generation of C1 to C3 molecules from different carbon-containing radicals, and interprets the physical origin of the huge H_2 production enhancement occurring in doped-composite titania-based catalysts.

Au and Pt Remain Unoxidized on a CeO_2-Based Catalyst during the Water-Gas Shift Reaction

Reina, TR; González-Castaño, M; López-Flores, V; Martínez, LMT; Zitolo, A; Ivanova, S; Xu, WQ; Centeno, MA; Rodríguez, JA; Odriozola, JA
Journal of the American Chemical Society, **144** (2022) 446-453
Enero, 2022 | **DOI:** 10.1021/jacs.1c10481

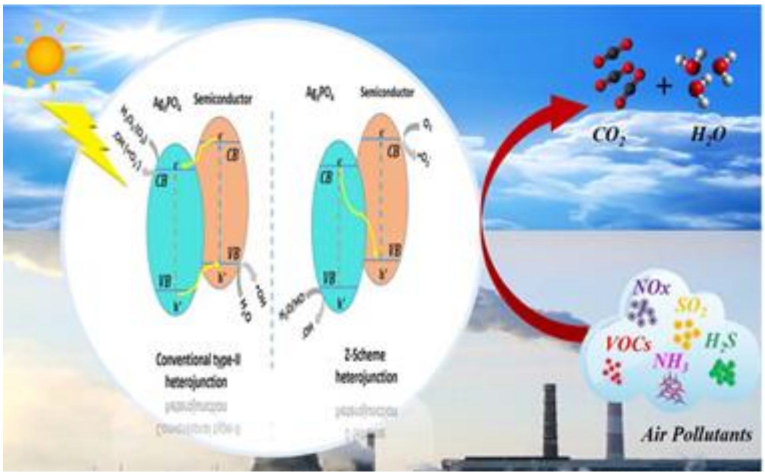


The active forms of Au and Pt in CeO_2-based catalysts for the water-gas shift (WGS) reaction are an issue that remains unclear, although it has been widely studied. On one hand, ionic species might be responsible for weakening the Ce-O bonds, thus increasing the oxygen mobility and WGS activity. On the other hand, the close contact of Au or Pt atoms with CeO_2 oxygen vacancies at the metal-CeO_2 interface might provide the active sites for an efficient reaction. In this work, using in situ X-ray absorption spectroscopy, we demonstrate that both Au and Pt remain unoxidized during the reaction. Remarkable differences involving the dynamics established by both species under WGS atmospheres were recognized. For the prereduced Pt catalyst, the increase of the conversion coincided with a restructuration of the Pt atoms into cuboctahedrical metallic particles without significant variations on the overall particle size. Contrary to the relatively static behavior of Pt-0, Au-0 nanoparticles exhibited a sequence of particle splitting and agglomeration while maintaining a zero oxidation state despite not being located in a metallic environment during the process. High WGS activity was obtained when Au atoms were surrounded by oxygen. The fact that Au preserves its unoxidized state indicates that the chemical interaction between Au and oxygen must be necessarily electrostatic and that such an electrostatic interaction is fundamental for a top performance in the WGS process.

Photocatalytic oxidation of pollutants in gas-phase via Ag_3PO_4-based semiconductor photocatalysts: Recent progress, new trends, and future perspectives

Y. Naciri; A. Hsini; A. Bouziani; R. Djellabi; Z. Ajmal; M. Laabd; J.A. Navío; A. Mills; C.L. Bianchi; H.Li; B. Bakiz; A. Albourine
Critical Reviews in Environmental Science and Technology, **52** (2022) 2339-2382
Julio, 2022 | **DOI:** 10.1080/10643389.2021.1877977

Air pollution has become a significant challenge for both developing and developed nations due to its close association with numerous fatal diseases such as cancer, respiratory, heart attack, and brain stroke. Over recent years, heterogeneous semiconductor photocatalysis has emerged as an effective approach to air remediation due to the ease of scale-up, ready application in the field, use of solar light and ready availability of a number of different effective photocatalysts. To date, most work in this area has been conducted using UV-absorbing photocatalysts, such as TiO_2 and ZnO; However, recent studies have revealed Ag_3PO_4 as an attractive, visible-light-absorbing alternative, with a bandgap of 2.43 eV. In particular, this material has been shown to be an excellent photocatalyst for the removal of many types

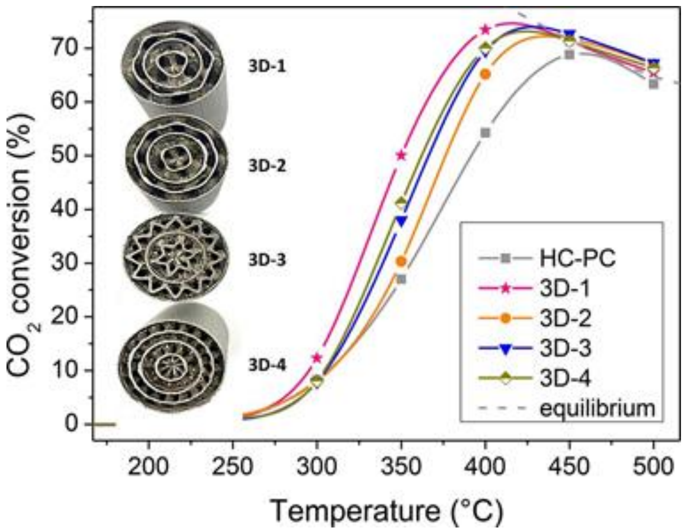


of pollutants in the gas phase. However, the widespread application of Ag_3PO_4 is restricted due to its tendency to undergo photoanodic corrosion and the poor reducing power of its photogenerated conductance band electrons, which are unable to reduce O_2 to superoxide $\bullet O_2^-$. These limitations are critically evaluated in this review. In addition, recent studies on the modification of Ag_3PO_4 via combination with the conventional heterojunctions or Z-scheme junctions, as well as the photocatalytic mechanistic pathways for enhanced gas-pollutants removal, are summarized and discussed. Finally, an overview is given on the future developments that are required in order to overcome these challenges and so stimulate further research into this promising field.

3D-printed structured catalysts for CO_2 methanation reaction: Advancing of gyroid-based geometries

González-Castaño, M; Baena-Moreno, F; De Miguel, JCN; Miah, KUM; Arroyo-Torralvo, F; Ossenbrink, R; Odriozola, JA; Benzinger, W; Hensel, A; Wenka, A; Arellano-García, H

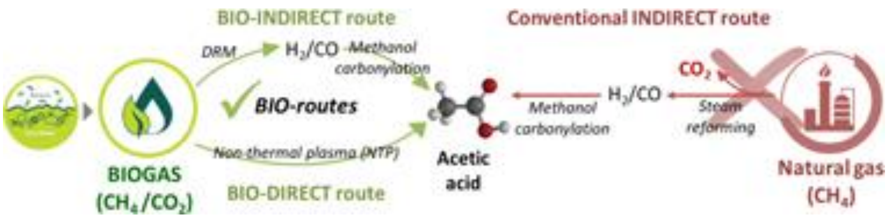
Energy Conversion and Management, **258** (2022) 115464
Abril, 2022 | **DOI:** 10.1016/j.enconman.2022.115464



This work investigates the CO_2 methanation rate of structured catalysts by tuning the geometr y of 3D-printed metal Fluid Guiding Elements (FGEs) structures based on periodically variable pseudo-gyroid geometries. The enhanced performance showed by the structured catalytic systems is mostly associated with the capability of the FGEs substrate geometries for efficient heat usages. Thus, variations on the channels diameter resulted in ca. 25% greater CO_2 conversions values at intermediate temperature ranges. The highest void fraction evidenced in the best performing catalyst (3D-1) favored the radial heat transfer and resulted in significantly enhanced catalytic activity, achieving close to equilibrium (75%) conversions at 400°C and 120 mL/min. For the 3D-1 catalyst, a mathematical model based on an experimental design was developed thus enabling the estimation of its behavior as a function of temperature, spatial velocity, hydrogen to carbon dioxide (H_2/CO_2) ratio, and inlet CO_2 concentration. Its optimal operating conditions were established under 3 different scenarios: 1) no restrictions, 2) minimum H_2:CO_2 ratios, and 3) minimum temperatures and H_2/CO_2 ratio. For instance, for the lattest scenario, the best CO_2 methanation conditions require operating at 431°C, 200 mL/min, H_2/CO_2 = 3 M ratio, and inlet CO_2 concentration = 10 %.

Sustainable routes for acetic acid production: Traditional processes vs a low-carbon, biogas-based strategy

Martín-Espejo, JL; Gandara-Loe, J; Odriozola, JA; Reima, TR; Pastor-Pérez, L
Science of the Total Environment, **840** (2022) 156663
Septiembre, 2022 | **DOI:** 10.1016/j.scitotenv.2022.156663



The conversion of biogas, mainly formed of CO_2 and CH_4, into high-value platform chemicals is increasing attention in a context of low-carbon societies. In this new paradigm, acetic acid (AA) is deemed as an interesting product for the chemical industry. Herein we present a fresh overview of the current manufacturing approaches, compared to potential low-carbon alternatives. The use of biogas as primary feedstock to produce acetic acid is an auspicious alternative, representing a step-ahead on carbon-neutral industrial processes. Within the spirit of a circular economy, we propose and analyse a new BIO-strategy with two noteworthy pathways to potentially lower the environmental impact. The generation of syngas via dry reforming (DRM) combined with CO_2 utilisation offers a way to produce acetic acid in a two-step approach (BIO-Indirect route), replacing the conventional, petroleum-derived steam reforming process. The most recent advances on catalyst design and technology are discussed. On the other hand, the BIO-Direct route offers a ground-breaking, atom-efficient way to directly generate acetic acid from biogas. Nevertheless, due to thermodynamic restrictions, the use of plasma technology is needed to directly produce acetic acid. This very promising approach is still in an early stage. Particularly, progress in catalyst design is mandatory to enable low-carbon routes for acetic acid production.

Recent advances on gas-phase CO_2 conversion: Catalysis design and chemical processes to close the carbon cycle

Torres-Sempere, G; Pastor-Pérez, L; Odriozola, JA; Yu, J; Duran-Olivencia, FJ; Bobadilla, LF; Reina, TR
Current Opinion in Green and Sustainable Chemistry, **36** (2022) 100647
Agosto, 2022 | **DOI:** 10.1016/j.cogsc.2022.100647

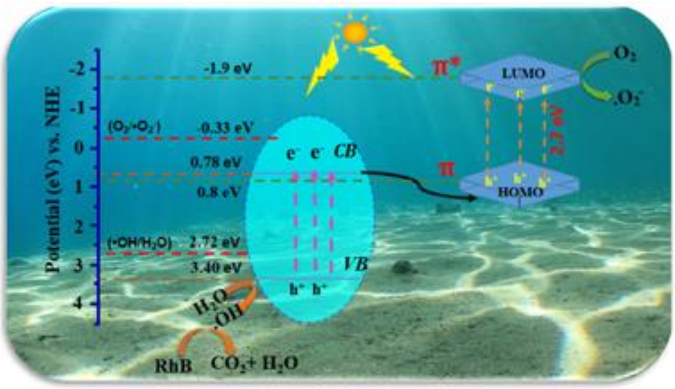
Chemical CO_2 recycling in the gas phase constitutes a straightforward approach for effective CO_2 conversion to added-value products like syngas or synthetic methane. In this scenario, some traditional processes such as the dry and bi-reforming of methane, the CO_2 methanation and the reverse water-gas shift have gained a renewed interest from the CO_2 utilisation perspective. Indeed, these reactions represent flexible routes to upgrade CO_2 and their application at an industrial scale could substantially reduce CO_2 emissions. The bottleneck for the implementation of these processes at the commercial level is the development of highly active and robust heterogeneous catalysts able to overcome CO_2 activation and deliver sufficient amounts of the upgrading products (i.e. syngas or synthetic natural gas) at the desired operating conditions. This review paper gathers the most recent advances in the design of new catalytic formulations for chemical CO_2 recycling in the gas phase and constitutes an overview for experts and newcomers in the field to get fundamental insights into this emerging branch of low-carbon technologies.

Assessment of pilot-plant scale solar photocatalytic hydrogen generation with multiple approaches: Valorization, water decontamination and disinfection

Ruiz-Aguirre, A; Villachica-Llamosas, JG; Polo-López, MI; Cabrera-Reina,A; Colón,G; Peral,J; Malato, S
Energy, **260** (2022) 125199
Diciembre, 2022 | **DOI:** 10.1016/j.energy.2022.125199
The main goal of the present study was to explore pilot-scale combination of H_2 generation with simultaneous water disinfection or decontamination. Performance of a TiO_2-CuO mixture for solar-to-hydrogen (STH) con-version was studied, focusing on treatment optimization (catalyst dose, proportion of semiconductors in the mixture and concentration of the sacrificial agent). Experiments were performed in a 25-L compound parabolic collector (2 m^2) solar pilot plant specifically designed for photocatalytic hydrogen generation. The best operating conditions were 100 mg L^{-1} TiO_2-CuO (10:1) with 0.075 M glycerol as the sacrificial agent. The best STH conversion attained was 0.9%. 25 mg L^{-1} imidacloprid was completely degraded (over 99%). The synergetic effect of anoxic conditions, TiO_2:CuO and solar radiation caused a significant reduction (> 5 Log) in concen-tration of E. coli, used as a model waterborne pathogen, in less than 10 min.

Z-scheme WO_3/PANI heterojunctions with enhanced photocatalytic activity under visible light: A depth experimental and DFT studies

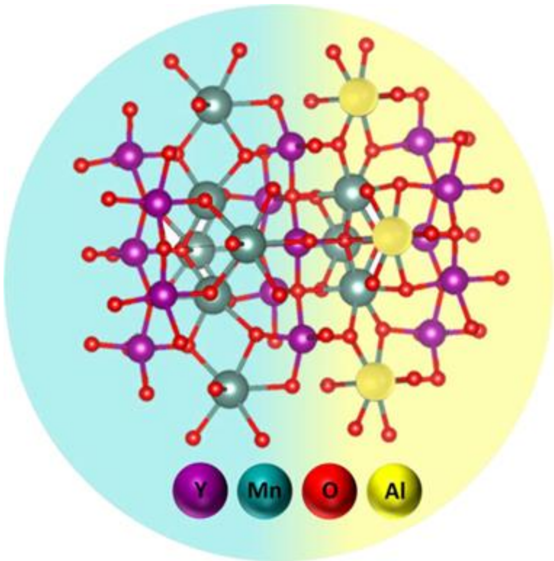
Y. Naciri; A.Hsini; A.Bouziani; K.Tanji; B.El Ibrahimi; M.N.Ghazza; B. Bakiz; A.Albourine; A.Benlhachemi; J.A. Navío
Chemosphere, **292** (2022) 133468
Abril, 2022 | **DOI:** 10.1016/j.chemosphere.2021.133468



A WO_3@PANI heterojunction photocatalyst with a various mass ratio of polyaniline to WO_3 was obtained via the in situ oxidative deposition polymerization of aniline monomer in the presence of WO_3 powder. The characterization of WO_3@PANI composites was carried via X-ray diffraction (XRD), scanning electron microscopy (SEM-EDS), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR), ultraviolet–visible diffuse reflection spectroscopy (DRS), X-ray photoelectron spectroscopy (XPS) and photoluminescence spectroscopy (PL). The photocatalytic efficiency of WO_3@PANI photocatalysts was assessed by following the decomposition of the Rhodamine B (RhB) dye under visible light irradiation (λ >420 nm). The results evidenced the high efficiency of the WO_3@PANI (0.5 wt %) nanocomposite in the photocatalytic degradation of RhB (90% within 120 min) under visible light irradiation 3.6 times compared to pure WO_3. The synergistic effect between PANI and WO3 is the reason for the increased photogenerated carrier separation. The superior photocatalytic performance of the WO_3@PANI catalyst was ascribed to the increased visible light in the visible range and the efficient charge carrier separation. Furthermore, the Density Functional Theory study (DFT) of WO_3@PANI was performed at the molecular level, to find its internal nature for the tuning of photocatalytic efficiency. The DFT results indicated that the chemical bonds connected the solid-solid contact interfaces between WO_3 and PANI. Finally, a plausible photocatalytic mechanism of WO_3@PANI (0.5 wt %) performance under visible light illumination is suggested to guide additional photocatalytic activity development.

CO_2 methanation on Ni/$YMn_{1-x}Al_xO_3$ perovskite catalysts

Safdar, M; González-Castaño, M; Penkova, A; Centeno, MA; Odriozola, JA; Arellano-García, H
Applied Materials Today, **29** (2022) 101577
Diciembre, 2022 | DOI: 10.1016/j.apmt.2022.101577

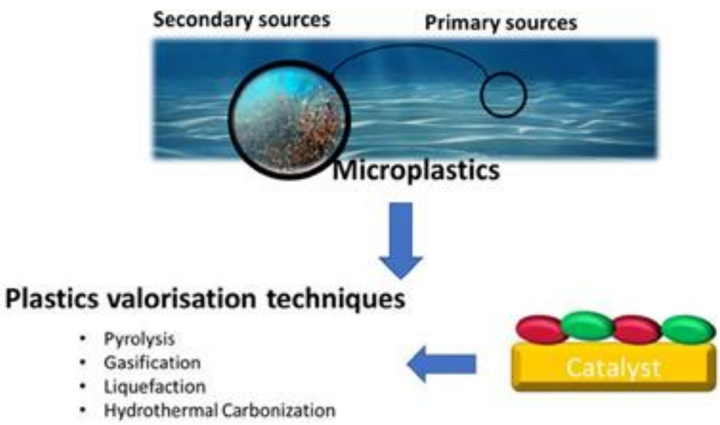


Seeking for advanced catalytic systems for the CO_2 methanation reaction, the use of Ni supported catalysts over redox materials is often proposed. Profiting the superior redox properties described for layered perovskite systems, this work has investigated a series Ni supported $YMn_{1-x}Al_xO_3$ (x = 0, 0.2, 0.5, 0.8, 1) perovskite catalysts. The obtained results evidenced the impact of the support nature on the systems redox properties and Ni-support interactions. Within the catalysts series, the greater methanation rates displayed by Ni/$YMn_{0.5}Al_{0.5}O_3$ catalyst (0.748 $mmol_{CO2,conv.}s^{-1}g_{Ni}^{-1}$ at 400 °C and 60 L/gh) were associated to the interplay between the support redox properties and superior Ni dispersion. The improved redox behavior attained through the Al-incorporation (up to x = 0.5) was associated to the layered perovskite structures which, being distorted and constituted by smaller crystal sizes, facilitated the behavior of Mn redox couples as surface species readily interconverted. Exhibiting catalytic performances comparable to precious metals based catalysts, this work proposes the Ni/$YMn_{0.5}Al_{0.5}O_3$ catalyst as an effective system for the CO_2 methanation reaction.

Materials challenges and opportunities to address growing micro/nanoplastics pollution: a review of thermochemical upcycling

Parrilla-Lahoz, S; Mahebadevan, S; Kauta, M; Zambrano, MC; Pawlak, JJ; Venditti, RA; Reina, TR; Duyar, MS

Materials Today Sustainability, **20** (2022) 100200
Diciembre, 2022 | **DOI:** 10.1016/j.mtsust.2022.100200

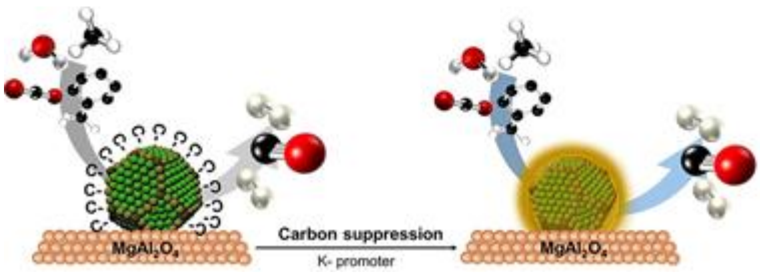


Micro/nanoplastics have sparked attention in recent years due to their widespread presence in the environment. Currently, several waste valorization approaches are under development in order to upcycle micro/nanoplastics. Thermal conversion technologies such as pyrolysis, gasification, liquefaction, or hydrothermal carbonization can yield high-value solid products, oil, and gases from plastics waste. The common thermal conversion technologies investigated focus on maximizing the production of oil and gases (such as H_2 and CH_4) for use as fuel. Except for hydrogen, when these products are used to generate energy, the carbon emissions generated are comparable to those produced by traditional fossil fuels. Herein, we present a review of the current efforts to capture and convert plastic waste into valuable products with an emphasis on identifying the need to develop processes specifically for micro/nano-plastics while also preventing the release of CO_2 emissions. We identify the development of efficient catalytic materials as a critical research need for achieving economically viable thermochemical conversion of micro/nanoplastics.

Catalytic reforming of model biomass-derived producer gas

Azancot, L; Bobadilla, LF; Centeno, MA; Odriozola, JA

Fuel, **320** (2022) 123843
Julio, 2022 | **DOI:** 10.1016/j.fuel.2022.123843



This work includes a complete study of the reaction of reforming a simulated producer gas stream comparing a Ni-based catalyst with another one promoted with potassium to enhance the resistance to coke formation. Although coke deposition is unavoidable in the presence of tars in the stream, the analysis of different reaction parameters revealed that operating at 750 °C, weight hourly space velocity (WHSV) of 60 L^{-1} g^{-1} h^{-1} and 10-20 vol% of steam is possible to minimize the accumulation of carbon deposits. Moreover, it was demonstrated that the addition of potassium helps to mitigate carbon formation, but a high concentration of steam leads to nickel sintering and/or partial oxidation of metallic nickel. On this basis, it was successfully evidenced that the Ni-K catalyst is an excellent candidate for obtaining clean syngas from producer gas reforming.

Hydrogen production from landfill biogas: Profitability analysis of a real case study

Vidal-Barrero, F; Baena-Moreno, FM; Preciado-Cardenas, C; Villanueva-Perales, A; Reina, TR

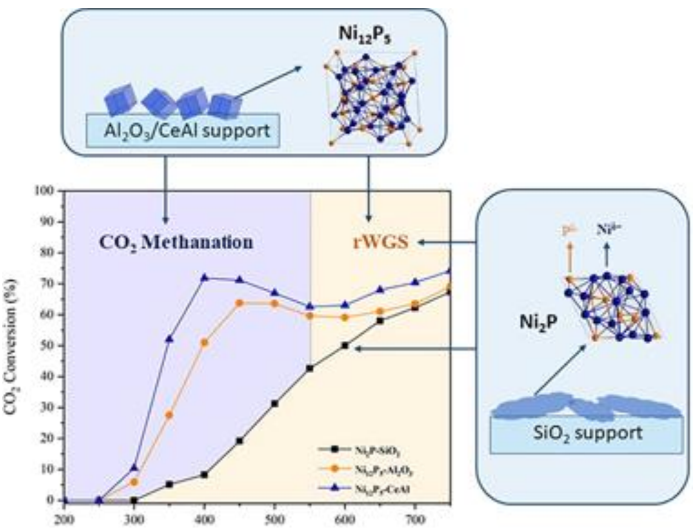
Fuel, **324** (2022) 124438
Septiembre, 2022 | **DOI:** 10.1016/j.fuel.2022.124438

Hydrogen is not only considered as a cornerstone within renewable energy portfolio but it is also a key enabler for CO_2 valorisation being a central resource for industrial decarbonization. This work evaluates the profitability of hydrogen production via combined biogas reforming and water-gas shift reaction, based on a real case scenario for landfill biogas plant in Seville (Spain). A techno-economic model was developed based on a process model and the discounted cash-flow method. A biogas flow of 700 m^3/h (input given by the landfill biogas plant) was used as plant size and the analysis was carried out for two different cases: (1) use of already available energy sources at the industrial plant, and (2) solar energy generation to power the process. The economic outputs obtained showed that under the current circumstances, this hydrogen production route is not profitable. The main reason is the relatively low current hydrogen prices which comes from fossil fuels. A revenues analysis indicates that hydrogen from biogas selling prices between 2.9 and 5.7 euro/kg would be needed to reach profitability, which are considerably higher than the current hydrogen cost (1.7 euro/kg). A subsidy scheme is suggested to improve the competitiveness of this hydrogen production process in the short-medium term. A cost analysis is also performed, revealing that electricity prices and investment costs have a high impact on the total share (23-40% and 8-22%, respectively). Other potential costs reduction such as catalyst, labour and manteinance & overhead are also evaluated, showing that cutting-down production costs is mandatory to unlock the potential of hydrogen generation from biogas. Our work showcases the techno-economic challenge that green energy policies face in the path toward sustainable societies.

Ni-Phosphide catalysts as versatile systems for gas-phase CO_2 conversion: Impact of the support and evidences of structure-sensitivity

Zhang, Q; Pastor-Pérez, L; Villora-Pico, JJ; Joyce, M; Sepulveda-Escribano, A; Duyar, MS; Reina, TR

Fuel, **323** (2022) 124301
Septiembre, 2022 | **DOI:** 10.1016/j.fuel.2022.124301

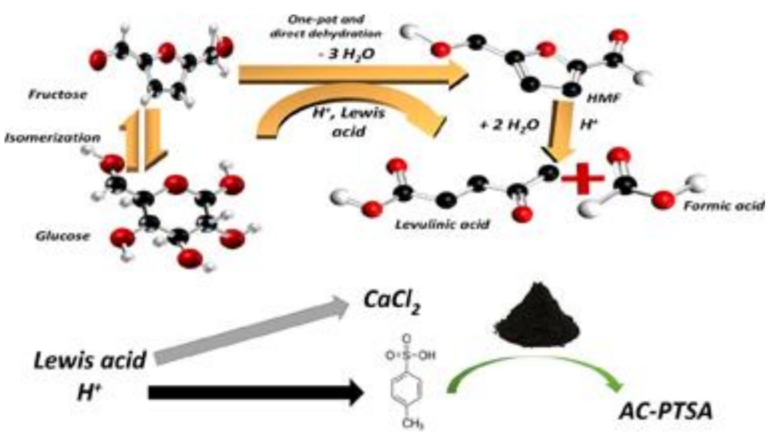


We report for the first time the support dependent activity and selectivity of Ni-rich nickel phosphide catalysts for CO_2 hydrogenation. New catalysts for CO_2 hydrogenation are needed to commercialise the reverse water-gas shift reaction (RWGS) which can feed captured carbon as feedstock for traditionally fossil fuel-based processes, as well as to develop flexible power-to-gas schemes that can synthesise chemicals on demand using surplus renewable energy and captured CO_2. Here we show that Ni_2P/SiO_2 is a highly selective catalyst for RWGS, producing over 80% CO in the

full temperature range of 350-750 °C. This indicates a high degree of suppression of the methanation reaction by phosphide formation, as Ni catalysts are known for their high methanation activity. This is shown to not simply be a site blocking effect, but to arise from the formation of a new more active site for RWGS. When supported on Al_2O_3 or CeAl, the dominant phase of as synthesized catalysts is $Ni_{12}P_5$. These $Ni_{12}P_5$ catalysts behave very differently compared to Ni_2P/SiO_2, and show activity for methanation at low temperatures with a switchover to RWGS at higher temperatures (reaching or approaching thermodynamic equilibrium behaviour). This switchable activity is interesting for applications where flexibility in distributed chemicals production from captured CO_2 can be desirable. Both $Ni_{12}P_5/Al_2O_3$ and $Ni_{12}P_5$/CeAl show excellent stability over 100 h on stream, where they switch between methanation and RWGS reactions at 50-70% conversion. Catalysts are characterized before and after reactions via X-ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), temperature-programmed reduction and oxidation (TPR, TPO), Transmission Electron Microscopy (TEM), and BET surface area measurement. After reaction, Ni_2P/SiO_2 shows the emergence of a crystalline $Ni_{12}P_5$ phase while $Ni_{12}P_5/Al_2O_3$ and $Ni_{12}P_5$/CeAl both show the crystalline Ni_3P phase. While stable activity of the latter catalysts is demonstrated via extended testing, this Ni enrichment in all phosphide catalysts shows the dynamic nature of the catalysts during operation. Moreover, it demonstrates that both the support and the phosphide phase play a key role in determining selectivity towards CO or CH_4.

Pursuing efficient systems for glucose transformation to levulinic acid: Homogeneous vs. heterogeneous catalysts and the effect of their co-action

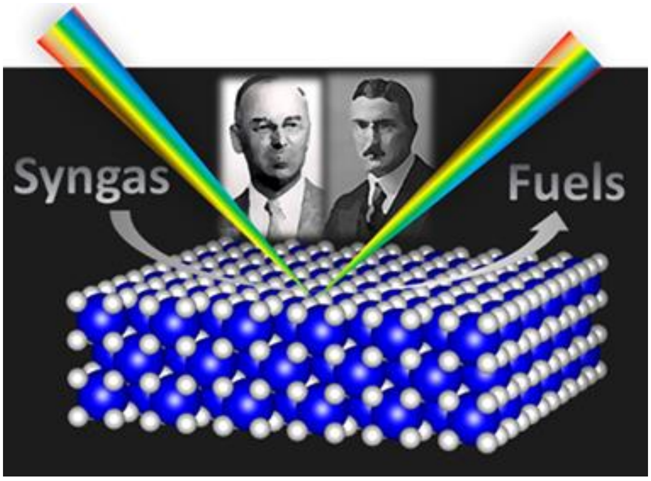
Bounoukta, CE; Megias-Sayago, C; Ivanova, S; Ammari, F; Centeno, MA; Odriozola, JA
Fuel, **318** (2022) 123712
Junio, 2022 | **DOI:** 10.1016/j.fuel.2022.123712



Exploring available catalytic systems to understand their behavior is a must to properly design efficient catalysts aiming to definitively drive biomass from laboratory to industrial scale. Glucose transformation to levulinic acid involves cascade reactions with specific requirements, different active sites in each case and secondary reactions hard to avoid which are intrinsically linked to the catalyst's nature and reaction conditions. In the present work, homogeneous, heterogeneous and heterogeneous/homogeneous catalysts are considered with the unique goal of improving levulinic acid yield while understanding the catalytic behaviour of cost-effective catalysts. The choice of the catalytic systems and the effect of the main reaction parameters on activity and selectivity is studied and discussed.

Understanding the promotional effect of Pt/CeO_2 in cobalt-catalyzed Fischer-Tropsch synthesis using operando infrared spectroscopy at moderated pressures

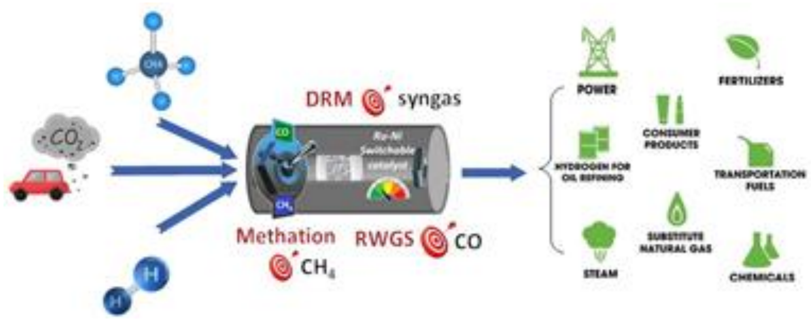
Bobadilla, LF; Egana, A; Castillo, R; Romero-Sarria, F; Centeno, MA; Sanz, O; Montes, M; Odriozola, JA
Fuel, **312** (2022) 122964
Marzo, 2022 | **DOI:** 10.1016/j.fuel.2021.122964



Fischer-Tropsch (FTS) reaction is a well-known catalytic process for the conversion of synthesis gas into liquid fuels. The addition of a water gas shift (WGS) catalyst to the FTS one has been postulate to notably increase the efficiency of the process. In order to investigate this issue, we conducted the FTS reaction over a $Co\text{-}Re/Al_2O_3$ catalyst combined with an optimal WGS Pt/CeO_2 catalyst. We observed a notable increase of CO conversion in presence of the Pt/CeO2 catalyst that a priori could be attributed to the WGS reaction. However, the WGS reaction is unfavourable at pressures higher than 1 bar and CO/CO_2 hydrogenation over Pt/CeO_2 could be more favoured under FTS reaction conditions. In order to gain insights on this fact and elucidate the role of Pt/CeO_2 in the FTS reaction we have performed an operando DRIFTS-MS study under close FTS reaction conditions at 4 bar over the Pt/CeO_2 catalyst.

Versatile Ni-Ru catalysts for gas phase CO_2 conversion: Bringing closer dry reforming, reverse water gas shift and methanation to enable end-products flexibility

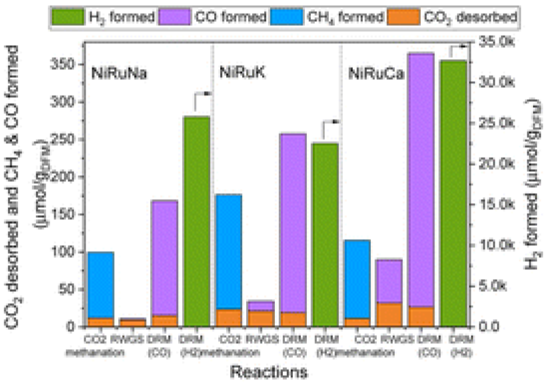
Merkouri, LP; le Sache, E; Pastor-Pérez, L; Duyar, MS; Reina, TR
Fuel, **315** (2022) 123097
Mayo, 2022 | **DOI:** 10.1016/j.fuel.2021.123097



Advanced catalytic materials able to catalyse more than one reaction efficiently are needed within the CO_2 utilisation schemes to benefit from end-products flexibility. In this study, the combination of Ni and Ru (15 and 1 wt%, respectively) was tested in three reactions, i.e. dry reforming of methane (DRM), reverse water-gas shift (RWGS) and CO_2 methanation. A stability experiment with one cycle of CO_2 methanation-RWGS-DRM was carried out. Outstanding stability was revealed for the CO_2 hydrogenation reactions and as regards the DRM, coke formation started after 10 h on stream. Overall, this research showcases that a multicomponent $Ni\text{-}Ru/CeO_2\text{-}Al_2O_3$ catalyst is an unprecedent versatile system for gas phase CO_2 recycling. Beyond its excellent performance, our switchable catalyst allows a fine control of end-products selectivity.

Feasibility of switchable dual function materials as a flexible technology for CO_2 capture and utilisation and evidence of passive direct air capture

Merkouri, LP; Reina, TR; Duyar, MS
Nanoscale, **14** (2022) 12620-12637
Agosto, 2022 | **DOI:** 10.1039/d2nr02688k

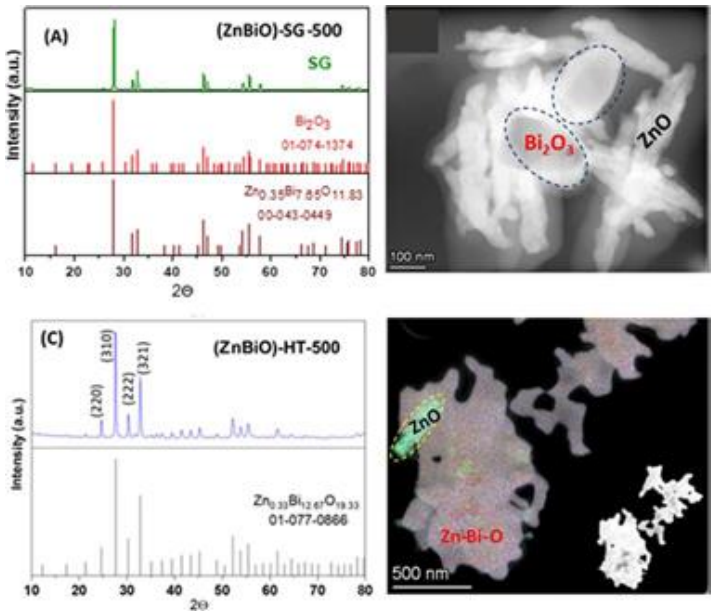


The feasibility of a Dual Function Material (DFM) with a versatile catalyst offering switchable chemical synthesis from carbon dioxide (CO_2) was demonstrated for the first time, showing evidence of the ability of these DFMs to passively capture CO_2 directly from the air as well. These DFMs open up possibilities in flexible chemical production from dilute sources of CO_2, through a combination of CO_2 adsorption and subsequent chemical transformation (methanation, reverse water gas shift or dry reforming of methane). Combinations of Ni Ru bimetallic catalyst with Na_2O, K_2O or CaO adsorbent were supported on CeO_2-Al_2O_3 to develop flexible DFMs. The designed multicomponent materials were shown to reversibly adsorb CO_2 between the 350 and 650 °C temperature range and were easily regenerated by an inert gas purge stream. The components of the flexible DFMs showed a high degree of interaction with each other, which evidently enhanced their CO_2 capture performance ranging from 0.14 to 0.49 mol kg^{-1}. It was shown that captured CO_2 could be converted into useful products through either CO_2 methanation, reverse water-gas shift (RWGS) or dry reforming of methane (DRM), which provides flexibility in terms of co-reactant (hydrogen vs. methane) and end product (synthetic natural gas, syngas or CO) by adjusting reaction conditions. The best DFM was the one containing CaO, producing 104 µmol of CH_4 per kg_{DFM} in CO_2 methanation, 58 µmol of CO per kg_{DFM} in RWGS and 338 µmol of CO per kg_{DFM} in DRM.

Insights into the structural and physicochemical properties of Zn-Bi-O composites for efficient photodegradation of caffeic acid, rhodamine B and methyl orange

F.Puga; J.A.Navío; J.M.Córdoba; F.Romero-Sarria; M.C.Hidalgo
Applied Surface Science, **581** (2022) 152351
Abril, 2022 | **DOI:** 10.1016/j.apsusc.2021.152351

Different Zn-Bi-O composites were synthesized following the starting chemical molar composition of $ZnBi2O_4$ spinels by a sol–gel method, (ZnBiO)-SG, and its subsequent hydrothermal treatment, (ZnBiO)-HT. The acquired X-ray diffractograms after sequential thermal treatments at a programmed rate indicate that both precursors evolved, after calcination at 500 °C, to materials (ZnBiO) with different stoichiometry. The use of different characterization techniques (both FT-IR and TEM), allowed us to establish that, with the sol–gel process a mixed ZnO/Bi2O3 oxide is generated, while after hydrothermal process a ternary Zn-Bi-O oxide is formed, with small amounts of residual ZnO. The



photocatalytic properties of the synthesized samples were evaluated using Caffeic acid, Rhodamine B and Methyl Orange as model substrates. It can be concluded that both catalysts showed excellent photocatalytic activity for the degradation of trans-caffeic acid under both UV and visible illumination. The leaching process (in particular of zinc), which is produced with the illumination time (in particular under UV illumination) in the presence of oxygen, raises the hypothesis of a foreseeable formation of complexes (photochemically stable or unstable) of caffeic acid with Zn^{2+} and Bi^{3+} ions. The plausible donor/acceptor interactions between the toxic molecules studied and the Zn^{2+} and Bi^{3+} ions, could condition the degradation processes, by means of a photoassisted process that would take place both, in the heterogeneous (photocatalytic) and homogeneous (photoassisted) phases. For the degradation processes of Rhodamine B and Methyl Orange, additional experimental conditions are studied that significantly improved their photocatalytic degradation.

Structure effect of modified biochar in Ru/C catalysts for sugar mixture hydrogenation

Santos, JL; Sanz-Moral, LM; Aho, A; Ivanova, S; Murzin, DY; Centeno, MA

Biomass & Bioenergy, **163** (2022) 106504
Agosto, 2022 | **DOI:** 10.1016/j.biombioe.2022.106504

This study deals with the production and activation of biochars and their use as supports for a series of ruthenium catalysts for hydrogenation of L-arabinose/D-galactose sugar mixture. The synthesized biochars differ in physicochemical properties and surface chemistry influencing ruthenium metal uptake and dispersion and as a consequence its catalytic behaviour. Selectivity exceeding 95% was observed for both hexitols. The catalytic performance of the prepared Ru supported catalysts is also compared to the already known Ru/activated carbon commercial catalyst.

Emerging natural and tailored perovskite-type mixed oxides-based catalysts for CO_2 conversions

Wu, J; Ye, RP; Xu, DJ; Wan, LZ; Reina, TR; Sun, H; Ni, Y; Zhou, ZF; Deng, XA

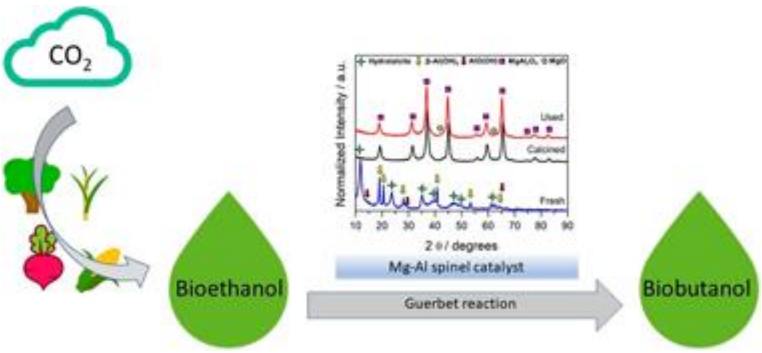
Frontiers in Chemistry, **10** (2022) 961355
Agosto, 2022 | **DOI:** 10.3389/fchem.2022.961355

The rapid economic and societal development have led to unprecedented energy demand and consumption resulting in the harmful emission of pollutants. Hence, the conversion of greenhouse gases into valuable chemicals and fuels has become an urgent challenge for the scientific community. In recent decades, perovskite-type mixed oxide-based catalysts have attracted significant attention as efficient CO_2 conversion catalysts due to the characteristics of both reversible oxygen storage capacity and stable structure compared to traditional oxide-supported catalysts. In this review, we hand over a comprehensive overview of the research for CO_2 conversion by these emerging perovskite-type mixed oxide-based catalysts. Three main CO_2 conversions, namely reverse water gas shift reaction, CO_2 methanation, and CO_2 reforming of methane have been introduced over perovskite-type mixed oxide-based catalysts and their reaction mechanisms. Different approaches for promoting activity and resisting carbon deposition have also been discussed, involving increased oxygen vacancies, enhanced dispersion of active metal, and fine-tuning strong metal-support interactions. Finally, the current challenges are mooted, and we have proposed future research prospects in this field to inspire more sensational breakthroughs in the material and environment fields.

Insights on Guerbet Reaction: Production of Biobutanol From Bioethanol Over a Mg-Al Spinel Catalyst

Crespo, MAP; Vidal-Barrero, F; Azancot, L; Reina, TR; Campoy, M

Frontiers in Chemistry, **10** (2022) 945596
Julio, 2022 | **DOI:** 10.3389/fchem.2022.945596

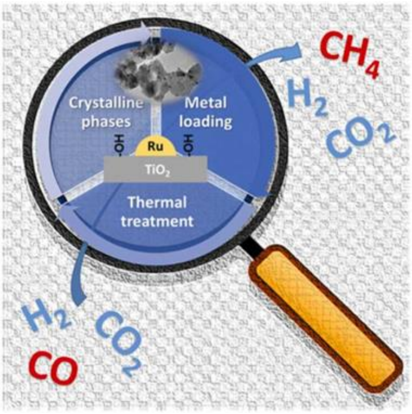


The production of biobutanol from bioethanol by the Guerbet reaction is an alternative pathway to renewable sources. The commercial viability of this green route requires improvements in the process development. This study experimentally examines the influence of operating conditions on the performance of a Mg-Al spinel catalyst prepared from hydrotalcite precursors. This catalyst demonstrates an exceptional performance in the Guerbet reaction with a promising activity/butanol selectivity balance, excellent long-term stability, and very-low-carbon footprint (CO_2 generation as by-products is minimal). This study showcases a systematic strategy to optimize the reaction parameters in the Guerbet reaction for biobutanol production using an advanced spinel catalyst. Upon carefully adjusting temperature, pressure, space velocity, and reactants co-feeding, very promising conversion (35%) and butanol selectivity values (48%) were obtained.

The effect of support surface hydroxyls on selective CO methanation with Ru based catalysts

Martínez, LMT; Muñoz, A; Pérez, A; Laguna, OH; Bobadilla, LF; Centeno, MA; Odriozola, JA

Applied Catalysis A: General, **641** (2022) 118678
Julio, 2022 | **DOI:** 10.1016/j.apcata.2022.118678

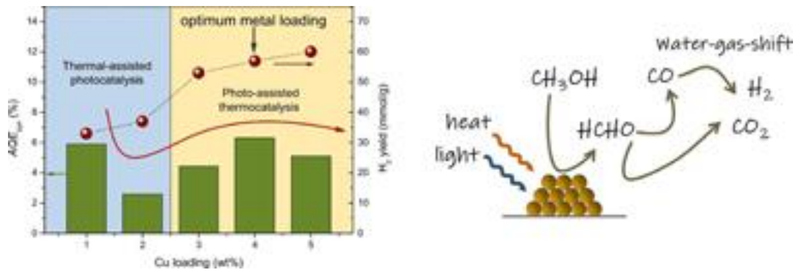


The aim of this work was to clarify the effect of the support on CO selective methanation with Ru/TiO_2 catalysts. TPR, XRD and TEM measurements confirmed that the changes in the activity and selectivity should be ascribed to anatase:rutile ratio, RuO_2 +TiO_2 solid solution formation, as well as the metal content and the thermal treatment used. All these characteristics result in active and selective catalysts in which the suppression of the reverse water gas shift reaction was observed. The catalytic performance must be explained by both the formation of more active Ru species as a result of support influence and the higher Ru dispersion. The study allows to conclude that for CO activation the role of support surface hydroxyls seems to be determinant for both the activity and selectivity of Ru/TiO_2 catalysts.

Tuning the co-catalyst loading for the optimization of thermo-photocatalytic hydrogen production over Cu/TiO_2

Platero, F; Caballero, A; Colón, G

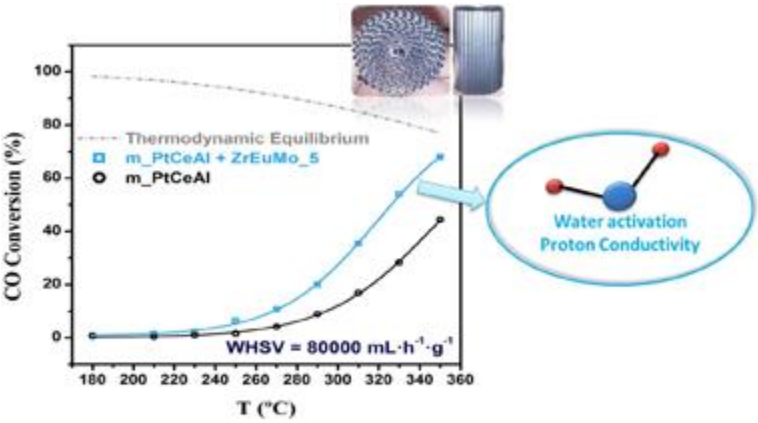
Applied Catalysis A-General, **643** (2022) 118804
Agosto, 2022 | **DOI:** 10.1016/j.apcata.2022.118804



We have optimized the H_2 production by methanol thermo-photocatalytic reforming in the gas phase using Cu/TiO_2 catalyst by tuning metal loading. Metal co-catalyst has been deposited by means of chemical reduction deposition. We have stated that thermo- and thermo-photocatalytic process leads to a notable H_2 production at 200 C. By in-situ FTIR studies we evidenced that formate formation follows a different evolution depending on the reforming experiment. These surface formate would lead to CO formation through dehydration reaction. At higher Cu content the low CO selectivity denote that water-gas-shift reaction would predominate and exalt H_2 yield. Thus, different optimum Cu content is found for each reforming experiment. While for the photocatalytic reforming Cu/TiO_2 (2 wt%) is the best catalyst of the series, we should increase the Cu content to Cu/TiO_2 (5 wt%) to achieve the optimum performance for thermo-photocatalytic reforming of methanol.

Boosting water activation determining-step in WGS reaction on structured catalyst by Mo-doping

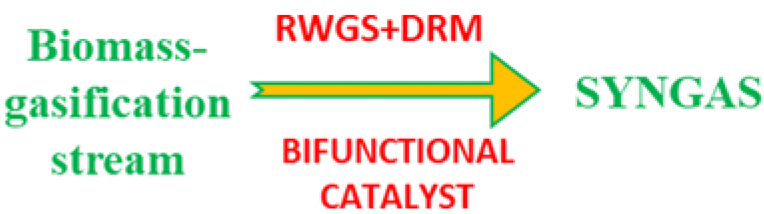
García-Moncada, N; Jurado, L; Martínez-Tejada, LM; Romero-Sarria, F; Odriozola, JA
Catalysis Today, **383** (2022) 193-204
Enero, 2022 | **DOI:** 10.1016/j.cattod.2020.06.003



Proton conductors Mo-Eu-Zr mixed oxide systems were synthesized and further mixed with a conventional Pt/CeO_2/Al2O_3 catalyst to develop a highly efficient water-gas-shift (WGS) catalyst. The designed catalyst, once structured, allows reach the equilibrium conversion at medium temperatures (~350 °C) at 80 L.g^{-1} h^{-1} space velocity. The ability of the proton conductor to maintain an elevated water concentration at the metal-support interface by Grotthuss' mechanism boosts the catalytic activity in WGS reaction.
The Mo-containing proton conductor is extensively characterized allowing to establish the formation of molybdenum oxide phases nucleating on top of the Eu sites in Eu-Zr oxide solid solution. $[MoO_4]^{2-}$ to $[Mo_7O_{24}]^{6-}$ clusters nucleates at low Mo contents resulting in a α-MoO_3 layer on increasing its content. In presence of H_2, Mobronzes are formed from similar to 200 °C enhancing water concentration at the surfaces and boosting the catalytic activity in the WGS reaction. These results pave the way for developing lower volume WGS reactors.

Catalytic Upgrading of Biomass-Gasification Mixtures Using Ni-Fe/ $MgAl_2O_4$ as a Bifunctional Catalyst

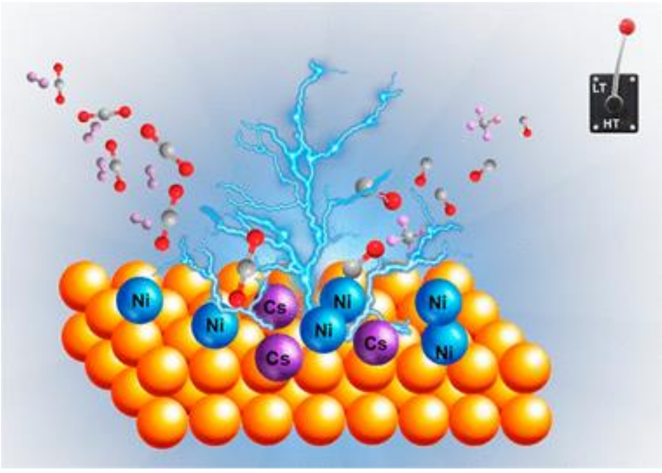
Tarifa, P; Reina, TR; González-Castaño, M; Arellano-García, H
Energy & Fuels, **36** (2022) 8267-8273
Agosto, 2022 | **DOI:** 10.1021/acs.energyfuels.2c01452



Biomass gasification streams typically contain a mixture of CO, H_2, CH_4, and CO_2 as the majority components and frequently require conditioning for downstream processes. Herein, we investigate the catalytic upgrading of surrogate biomass gasifiers through the generation of syngas. Seeking a bifunctional system capable of converting CO_2 and CH_4 to CO, a reverse water gas shift (RWGS) catalyst based on Fe/$MgAl_2O_4$ was decorated with an increasing content of Ni metal and evaluated for producing syngas using different feedstock compositions. This approach proved efficient for gas upgrading, and the incorporation of adequate Ni content increased the CO content by promoting the RWGS and dry reforming of methane (DRM) reactions. The larger CO productivity attained at high temperatures was intimately associated with the generation of $FeNi_3$ alloys. Among the catalysts' series, Ni-rich catalysts favored the CO productivity in the presence of CH_4, but important carbon deposition processes were noticed. On the contrary, 2Ni-Fe/$MgAl_2O_4$ resulted in a competitive and cost-effective system delivering large amounts of CO with almost no coke deposits. Overall, the incorporation of a suitable realistic application for valorization of variable composition of biomass-gasification derived mixtures obtaining a syngas-rich stream thus opens new routes for biosyngas production and upgrading.

Design of Full-Temperature-Range RWGS Catalysts: Impact of Alkali Promoters on Ni/CeO_2

Gandara-Loe, J; Zhang, Q; Villora-Pico, JJ; Sepulveda-Escribano, A; Pastor-Pérez, L; Reina, TR
Energy & Fuels, **36** (2022) 6362-6373
Junio, 2022 | **DOI:** 10.1021/acs.energyfuels.2c00784

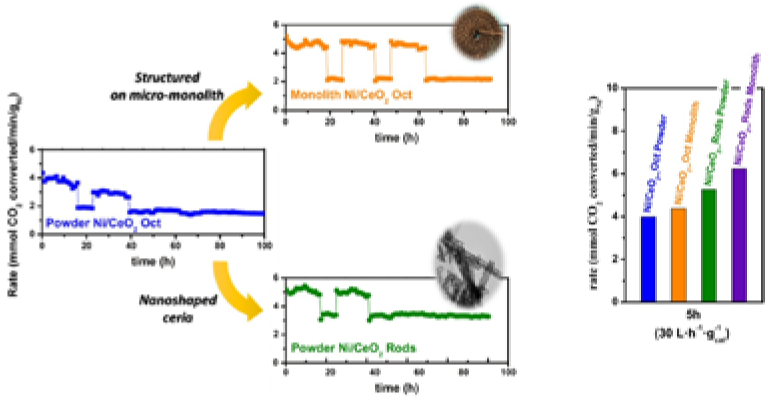


Reverse water gas shift (RWGS) competes with methanation as a direct pathway in the CO_2 recycling route, with methanation being a dominant process in the low-temperature window and RWGS at higher temperatures. This work showcases the design of multi-component catalysts for a full-temperature-range RWGS behavior by suppressing the methanation reaction at low temperatures. The addition of alkali promoters (Na, K, and Cs) to the reference Ni/CeO_2 catalyst allows identifying a clear trend in RWGS activation promotion in both low- and high-temperature ranges. Our characterization data evidence changes in the electronic, structural, and textural properties of the reference catalyst when promoted with selected dopants. Such modifications are crucial to displaying an advanced RWGS performance. Among the studied promoters, Cs leads to a more substantial impact on the catalytic activity. Beyond the improved CO selectivity, our best performing catalyst maintains high conversion levels for long-term runs in cyclable temperature ranges, showcasing the versatility of this catalyst for different operating conditions. All in all, this work provides an illustrative example of the impact of promoters on fine-tuning the selectivity of a CO_2 conversion process, opening new opportunities for CO_2 utilization strategies enabled by multi-component catalysts.

Enhanced catalytic activity and stability of nanoshaped Ni/CeO_2 for CO_2 methanation in micro-monoliths

García-Moncada, N; Navarro, JC; Odriozola, JA; Lefferts, L; Faria, JA
Catalysis Today, **383** (2022) 205-215
Enero, 2022 | **DOI:** 10.1016/j.cattod.2021.02.014

Coupling inherently fluctuating renewable feedstocks to highly exothermic catalytic processes, such as CO_2 methanation, is a major challenge as large thermal swings occurring during ON- and OFF- cycles can irreversible deactivate the catalyst via metal sintering and pore collapsing. Here, we report a highly stable and active Ni catalyst supported on CeO_2 nanorods that can outperform the commercial CeO_2 (octahedral) counterpart during CO_2 methanation at variable reaction conditions in both powdered and



μ-monolith configurations. The long-term stability tests were carried out in the kinetic regime, at the temperature of maximal rate (300 °C) using fluctuating gas hourly space velocities that varied between 6 and 30 L $h^{-1}.g_{cat}^{-1}$. Detailed catalyst characterization by mu-XRF revealed that similar Ni loadings were achieved on nanorods and octahedral CeO_2 (c.a. 2.7 and 3.3 wt. %, respectively). Notably, XRD, SEM, and HR-TEM-EDX analysis indicated that on CeO_2 nanorods smaller NiClusters with a narrow particle size distribution were obtained (~ 7 ± 4 nm) when compared to octahedral CeO_2 (~ 16 ± 13 nm). The fast deactivation observed on Ni loaded on commercial CeO_2 (octahedral) was prevented by structuring the reactor bed on μ-monoliths and supporting the Ni catalyst on CeO_2 nanorods. FeCrAlloy (R) sheets were used to manufacture a multichannel mu-monolith of 2 cm in length and 1.58 cm in diameter, with a cell density of 2004 cpsi. Detailed catalyst testing revealed that powdered and structured Ni/ CeO_2 nanorods achieved the highest reaction rates, c.a. 5.5 and 6.2 mmol CO_2 $min^{-1}.g_{Ni}^{-1}$ at 30 L $h^{-1}.gcat^{-1}$ and 300 °C, respectively, with negligible deactivation even after 90 h of fluctuating operation.

Fast photodegradation of rhodamine B and caffeine using ZnO-hydroxyapatite composites under UV-light illumination

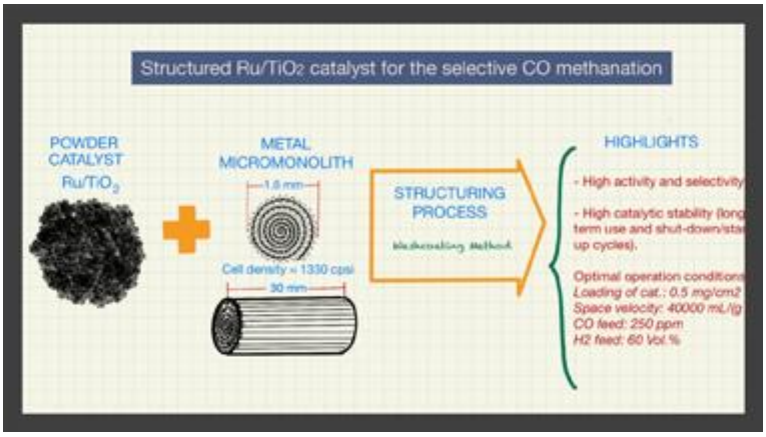
KarimTanji, J.A.Navio, Abdellah Chaqroune, Jamal Naja, F.Puga, M.C.Hidalgo, Abdelhak Kherbeche

Catalysis Today, **388** (2022) 176-186
Abril, 2022 | **DOI:** 10.1016/j.cattod.2020.07.044

Zinc oxide-hydroxyapatite composites were prepared using wet impregnation method. Firstly, a natural phosphate ore rich in silica and calcium phosphate was sieved to separate silica phase from phosphate phase. Then, through a chemical precipitation method, a pure hydroxyapatite (HAP) was obtained, which was used as a support for ZnO immobilization and applied for the photodegradation of two toxic contaminants: a transparent molecule (caffeine) and dye molecule (rhodamine B). During the present work two weight ratio percentages of zinc oxide were used: 25 wt.% and 50 wt.% of ZnO relative to HAP. The samples were characterized by X-ray diffraction (XRD), Fourier Transform Infrared (FTIR), X-ray Fluorescence (XRF), BET surface area (SBET), Scanning Electron Microscopy (SEM-EDS) and by Transmission Electron Microscopy (TEM-STEM). The immobilization of ZnO on HAP surface followed by thermal treatment at 400 °C for 2 h to get a homogenous dispersion of ZnO on the hydroxyapatite support. At high ZnO impregnation percentage, photodegradation performances of ZnO-HAP under UV illumination were fast and superior than the ZnO photocatalyst alone. The results showed that due to the presence of HAP, the conversion of both molecules became faster and greater, since it promotes the synergic phenomena of adsorption and photocatalysis. The toxicity of the treated substrate solutions obtained in the corn kernels germination test indicated a low toxicity after the photodegradation processes, probably due to a high mineralization degree.

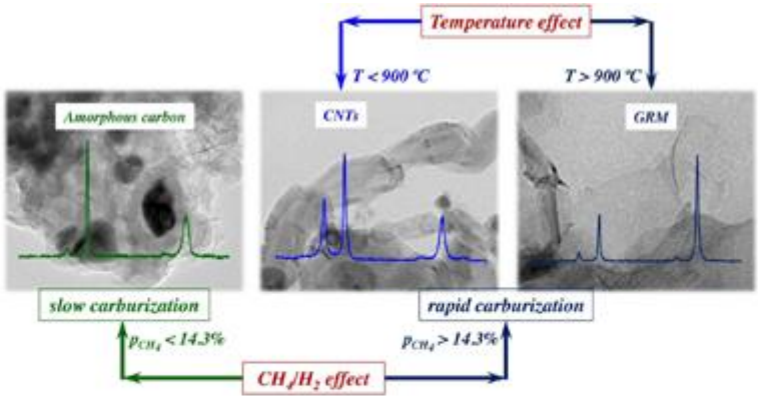
Metal micromonoliths for the cleaning of H_2 by means of methanation reactions

Laguna, OH; Muñoz-Murillo, A; Bobadilla, LF; Martínez, LM; Montes, M; Centeno, MA; Odriozola, JA
Catalysis Today, **383** (2022) 216-225
Enero, 2022 | **DOI:** 10.1016/j.cattod.2021.04.026



The present manuscript presents for the first time the structuring of a Ru/TiO_2 catalyst that was achieved by means of the washcoating procedure using homemade metal micromonoliths (Fecralloy (R)) of 1330 cpsi. For this, an optimized formulation of the slurried catalyst as well as a reproducible protocol for the coating of the micromonoliths were successfully achieved. The obtained structured systems were tested in the selective CO methanation reaction and the effect of different variables over the catalytic performance were analyzed such as the amount of loaded catalyst in the micromonoliths, the temperature of reaction, the space velocity, and the amount of CO and H_2 within the feed-stream. The study of all of these parameters allowed to establish optimal conditions to maximize the performance of the structured Ru/TiO_2 catalyst and subsequently, this was tested under those cited conditions in long-term tests (similar to 375 h), including shut-down/start-up cycles, aiming to evaluate its catalytic stability. The system presented a considerable stability along the different test without loss of catalytic activity, being specially remarkable its resistance to the inclusion of shut-down/start-up cycles. Therefore, this study lays the foundations for future development of more sophisticated structured systems for the selective CO methanation based on the structuring strategy proposed.

Performance of AISI 316L-stainless steel foams towards the formation of graphene related nanomaterials by catalytic decomposition of methane at high temperature
Cazana, F; Latorre, N; Tarifa, P; Royo, CJ; Sebastian, V; Romeo, E; Centeno, MA; Monzon, A
Catalysis Today, **383** (2022) 236-246
Enero, 2022 | **DOI:** 10.1016/j.cattod.2020.12.003

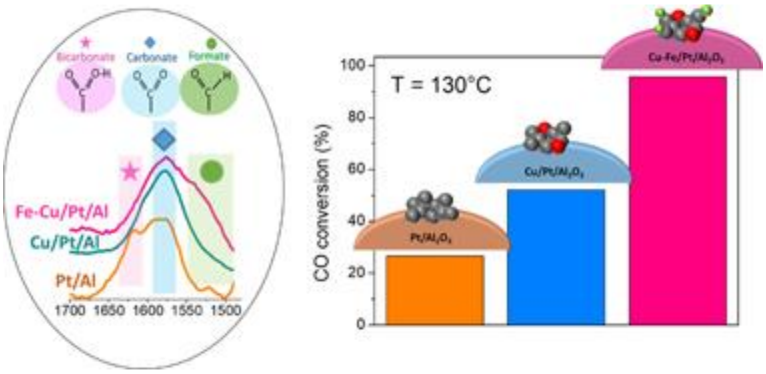


This work explores the preparation of graphene-related materials (GRMs) grown on stainless steel foams via catalytic decomposition of methane (CDM). The main active phases for the reaction are the Fe nanoparticles segregated from the stainless-steel after the activation stage of the foam. The effect of the feed composition and reaction temperature has been studied in order to maximize the productivity, stability and selectivity to GRMs. The maximum productivity attained was 0.116 g(C)/g(foam) h operating at 950 °C with a feed ratio of CH4/H-2 = 3 (42.9 %CH4:14.3 %H-2). The carbonaceous nanomaterials (CNMs) obtained were characterized by X-Ray diffraction, Raman spectroscopy and by transmission and scanning electron microscopy. The parameters of the kinetic model developed are directly related to the relevant stages of the process, including carburization, diffusion-precipitation and deactivation-regeneration. The balance among these sequential stages determines the overall performance of the activated foam. In conditions of rapid carburization of the Fe NPs (p(CH4) > 14 %), the productivity to CNMs is favoured, avoiding an initial deactivation of the active sites by fouling with amorphous carbon. After a rapid carburization, the selectivity to the different CNMs is governed by the ratio CH4/H-2, and mainly by the temperature. Thus, the formation of GRMs, mainly Few Layer Graphene (FLG) and even graphene, is favoured at temperatures above 900 °C. At lower temperatures, carbon nanotubes are formed.

Structured and micro-structured catalysts: A fascinating future for a sustainable world – A special issue in tribute to the careers of Professors Mario Montes and José Antonio Odriozola
M.A.Centeno; L.M.Gandía; F.Romero-Sarria; O.Sanz
Catalysis Today, **383** (2022) 1-4
Enero, 2022 | **DOI:** 10.1016/j.cattod.2021.09.034

Unravelling the role of Fe in trimetallic Fe-Cu-Pt/Al_2O_3 catalysts for CO-PROX reaction
Palma, S; González-Castaño, M; Romero-Sarria, F; Odriozola, JA
Molecular Catalysis, **517** (2022) 112015
Enero, 2022 | **DOI:** 10.1016/j.mcat.2021.112015

This work proposes a trimetallic Fe-Cu/Pt/Al2O3 catalyst as an appealing system for preferential oxidation of CO (CO-PROX) reaction. The excellent conversion rates achieved by the Fe-Cu/Pt/Al_2O_3



catalysts under realistic reforming-surrogated feed streams along with the catalyst stability, reproducibility, and scalability showcase a very competitive system for CO-PROX reaction units. Furthermore, the systematic analysis conducted for Pt/Al_2O_3, Cu/Pt Al_2O_3, and Fe-$Cu/Pt/Al_2O_3$ catalysts enabled establishing meaningful relationships between catalytic behaviour and the catalyst surface to reactants interactions. Thus, the enhanced CO oxidation performances attained by the incorporation of Fe species into bimetallic $Cu/Pt/Al_2O_3$ catalysts were associated to superior surface electron densities and inhibited CO adsorption process over Pt surfaces. Remarkably, operando-DRIFTS spectroscopy evidenced significantly larger H-containing surface species developed over the trimetallic system. The enhanced abilities for developing thermally instable intermediates favoured by small amounts of Fe should indeed determine the enhanced catalysts behaviours displayed by the trimetallic Fe-$Cu/Pt/Al_2O_3$ catalyst.

Effective photocatalytic conversion of formic acid using iron, copper and sulphate doped TiO_2

Zouheir, M; Tanji, K; Navío, JA; Hidalgo, MC; Jaramillo-Paez, CA; Kherbeche, A
Journal of Central South University, **29** (2022) 3592-3607
Noviembre, 2022 | **DOI:** 10.1007/s11771-022-5172-9

In this paper, the combined addition of copper or iron and sulphate ions onto TiO_2 prepared by a simple sol-gel method is studied for formic acid photocatalytic conversion. A wide structural and morphological characterization of the different photocatalysts was performed by X-ray diffraction (XRD), N_2-physisorption for BET surface area measurements, scanning and transmission electronic microscopies (SEM and TEM), UV-Vis diffuse spectroscopy (DRS) and X-ray photoelectron spectroscopy (XPS), in order to correlate the physico-chemical properties of the materials to their photocatalytic efficiencies for formic acid oxidation. Results have shown important differences among the catalysts depending on the metal added. Sulphated TiO_2/Cu (1%Cu) was the best photocatalyst obtaining about 100% formic acid conversion in only 5 min. The appropriate physico-chemical features of this photocatalyst, given by the addition of combined copper and sulphate ions, explain its excellence in photocatalytic reaction.

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

Puga, F; Navío, JA; Hidalgo, MC
Photochemical & Photobiological Sciences, **22** (2022) 549-566
Noviembre, 2022 | **DOI:** 10.1007/s43630-022-00334-9

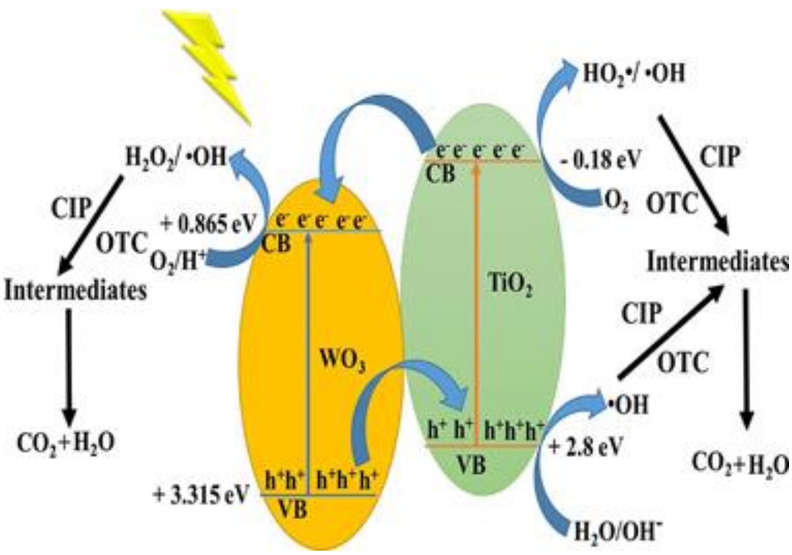
$AgBr/NaTaO_3$ composites, with different molar % of $NaTaO_3$ (Br/NTO(X%)), have been synthesized by simple precipitation methods; bare $NaTaO_3$ was synthesized by hydrothermal procedure, while AgBr was synthesized by a precipitation procedure using cetyl-tri-methyl-ammonium bromide (CTAB) and $AgNO_3$. 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.

Enhanced photocatalytic activity of TiO_2/WO_3 nanocomposite from sonochemical-microwave assisted synthesis for the photodegradation of ciprofloxacin and oxytetracycline antibiotics under UV and sunlight

Moghni, N; Boutoumi, H; Khalaf, H; Makaoui, N; Colón, G

Journal of Photochemistry and Photobiology A-Chemistry, **428** (2022) 113848
Junio, 2022 | **DOI:** 10.1016/j.jphotochem.2022.113848

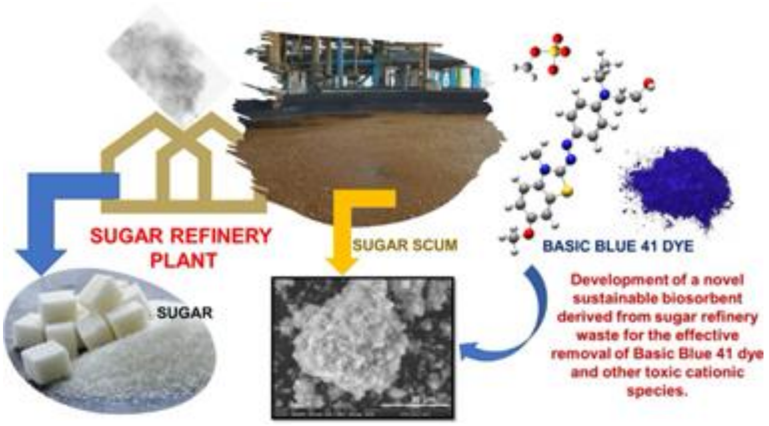


The TiO_2/WO_3 photocatalysts were prepared by a simple assisted sonochemical - microwave combination. The wide surface and structural characterization of synthesized material confirmed that the adopted preparation method resulted in nanoparticulated crystallite anatase phase of TiO_2 with a large surface area (> 200 m^2/g), and the dispersion of WO_3 on the surface of TiO_2. The photoactivity was assessed for the photodegradation of ciprofloxacin (CIP) and oxytetracycline (OTC) antibiotics under UV and sunlight irradiation. The mineralization rate, toxicity assessment, pollutant concentration effect on photodegradation efficiency, and reusability potential under sunlight were all investigated. Results showed that TiO_2 doped with 5 wt% of WO_3 exhibited the best photocatalytic activity under UV (100% degradation) and solar light. Rate constants for CIP and OTC degradation showed that TiO_2/WO_3 significantly improved with respect to bare TiO_2. The antibacterial study revealed that the photodegraded solutions became less toxic than the initial CIP and OTC solutions showing a significant decrease in the inhibition zone diameter and mineralization rates. The prepared TiO_2/WO_3 maintained high performances in the presence of high concentrations of pollutants as well as good stability after four consecutive uses. The increased photocatalytic activity is attributed to the incorporation of WO_3, which extends the light absorption range and decreases the rate of electron -hole recombination.

Insights into the physicochemical properties of Sugar Scum as a sustainable biosorbent derived from sugar refinery waste for efficient cationic dye removal

F. Atmani, M.M. Kaci, N. Yeddou-Mezenner, A. Soukeur, I. Akkari, J.A. Navío

Biomass Conversion and Biorefinery (2022)
Abril, 2022 | **DOI:** 10.1007/s13399-022-02646-3



The objective of this study was to determine the ability of sugar scum (SS), an industrial waste, as a novel biosorbent for the removal of Basic Blue 41 (BB 41) from aqueous solutions. The biosorbent was characterized by SEM/EDS, BET, FTIR, and pH_{pzc} measurements, respectively. To reach a maximum adsorption capacity of 26.45 $mg.g^{-1}$, impacting operational factors such as pH, biosorbent dose, contact duration, starting dye concentration, and temperature were adjusted, when the removal efficiency reached 84% during 60 min at pH 10, 1.5 $g.L^{-1}$ of biosorbent and $C_o = 10$ $mg.L^{-1}$. The experimental data were modeled by various isotherm models, whereas the best fit was found for Freundlich with a high correlation coefficient ($R^2 = 0.991$). Other kinetic models including pseudo-first, pseudo-second order, and intra-particle diffusion models were tested to fit the kinetic data. The biosorption of BB 41 onto SS was spontaneous ($\Delta G° < 0$) and exothermic ($\Delta H° < 0$), while the biosoprtion mechanism of BB41 over SS was proposed with repeated reuse showing that SS could be regenerated after four successive runs. Furthermore, this study revealed that sugar scum is an underutilized bioresource in Algeria, with the potential to provide low-cost environmental removal of additional contaminants in the wastewater treatment domain.

H_2 Photoproduction Efficiency: Implications of the Reaction Mechanism as a Function of the Methanol/Water Mixture

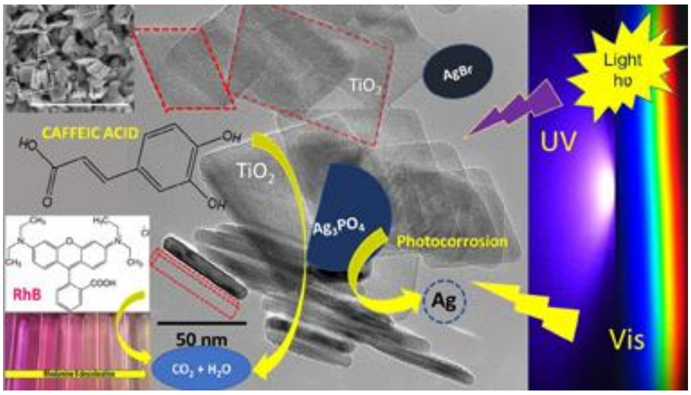
Barba-Nieto, I; Colón, G; Kubacka, A; Fernandez-García, M

Catalysts, **12** (2022) 402
Abril, 2022 | **DOI:** 10.3390/catal12040402

The influence of the reaction pathway of the sacrificial molecule oxidation to generate hydrogen is here investigated for lean and rich methanol reaction mixtures. Pt-TiO2 powders promoted or not with tin sulfide were used as catalysts. With the help of in situ infrared experiments under reaction conditions, methanol evolution was shown to take place by hole-related oxidation steps, with alkoxy and carbon-centered species as key radical species. The study analyzed quantitatively the fate and chemical use of the photons absorbed by the solids with the help of the quantum efficiency and the useful fraction of photons observables. Within this framework, the role of the sulfide component to promote photoactivity is interpreted, braiding chemical and photonic information.

Exploring the photocatalytic activities of a highly {0 0 1} faceted TiO_2 sensitized by coupling with AgBr or Ag_3PO_4

F.Puga; J.A.Navío; M.A.Paulete-Romero; J.M.Córdoba; M.C.Hidalgo
Materials Science and Engineering: B, **276** (2022) 115555
Febrero, 2022 | **DOI:** 10.1016/j.mseb.2021.115555



TiO_2 with high {0 0 1} facet exposure was coupled with AgBr or Ag_3PO_4. Catalysts were widely characterized and tested with rhodamine B (RhB) or caffeic acid under UV and visible light. Combination of the used sensitizer (AgBr or Ag_3PO_4) with TiO_2, not only enhances the high photocatalytic activity shown in the UV for TiO_2, but it also largely increases the degradation activity under visible illumination. A synergistic effect toward photocatalytic degradation in the visible light was observed when coupling AgBr and TiO_2, with the photocatalytic degradation profiles being strongly related to the molar percentages of the coupled materials and to the nature of the contaminant. The recycling of the coupled materials allows us to conclude that the AgBr(50%)/TiO_2 sample presents better results in the consecutive reuse cycles and percentages of RhB dye mineralization, in contrast to those observed for the Ag_3PO_4(50%)/TiO_2 composite.

Visible light photodegradation of blue basic 41 using cobalt doped ZnO: Box–Behnken optimization and DFT calculation

K. Tanji; M. Zouheir; Y. Naciri; H. Ahmoum; A. Hsini; O. Mertah; A. El Gaidoumi; J.A. Navio; M.C. Hidalgo; A Kherbeche
Journal of the Iranian Chemical Society, **19** (2022) 2779-2794
Enero, 2022 | **DOI:** 10.1007/s13738-022-02496-w

$Co_xZn_{1-x}O$ system ($0 \leq x \leq 0.2$) was synthesized using the solution combustion method with urea as a fuel source. Photocatalytic tests were performed under visible light to assess the Basic Blue 41 (BB41) conversion. Various characterization techniques, including XRD, FT-IR analysis, SEM, EDS, XRF, BET-surface area, and DRS were used to investigate the composition, structure, and morphology of the synthesized catalysts. In addition, the density functional theory calculation was used in order to study the electronic properties of the ZnO structure. The Box–Behnken model was valid for describing the degradation of BB41 dye according to the analysis of variances results. A maximum conversion of 100% for BB41 dye has been reached with high mineralization and important removal of chemical oxygen demand. The optimum conditions for BB41 conversion are reported. On the other hand, the reuse tests of the best catalyst showed high-performance stability after five cycles. Furthermore, the activity of superoxide ions ($O_2^{\cdot-}$) and hydroxyl radicals ($OH^{\cdot}$) as the spices responsible for BB41 dye conversion was well confirmed by the free radicals scavenging tests. The use of Box–Behnken optimization and DFT calculation applied to the synthesized catalysts proves to be a very suitable procedure to establish the operating conditions under which the synthesis strategy of the $Co_xZn_{1-x}O$ catalyst in its activity in the visible region performs an excellent efficiency for the degradation of organic dyes and makes contributions to the current literature related to the field of environmental technology.

Development of Power-to-X Catalytic Processes for CO_2 Valorisation: From the Molecular Level to the Reactor Architecture

Bobadilla, LF; Azancot, L; Luque-Alvarez, LA; Torres-Sempere, G; González-Castano, M; Pastor-Pérez, L; Ramírez-Reina, T; Ivanova, S; Centeno, MA; Odriozola, JA
Chemistry, **4** (2022) 1250-1280
Diciembre, 2022 | **DOI:** 10.3390/chemistry4040083

Nowadays, global climate change is likely the most compelling problem mankind is facing. In this scenario, decarbonisation of the chemical industry is one of the global challenges that the scientific community needs to address in the immediate future. Catalysis and catalytic processes are called to play a decisive role in the transition to a more sustainable and low-carbon future. This critical review analyses the unique advantages of structured reactors (isothermicity, a wide range of residence times availability, complex geometries) with the multifunctional design of efficient catalysts to synthesise chemicals using CO_2 and renewable H_2 in a Power-to-X (PTX) strategy. Fine-chemistry synthetic methods and advanced in situ/operando techniques are essential to elucidate the changes of the catalysts during the studied reaction, thus gathering fundamental information about the active species and reaction mechanisms. Such information becomes crucial to refine the catalyst's formulation and boost the reaction's performance. On the other hand, reactors architecture allows flow pattern and temperature control, the management of strong thermal effects and the incorporation of specifically designed materials as catalytically active phases are expected to significantly contribute to the advance in the valorisation of CO_2 in the form of high added-value products. From a general perspective, this paper aims to update the state of the art in Carbon Capture and Utilisation (CCU) and PTX concepts with emphasis on processes involving the transformation of CO_2 into targeted fuels and platform chemicals, combining innovation from the point of view of both structured reactor design and multifunctional catalysts development.

Preferential CO oxidation in hydrogen-rich gases over Ag catalysts supported on different supports

Todorova, S; Kolev, H; Karakirova, Y; Filkova, D; Grahovski, B; Aleksieva, K; Holgado, JP; Kadinov, G; Caballero, A
Reaction Kinetics Mechanisms and Catalysis, **135** (2022) 1405-1422
Marzo, 2022 | **DOI:** 10.1007/s11144-022-02158-1

The monometallic silver supported on SiO_2, Al_2O_3, ZSM-5 (Si:Al = 100) and bi-metallic AgCe/SiO_2 samples were studied in the reaction of the preferential CO oxidation. It was established that the supported silver catalysts are promising systems for selective oxidation of CO at low temperatures and the addition of cerium oxide increases the catalytic activity and selectivity most probably because of the increase in the silver dispersion; the homogeneous distribution of Ag and ceria on the silica support; formation of $Ag_n^{\delta+}$ clusters; increase in bulk and subsurface oxygen.

Research on properties and catalytic behaviour in CO hydrogenation at atmospheric and high pressure of bimetallic systems (10%Co+0.5%Pd)/TiO_2 (Al_2O_3)

Shopska, M; Caballero, A; Platero, F; Todorova, S; Tenchev, K; Fabian, M; Aleksieva, K;Kolev, H; Kadinov, G

Reaction Kinetics Mechanisms and Catalysis, **135** (2022) 589-618
Marzo, 2022 | **DOI:** 10.1007/s11144-022-02194-x

The properties of prereduced (10%Co + 0.5%Pd)/Al_2O_3 (TiO_2) systems in the CO hydrogenation reaction at atmospheric and high pressure were studied. At atmospheric pressure, alumina-supported catalysts were more selective toward methane but those using titania were more active. Alumina containing samples demonstrated high temperature H_2 desorption, firmly held surface carbonate species, high tendency to agglomeration. During the reaction metal surface reconstruction and increased formation of CH_2 groups occurred being more pronounced with titania-supported catalysts. Stability tests at 250 °C showed opposite behaviour of both systems. Monodentate carbonate intermediates adsorbed on sites of moderate strength prevailed on titania samples, while formate species predominated on high strength sites of alumina-supported catalysts. High pressure catalytic tests revealed dependence of activity on T_{red}, synthesis of C_{2+} hydrocarbons, decreased CO_2 production, a higher CH_4/CO_2 ratio for alumina containing system. Due to SMSI, increased CO_2 production on titania samples was preserved. Titania-supported catalysts revealed a stronger decrease of CO conversion rising T_{red} while alumina catalysts had almost unchanged activity. CO conversion decreased with time due to difficulties in surface diffusion of reagents/intermediates/products and metal particle agglomeration. Concerning T-red comparison of product distribution showed a steady trend. Because of stable CO and CHx surface species, titania containing catalysts produced lower content of C_{5+} compounds. Alumina-supported samples showed a higher selectivity to C_{5+} compounds at the expense of methane. A higher selectivity ratio for CH_4 and CO_2 determined in catalytic CO hydrogenation over a certain catalyst at atmospheric pressure could indicate that a given sample is predisposed to form C_{2+} hydrocarbons at a higher pressure.

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

The 13th International Symposium of the Romanian Catalysis Society | RomCat2022
22-24 junio [Baile Govora, Rumania]

Póster: **Selective gas phase dehydrogenation of formic acid over Pd-Ru based catalysts.** E.R. López; M.B. Ruz; M.R. Peláez; M.I. Domínguez; S. Ivanova; M.A. Centeno

Summer School of the Romanian Catalysis Society: Catalysis for Promising Future
26 junio [Baile Govora, Rumania]

Conferencia Invitada: **Structured and micro-structured catalysts: A fascinating future for a sustainable world.** M.A. Centeno

9th International Symposium on Carbon for Catalysis | CarboCat-IX
28 – 30 junio [Zaragoza, España]

Conferencia Invitada: **Development of GICs-derived catalysts and their application in the synthesis of graphene-related materials.** F. Cazaña; W. Henao; P. Tarifa; N. Latorre; J.J. Delgado; M.A. Centeno; E. Romeo; A. Monzón

Comunicación Oral: **Selective hydrodeoxygenation of levulinic acid over Ru supported on functionalized carbon nanofibers.** Ch.E. Bounoukta; C. Megias-Sayago; N. Rendón Marquez; F. Ammari; A. Penkova; S. Ivanova; M.A. Centeno; J.A. Odriozola

Póster: **Hydrogen yield improvement via pH control in the reaction of formic acid dehydrogenation.** J.L. Santos; E. Ruiz López; M.I. Domínguez; S. Ivanova; M.A. Centeno; J.A. Odriozola

Póster; **N-doped carbon xerogels for HMF production.** M. Andrades; G. Delgado; C.E. Bounoukta; S. Ivanova; M.I. Domínguez; L.M. Martínez T.; M.A. Centeno

Póster. **Understanding the effect of palladium size on formic acid dehydrogenation.** J.L. Santos; S. Ivanova; L.M. Martínez T.; M.A. Centeno; J.A. Odriozola

Póster. **Co-catalyst effect of calcium chloride and sulfonated activated carbons in the dehydration of glucose to HMF.** Ch. E. Bounoukta; S. Ivanova; F. Ammari; A. Penkova; M.A. Centeno; J.A. Odriozola

VI Forum: Advances of Nanotechnology in Biomedicine and Environment and the 3rd International Symposium on Nanotechnology
7 – 9 diciembre [Online, Juárez, México]

Conferencia Invitada: **Viabilidad del ácido fórmico como vector de energía: De la biomasa al hidrógeno verde.** M.A. Centeno

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

A. Caballero (Presidente del Comité Oganizador / Presidente Comité Científico)
G. Colón (Comité Organizador)
J.P. Holgado (Comité Organizador)
R. Pereñíguez (Comité Organizador)

COMUNICACIONES / COMMUNICATIONS

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

Comunicación Oral: **Nickel based hexaluminates: a new type of OCM catalysts.** J.P. Holgado, N. Touahri, A. Bennada, A. Caballero

Comunicación Oral: **Unraveling the effect of Re as promotor on Mo/ZSM-5 for methane dehydroaromatization reaction.** A. López-Martín, A. Caballero, G. Colón

Póster: **Efecto de la adición de Ru como promotor en catalizadores Co/TiO_2 para la síntesis de Fischer-Tropsch.** F.J. Platero, A. López-Martín, J.P. Holgado, G. Colón, A. Caballero

Póster: **Influencia en la reducibiliad y actividad en DRM al sustituir con aluminio la perovskita $LaNiO_3$.** F. Maldonado, F. Platero, R. Pereñiguez

Póster: **Adsorción de ciprofloxacina con perovskitas de lantano y bismuto.** J. Morillo, E. Otal, G. Molina, A. Caballero, R.M. Pereñíguez, J. Usero

XV Reunión del Grupo Español del Carbón
24 – 27 abril [Granada, España]

Comunicación Oral: **Estudio del efecto de las propiedades de textura del carbón en la deshidrogenación de ácido fórmico.** J.L. Santos; S. Ivanova; M. A. Centeno; J.A. Odriozola

Póster: **Nuevo método de preparación de microreactores integrales de carbón basados en sistemas de impresión 3D.** N. Rodríguez; G. Delgado; M.I. Domínguez; J.L. Santos; Y.Y. Agamez; J. de Jesús Díaz; J.A. Odriozola; M. A. Centeno

Póster: **Desarrollo de catalizadores basados en GICS y su aplicación en la síntesis de materiales grafénicos.** F. Cazaña; W.A. Henao; P. Tarifa; N. Latorre; J.J. Delgado; M.A. Centeno; E. Romeo; A. Monzón

Póster: **Deshidratación de glucosa a 5-hidroximetilfurfural sobre carbones bifuncionales.** C.E. Bounoukta; C. Megías-Sayago; F. Ammari; S. Ivanova; A. Monzón; M. A. Centeno; J.A. Odriozola

V Encuentro de Jóvenes Investigadores de la SECAT
11 – 13 julio [Alicante, España]

Comunicación Oral: **Efecto de la estructura de espumas de acero inoxidable sobre el crecimiento de NMCs por CCVD.** M. González Martín; F. Cazaña Pérez; N. La Torre Sierra; E. Romeo Salazar; M.A. Centeno Gallego; A. Monzón Bescós

Comunicación Oral: **Catalizadores bimetálicos de Pd y Co para la reacción de deshidrogenación del ácido fórmico.** M. Ribota Peláez; S. Ivanova; M.I. Dominguez Leal; L.M. Martínez Tejada; M.A. Centeno Gallego

VII Jornadas del Instituto Universitario de Investigación en Ciencias Ambientales de Aragón (IUCA)
6 octubre [Zaragoza, España]

Póster: **Desinfección de agua para su reuso: Activación del peroxidisulfato por Ag/ZnO bajo luz solar.** S.D. Jojoa.-Sierra; A.F. Silvera; C. Jaramillo-Páez; M.C. Hidalgo; M.P. Ormad; J.A. Navío; R. Mosteo

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título: **Elucidación de las especies activas en la reacción dehidroaromatización de metano a aromáticos sobre sistemas Mo-M/Zeolita: Efecto de la activación y de la adición de un segunto metal**
Autor: Ángeles María López Martín
Directores: Alfonso Caballero Martínez, Gerardo Colón Ibáñez
Centro: Universidad de Sevilla
Fecha Defensa: 20 de abril de 2022

Título: **Nanomateriales con propiedades fotocatalíticas mejoradas para tratamientos de purificación de aguas**
Autor: Felipe Rubén Puga Martínez
Directores: José Antonio Navío Santos, María del Carmen Hidalgo López
Centro: Universidad de Sevilla
Fecha Defensa: 29 de noviembre de 2022

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título: **Sintesis y caracterización de nanopartículas basadas en Eu^{3+}:$NaBi(MoO_4)_2$ con posibles aplicaciones en biomedicina**
Autor: Sara Ruiz Herrera
Tutores: Nuria O. Nuñez Álvarez, José Antonio Navío Santos
Grado: Trabajo Fin de Máster
Centro: Universidad de Sevilla
Fecha Defensa: 12 de julio de 2022

Título: **Producción de ácido fórmico a partir de glucosa**
Autor: Ana Montes
Tutores: Miguel Ángel Centeno, María Isabel Domínguez Leal
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 23 de septiembre de 2022

Título: **Catalizadores para la hidrogenación de CO_2 a ácido fórmico**
Autor: Alberto Moreno
Tutores: Leidy Marcela Martínez Tejada, Miguel Ángel Centeno
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 23 de septiembre de 2022

Título:	**Desarrollo de heteroestructuras fotofuncionales soportadas sobre biocarbones**
Autor:	José Enrique Lorca Arias
Tutores:	José Manuel Córdoba Gallego, María del Carmen Hidalgo López
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	26 de septiembre de 2022

Título:	**Catalizadores de carbón dopado con N producidos a partir de quitosano para la reacción de deshidrogenación de ácido fórmico**
Autor:	María Andrades García
Tutores:	Leidy Marcela Martínez Tejada, Miguel Ángel Centeno
Grado:	Trabajo Fin de Máster
Centro:	Universidad de Sevilla
Fecha Defensa:	6 de julio de 2022

Título:	**Catalizadores heterogéneos para la producción de ácido succínico a partir de ácido levulinico**
Autor:	Luis Alejandro Arriaga
Tutores:	Leidy Marcela Martínez Tejada, María Isabel Domínguez Leal
Grado:	Trabajo Fin de Máster
Centro:	Universidad de Sevilla
Fecha Defensa:	8 de diciembre de 2022

DOCENCIA / TEACHING

Investigadores de esta unidad participan en el Máster en Ciencia y Tecnología de Nuevos Materiales y en titulaciones de Grado y doble Grado de la Universidad de Sevilla (ver ACTIVIDADES DIVULGATIVAS Y FORMATIVAS)

PREMIOS Y RECONOCIMIENTOS / PRIZES AND ACKNOWLEDGEMENTS

Premio FISIOCAT 2022 Junior
Dr. Tomás Ramírez Reina
Premio a la Trayectoria Científica de Excelencia

X Edición Premio Losada Villasante
Dr. Tomás Ramírez Reina
Premio a la Investigación en Economía Circular por el trabajo "Nanocatalizadores de oro para la producción de hidrógeno verde: Hacia un modelo energético sostenible"

El premiado Tomás Ramírez Reina junto al responsable de su Grupo de Investigación, profesor José Antonio Odriozola Gordón

ESTANCIAS Y VISITAS 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

Pontificia Universidad Javeriana
Bogotá, Colombia — **Diana Lorena Lugo Castañeda** — 16/08/22 - 10/12/22

Institut Universitaire de Technologie (IUT) Robert Schuman. Universidad de Estrasburgo
Estrasburgo, Francia — **Claire Dumas** — 01/04/22 - 01/06/22

Universidad de la Plata
Buenos Aires, Argentina — **Federico Martín Pérz** — 01/03/22 - 01/05/22

School of Chemistry and Chemical Engineering. University of Surrey
Surrey, Inglaterra — **Anamika Kuswah** — 01/10/22 - 30/11/22

	Angie Merkouri	01/10/22 - 30/11/22
Politecnico di Milano Milán, Italia	**Alessandra Masseto**	14/02/22 - 01/10/22
Universidad Pedagógica y Tecnológica de Colombia Tunja, Colombia	**Mónica Hernández Laverde**	24/02/22 - 26/05/22

EQUIPAMIENTO CIENTÍFICO AVAILABLE EQUIPMENT

- Molino de bolas de movimiento planetario PM100 de RETSCH
- Espectrofotómetro Infrarrojos: Thermo-Nicolet Nexus FT-IR; Thermo-Nicolet 380 FT-IR
- Accesorio DRIFTS, celdas de alta y baja temperatura
- Sistema de vacío cuarzo/vidrio para adsorción de moléculas sonda seguido por FT-IR
- Espectrómetro de masas: Balzers Thermostar
- Sistema TPR-TPO (con posibilidad de realizar pulsos) seguido de espectrómetro de masas (Balzers) y detector de conductividad térmica. PID Eng&Tech.
- Equipos comerciales de actividad catalítica Microactivity Reference PID Eng&Tech (4)
- Microscopio metalográfico: Leica DMIRM
- Rotavapor: Heidolph Hei-VAP Value
- Equipo de ultra-alto vacío para espectroscopía XPS y Auger equipado con cañón de argón para realizar devastado iónico.
- Estufas: P-Selecta; P-Selecta digiheat
- Ph-metros: Crison pH burette 24; Crison phMeter Basic 20; Crison micropH2000.
- Cromatógrafos (2): Agilent Technologies 7890 A GC System; Agilent Technologies 6890 N Network GC System.
- Micro-cromatógrafos, microGC (2): Micro Gas Cromatograph CP-4900 Varian (2)
- HPLC: Varian 356-LC, Solvent Delivery Module Varian ProStar.
- Horno de soldadura: Microtest Máquina de ensayos EM2/200/FR
- Baño de ultrasonidos: P-Selecta Ultrasons Medi-II
- Horno Energon
- Horno para tratamiento de aceros a alta temperatura equipado con medidores de flujo e inyector de agua.
- Planta Piloto de Integración de reacciones catalíticas Reference PID Eng&Tech
- Espectrómetro Uv-Vis (Varian Cary 100, con esfera integradora para
- muestras sólidas)
- Analizador de Carbón Orgánico (TOC-V CHP Shimadzu 5000ª)
- Cromatógrafo (HPLC Agilent Technologies 1200)
- Espectrómetro IR (Varian 660-IR FTIR Spectrometer)
- Dip-Coater con cámara de temperatura (SS-00 AB Table Dry Oven MTI
- Corporation)
- Espectrofotómetro FTIR con celdas DRIFTS y ATR.
- Sistema de análisis TPR/TPO con detector TCD y espectrómetro de masas.
- 6 reactores catalíticos de gases con detección por cromatografía de gases y espectrometría de masas.

- 2 reactores catalíticos de líquidos que permiten el seguimiento de hasta 8 reacciones de forma simultánea con control de temperatura y flujo de gases.
- 4 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.
- Espectrofotómetros FTIR con accesorios DRIFTS, ATR y sistema de vacío en cuarzo/vidrio para adsorción de moléculas sonda
- Espectrómetros de masas
- Sistemas TPR-TPO (con posibilidad de realizar pulsos) seguido de espectrómetro de masas y detector de conductividad térmica.
- Microscopio metalográfico
- Rotavapor
- Estufas
- pH-metros
- Cromatógrafos de Gases
- Micro-cromatógrafos, microGC
- Cromatografos HPLC
- Horno de soldadura: Microtest Máquina de ensayos EM2/200/FR
- Baño de ultrasonidos
- Hornos
- Horno para tratamiento de aceros a alta temperatura equipado con medidores de flujo e inyector de agua.
- Planta Piloto de Integración de reacciones catalíticas Reference PID Eng&Tech
- Espectrómetro UV-Vis, con esfera integradora para muestras sólidas)
- Analizador de Carbón Orgánico
- Dip-Coater con cámara de temperatura
- Reactores catalíticos de gases con detección por cromatografía de gases y espectrometría de masas.
- Reactores catalíticos de líquidos que permiten el seguimiento de hasta 8 reacciones de forma simultánea con control de temperatura y flujo de gases.
- 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.

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

Personal / Personnel

Catedráticos	Dr. Miguel Ángel Castro Arroyo
	Dr. Manuel Jiménez Melendo
	Dra. Pilar Malet Maenner
	Dr. Julián Martínez Fernández
	Dr. Antonio Ramírez de Arellano-López
	Dr. Joaquín Ramírez Rico
Investigadores Científicos	Dra. María Dolores Alba Carranza
Científicos Titulares	Dr. José Jesús Benítez Jiménez
Profesores Titulares	Dr. Alfonso Bravo León
Doctores Contratados	Dra. Esperanza Pavón González
Investigadores en Formación	Lda. Ana Castro Chincho
	Gda. Sol Fernández Muñoz
	Gda. Irene Lamata Bermejo
	Gdo. Marcos Vázquez 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)

MINISTERIO DE CIENCIA E INNOVACIÓN | Financiado por la Unión Europea NextGenerationEU | Plan de Recuperación, Transformación y Resiliencia | AGENCIA ESTATAL DE INVESTIGACIÓN

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)

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_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

transferencia 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.

Biomasa para la desalación por desionización capacitiva y almacenamiento de energía
Biomass for DEsalination via CApacitive Deionization and Energy Storage, "BioDECADES"

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-1380856	01-01-2022 31-12-2022	Junta de Andalucía	80.000 €

Investigador Principal Research Head	Componentes Research Group
Joaquín Ramírez Rico	Alfonso Bravo León Manuel Jiménez Melendo Julián Martínez Fernández

RESUMEN / ABSTRACT

La presión sobre nuestros recursos hídricos, el calentamiento global y la escasez de combustibles fósiles son tres de los principales desafíos que, como sociedad, tendremos que abordar en la próxima década. Las soluciones a estos desafíos se basan en el desarrollo de nuevas tecnologías que permitan el uso eficiente y la reutilización de los recursos hídricos, así como en nuevos sistemas de almacenamiento de alta potencia y alta densidad de energía que se combinen con fuentes renovables. Estos dos temas aparentemente dispares dependen de una tecnología: electrodos y adsorbentes de carbono. Tanto los sistemas de desalinización y purificación como los supercondensadores y las baterías usan materiales basados en carbono con propiedades controladas mediante procesos físico-químicos. Una de las rutas más interesantes para la síntesis de estos materiales es la pirólisis de biomasa, un precursor barato y ampliamente disponible. La desionización capacitiva (CDI) es una tecnología emergente para aplicaciones en desalación que utiliza una pequeña diferencia de potencial eléctrico entre dos electrodos de carbono para eliminar iones de una solución mediante electrosorción. El pequeño potencial necesario para el proceso permite alimentar un dispositivo de CDI mediante paneles solares, lo que hace que esta tecnología sea útil en sistemas portátiles o fácilmente desplegables. Los supercondensadores y las baterías también se basan en mecanismos de adsorción y/o intercalación para almacenar carga eléctrica, en un proceso que es esencialmente el mismo, pero adaptado en este caso a maximizar la densidad de energía almacenada. Ambas tecnologías se basan en el uso de electrodos de carbono, con propiedades y estructura adaptadas a cada una de las aplicaciones.

El objetivo principal de esta propuesta es explorar el uso de residuos de biomasa como precursores de materiales de carbono con propiedades controladas para aplicaciones electroquímicas relacionadas la energía y el medio ambiente, con un enfoque en dos aplicaciones principales: almacenamiento de energía en sistemas de supercondensadores y baterías, y desalación por CDI. La

ruta de preparación de será la pirólisis de precursores de biomasa, centrándonos en productos de desecho de explotaciones agrícolas. Para la obtención de electrodos monolíticos usaremos madera y tableros prensados de fibra. Desarrollaremos métodos físicos y químicos con el fin de controlar sus propiedades para mejorar su capacitancia o selectividad de iones.

Construiremos un dispositivo de CDI a escala laboratorio para determinar el comportamiento de desalinización y correlacionarlo con información microscópica obtenida por técnicas avanzadas como microscopía electrónica, experimentos de difracción de dispersión total, isotermas de adsorción de nitrógeno y otros. Estudiaremos las propiedades electroquímicas de estos materiales y las correlacionaremos con la estructura y las condiciones de procesado. Nuestro objetivo será optimizar los electrodos de carbono derivados de la biomasa para aplicaciones específicas y desarrollar materiales de carbono derivados de la biomasa 'a la carta'.

Water resources, global warming and the decline of fossil fuels are three of the main challenges that we as a society will have to address in the next decade. Solutions to these challenges rely on the development of new technologies that allow the efficient use and reuse of water resources, as well as on new, high power and high energy density storage systems to be coupled with renewable sources. These two seemingly unrelated topics currently rely on one technology: carbon adsorbents and electrodes. Both desalination and purification systems as well as supercapacitors and batteries use materials that are based on carbon, their structure modified through physical and/or chemical processes. Biomass is a cheap, widely available precursor for carbon materials, which can be obtained by pyrolysis. Both the choice of biomass as well as the actual process will determine the final properties of the carbon electrode, which can be tailored for targeted applications.

Capacitive deionization (CDI) is an emerging desalination technology with tunable salt removal levels, that uses a small voltage applied across two carbon electrodes to remove ions from solution by means of Electrosorption. The small amount of energy required means that such a system can be powered by a solar panel, making this technology useful in portable and deployable systems. Supercapacitors and batteries also rely on adsorption and/or intercalation mechanisms to store electric charge, in a process that is essentially the same but with a different final target as CDI. Both technologies rely on the use of carbon electrodes, with properties and structure tailored to each of the applications.

This proposal's main objective is to use biomass residue as a precursor to develop tailored carbon electrodes for electrochemical applications related to energy and environmental technologies, with a focus on two main applications: energy storage in supercapacitor systems and batteries, and desalination via CDI. The main proposed synthesis approach for this electrodes 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. In the case of monolithic electrodes, wood and wood-derived fiberboards will be the main focus. Chemical methods will be developed to functionalize the resulting carbons, to improve their capacitance or ion selectivity.

We will build a CDI testing rig to determine desalination behavior, and to correlate this with microscopic information obtained from advanced techniques such as electron microscopy, total scattering diffraction experiments, nitrogen adsorption isotherm, and others. We will test the electrochemical energy storage behavior and correlate it with structural properties and processing conditions. Our goal will be to optimize carbon electrodes derived from biomass for targeted applications, and to develop a menu of biomass derived carbon materials.

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

Aspectos genéticos y biofísicos de la formación de la cutícula del fruto de tomate

Código/Code:	RTI2018-094277-B-C22
Periodo/Period:	01-01-2019 / 30-06-2022
Organismo Financiador/Financial source:	Ministerio de Ciencia e Innovacion
Importe total/Total amount:	193.600 €
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

Development of formulations bases on tomato pomace extracts from the preparation of post harvest coatings on fruits and vegetables

Periodo/Period:	10-02-2022 / 09-09-2022
Organismo Financiador/Financial source:	DECCO WORLDWIDE POST-HARVEST HOLDINGS BV
Importe total/Total amount:	29.000 €
Investigador responsable/Research head:	José Jesús Benítez

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

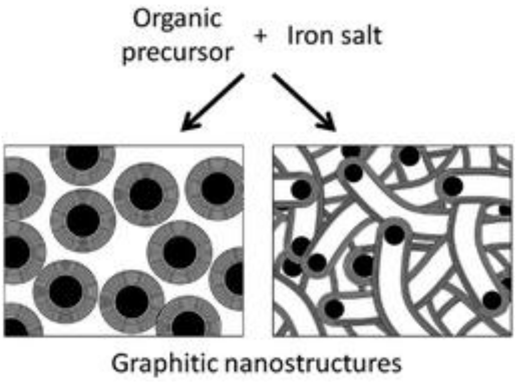
Periodo/Period:	31-08-2022 / 31-03-2023
Organismo Financiador/Financial source:	Fundación Ayuda en Acción
Importe total/Total amount:	31.476 €
Investigador responsable/Research head:	Susana Guzmán Puyol (IHSM)
Participante del ICMS como investigador:	José Jesús Benítez

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Iron-catalyzed graphitization for the synthesis of nanostructured graphitic carbons

Hunter, RD; Ramírez-Rico, J; Schnepp, Z

Journal of Materials Chemistry A, **10** (2022) 4489-4516
Febrero, 2022 | **DOI:** 10.1039/d1ta09654k

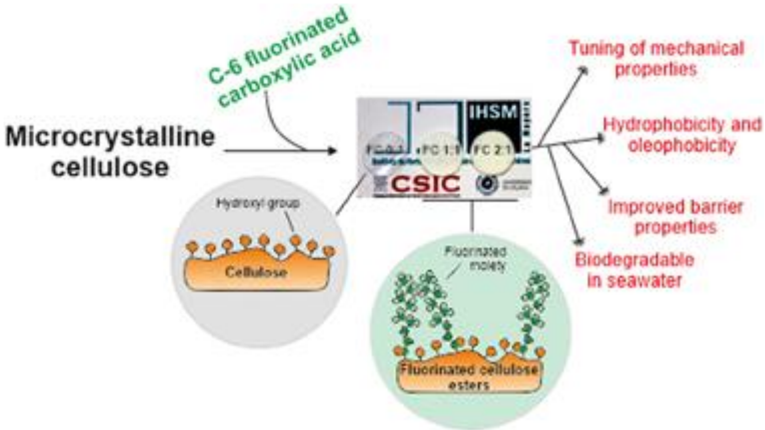


Carbons are versatile and diverse materials that have numerous applications across energy and environmental sciences. Carbons with a graphitic structure are particularly appealing due to their high chemical stability, large surface areas and high thermal and electronic conductivity. Numerous methods exist to produce nanostructured graphitic carbons but some of these can be energy-intensive and/or have problems with scalability. One option that is being increasingly explored is the process of iron-catalyzed graphitization. This simply involves the pyrolysis of carbon-rich precursors in the presence of an iron catalyst and has been used to produce carbons with a wide range of structures and properties. This review will examine the current field of iron-catalyzed graphitization, with a focus on molecular organic or biomass precursors. Bio-derived precursors are particularly attractive as a potential option for sustainable production of graphitic carbons. We start with a brief introduction to some key carbon structures, the current applications in which they are employed and some of the key methods that have been developed to produce nanostructured graphitic carbons. We will then review the history of catalytic graphitization before evaluating the wide range of conditions and precursors that have been employed in catalytic graphitization. Finally, this review will investigate the current challenges facing iron-catalyzed graphitization, looking particularly at the limitations of the current understanding of the mechanistic aspects of graphitization, with a view to outlining where research in this field might progress.

Greaseproof, hydrophobic, and biodegradable food packaging bioplastics from C6-fluorinated cellulose esters

Guzman-Puyol, S; Tedeschi, G; Goldoni, L; Benitez, JJ; Ceseracciu, L; Koschella, A; Heinze, T; Athanassiou, A; Heredia-Guerrera, JA

Food Hydrocolloids, **128** (2022) 107562
Julio, 2022 | **DOI:** 10.1016/j.foodhyd.2022.107562



Tridecafluorononanoic acid (TFNA), a C6-fluorinated carboxylic acid, was esterified with cellulose at different molar ratios (0:1, 1:1, 2:1, and 3:1) in a trifluoroacetic acid (TFA):trifluoroacetic anhydride (TFAA):$CHCl_3$ (2:1:1, v:v:v) solvent mixture. Free-standing films were obtained for all formulations and are presented as alternatives to composites and blends of paper with fluorinated molecules. Mechanical properties were investigated by tensile tests, and a plasticizer effect of fluorinated chains was observed. Interestingly, the wettability of these new cellulose derivatives was similar or even better than other common cellulose derivatives and fluorinated poly-mers employed in food packaging. Hydrodynamic properties were also improved by addition of TFNA, resulting in materials with water vapor permeability values comparable to other cellulose-based food packaging materials. In addition, films with the higher amounts of TFNA showed the required oil resistance for papers used in food packaging applications, as determined by the Kit Test. Finally, the biodegradation of these C6-fluorinated cel-lulose esters, assessed by biological oxygen demand (BOD) in seawater, was higher than typical bio-based polymers used in food packaging. The bioplastic synthesized at a molar ratio 1:1 (TFNA:cellulose) showed excellent performances in terms of greaseproof, hydrophobicity, ductility, and biodegradability, representing a sustainable alternative to typical plastics used in food packaging.

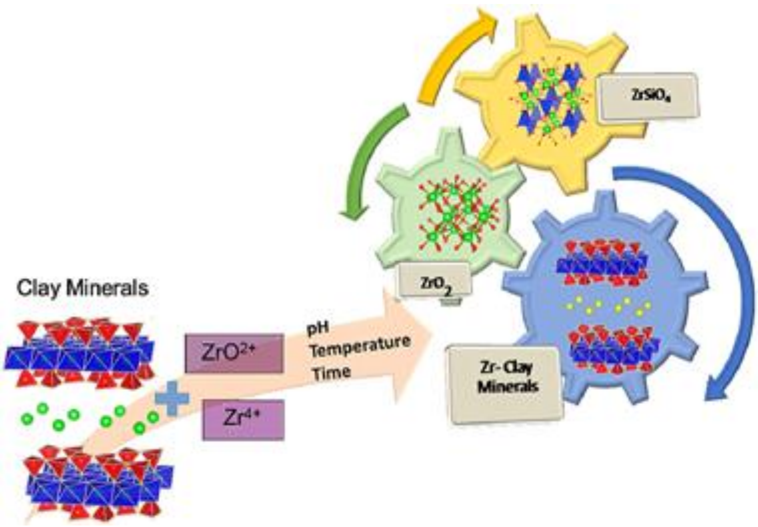
Flame confinement in biomass combustion systems for particles abatement

Ciria, D; Orihuela, MP; Moreno-Naranjo, P; Chacartegui, R; Ramírez-Rico, J; Becerra, JA
Energy Conversion and Management, **264** (2022) 115706
Julio, 2022 | **DOI:** 10.1016/j.enconman.2022.115706

This work explores the use of open-pore, inert ceramic foams with different pore sizes as particle abatement systems in small biomass combustion systems. Porous foams made of silicon carbide with pore sizes 10 to 60 pores-per-inch were installed in an in-house designed combustion unit operated with wood pellets. Their effects on the temperature distribution inside the chamber, particulate and gases emissions were studied using different airflow rates in the reaction-limited regime (low equivalence ratio) to minimise stoichiometric factors. The influence of pore size, foam position with respect to the flame and space velocity were assessed. The confinement of the flame with inert foams was found to substantially modify the temperature distribution in the combustion chamber, improve the air-fuel mixture, and favour the thermal decomposition of the pellet, leading to a reduction in particulate emissions when compared to free-flame combustion at the same experimental conditions. In general, the amount of particulate matter was found to decrease by up to one order of magnitude as the pore size of the foam was reduced, while the temperature gradient in the combustion chamber was increased. Nitrogen oxides and carbon dioxide emissions were essentially unchanged, irrespectively of the pore size of the foam. It is expected that these values will be improved with longer residence times, as happens in operations with reduced excess air ratios. These results suggest that it is possible to control pollutants derived from domestic heating within the most restrictive current regulations on particulate emissions by integrating flame confinement designs with better operating practices and efficient abatement systems.

Insight into the role of temperature, time and pH in the effective zirconium retention using clay minerals

Pavon, E; Alba, MD
Journal of Environmental Chemical Engineering, **308** (2022) 114635
Abril, 2022 | **DOI**: 10.1016/j.jenvman.2022.114635



The use of zirconium in chemical industries generates a potential risk of Zr contamination in the environment, with particular concern for the decommissioning of uranium-graphite reactors. Among the natural adsorbents employed for the treatment of nuclear waste, clay minerals showed a very high affinity adsorption for radionuclides, but the influence of the chemical composition, pressure, temperature and time reaction have not yet been analysed on deep. Thus, the objective of this research is to explore several experimental conditions for an actual prediction of the behaviour of zirconium immobilization by clay minerals. The results have shown that factors such as zirconium cation nature (Zr4+ or ZrO2+), temperature, time and pH influence the extent of zirconium immobilization by clay minerals and the zirconium phases generated. At moderate conditions, zirconium tectosilicates are formed and evolve to zircon at high temperature and a longer time reaction.

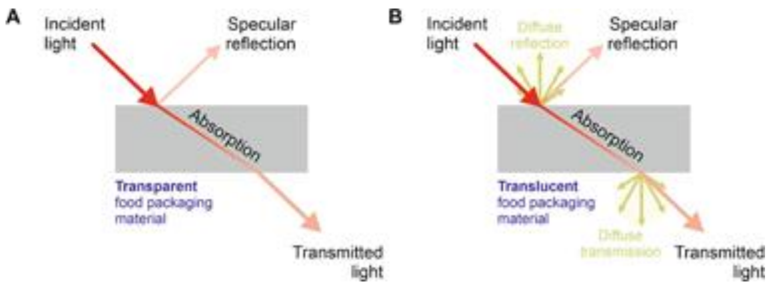
Transparent, UV-blocking, and high barrier cellulose-based bioplastics with naringin as active food packaging materials

Guzman-Puyol, S; Hierrezuelo, J; Benitez, JJ; Tedeschi, G; Porras-Vazquez, JM; Heredia, A; Athanassiou, A; Romero, D; Heredia-Guerrero, JA
International Journal of Biological Macromolecules, **209** (2022) 1985-1994
Mayo, 2022 | **DOI:** 10.1016/j.ijbiomac.2022.04.177

Free-standing, robust, and transparent bioplastics were obtained by blending cellulose and naringin at different proportions. Optical, thermal, mechanical, antioxidant, and antimicrobial properties were systematically investigated. In general, the incorporation of naringin produced important UV blocking and plasticizer effects and good antioxidant and antibacterial properties. Moreover, the barrier properties were characterized by determination of their water and oxygen transmission rates, finding that both parameters decreased by increasing the naringin content and reaching values similar to other petroleum-based plastics and cellulose derivatives used for food packaging applications. Finally, the biodegradability of these films was determined by measurement of the biological oxygen demand (BOD) in seawater, demonstrating an excellent decomposition in such conditions.

Transparency of polymeric food packaging materials

Guzman-Puyol, Susana; Benitez, Jose J; Heredia-Guerrero, Jose A
Food Research International, **161** (2022) 111792
Noviembre, 2022 | **DOI:** 10.1016/j.foodres.2022.111792

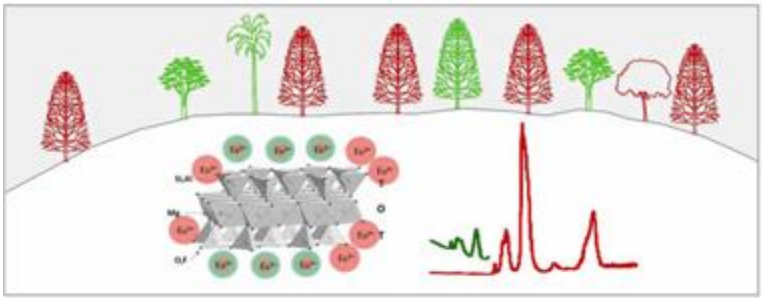


Transparency is a very important technical parameter to evaluate and validate certain food packaging materials. In the recent scientific literature, several methods (i.e. transmittance, opacity, haze, and absorbance) have been used and such variety hinders a direct comparison of results from different authors. In this Review, we describe and discuss the most widely employed methods to measure transparency, with special emphasis on two main parameters: transmittance and opacity. Moreover, a comparison of the different techniques is addressed and the typical values of transmittance and opacity of common transparent food packaging materials are provided. Our current opinion is that transparency should be expressed as transmittance in the visible range due to both the quickness and easiness of the measurement and the standardization of data. This information should be accompanied by the thickness value and a graphical image of the analysed samples for a useful and complete characterization.

Exploring the local environment of the engineered nanoclay Mica-4 under hydrothermal conditions using Eu(3+)as a luminescent probe

Martín-Rodríguez, R; Aguado, F; Alba, MD; Valiente, R; Pavon, E; Perdigon, AC
Journal of Alloys and Compounds, 921 (2022) 166086
Noviembre, 2022 | DOI: 10.1016/j.jallcom.2022.166086

High charge mica $Na_4Al_4Si_4Mg_6O_{20}F_4$, Mica-4, is a promising candidate as a filling material to immobilize high-level radioactive waste in deep geological repositories due to its extraordinary adsorption capacity. In contrast to traditional clay materials, the structural composition of this mica, with a high content of alu-minum in the tetrahedral sheet, enhances its chemical reactivity, favoring the formation of new



crystalline phases under mild hydrothermal conditions, and thus providing a definitive isolation of the radionuclides in the engineered barrier. Moreover, this synthetic clay has some features that allow its use as an optical sensor by doping with luminescent rare earth cations such as Eu^{3+}. In this paper we discuss the local structure of the nanoclay Mica-4 using Eu^{3+} as a local probe to track the physical and chemical modifica-tions under hydrothermal conditions. For that purpose, a set of hydrothermal experiments has been carried out heating Mica-4 and an aqueous $Eu(NO_3)_3$ solution in a stainless steel reactor at different temperatures and times. Optical properties of the as-treated samples were characterized by spectroscopic measurements. The fine peak structure of emission and the relative intensity of different Eu^{3+} transitions as well as the luminescence lifetime have been correlated with the structure and composition of this nanoclay, and the interaction mechanisms between the lanthanide ions and the clay mineral at different temperatures and times. Special attention has been paid to understanding the role of the aluminum content, which may act as either an aggregating or dispersing agent, in the optical features and reactivity of the system.

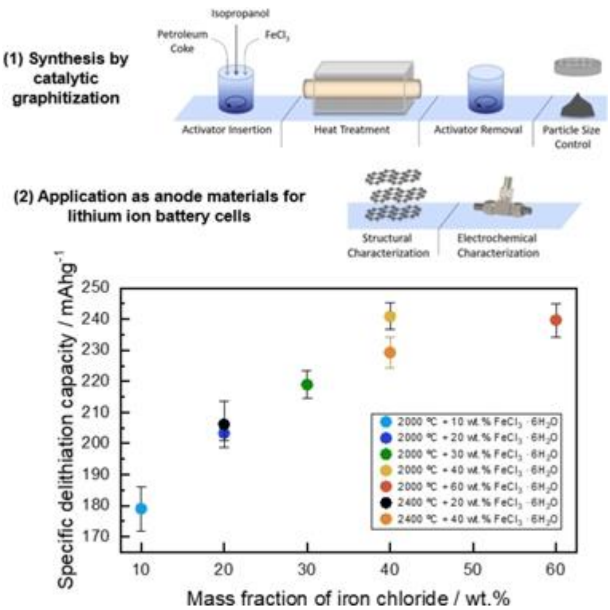
The Response of Tomato Fruit Cuticle Membranes Against Heat and Light

Benitez, JJ; Moreno, AG; Guzman-Puyol, S; Heredia-Guerrero, JA; Heredia, A; Dominguez, E
Frontiers in Plant Science, **12** (2022) 807723
Enero, 2022 | **DOI:** 10.3389/fpls.2021.807723

Two important biophysical properties, the thermal and UV-Vis screening capacity, of isolated tomato fruit cuticle membranes (CM) have been studied by differential scanning calorimetry (DSC) and UV-Vis spectrometry, respectively. A first order melting, corresponding to waxes, and a second order glass transition (T_g) thermal events have been observed. The glass transition was less defined and displaced toward higher temperatures along the fruit ripening. In immature and mature green fruits, the CM was always in the viscous and more fluid state but, in ripe fruits, daily and seasonal temperature fluctuations may cause the transition between the glassy and viscous states altering the mass transfer between the epidermal plant cells and the environment. CM dewaxing reduced the T_g value, as derived from the role of waxes as fillers. T_g reduction was more intense after polysaccharide removal due to their highly interwoven distribution within the cutin matrix that restricts the chain mobility. Such effect was amplified by the presence of phenolic compounds in ripe cuticle membranes. The structural rigidity induced by phenolics in tomato CMs was directly reflected in their mechanical elastic modulus. The heat capacity (Cp_{rev}) of cuticle membranes was found to depend on the developmental stage of the fruits and was higher in immature and green stages. The average Cp_{rev} value was above the one of air, which confers heat regulation capacity to CM. Cuticle membranes screened the UV-B light by 99% irrespectively the developmental stage of the fruit. As intra and epicuticular waxes contributed very little to the UV screening, this protection capacity is attributed to the absorption by cinnamic acid derivatives. However, the blocking capacity toward UV-A is mainly due to the CM thickness increment during growth and to the absorption by flavone chalconaringenin accumulated during ripening. The build-up of phenolic compounds was found to be an efficient mechanism to regulate both the thermal and UV screening properties of cuticle membranes.

Insights into the Impact of Activators on the 'Catalytic' Graphitization to Design Anode Materials for Lithium Ion Batteries

Hanhart, V; Frankenstein, L; Ramírez-Rico, J; Diozios, V; Winter, M; Gomez-Martín, A; Placke, T
Chemelectrochem, **9** (2022) e202200819
Noviembre, 2022 | **DOI:** 10.1002/celc.202200819



In this work, we systematically investigate the 'catalytic' graphitization of a biomass precursor (coffee ground) using 10-60 wt.% of the activator iron (III) chloride hexahydrate in a temperature range of 1000 °C-2400 °C. Special focus is put on the correlation of synthesis conditions, e.g., heat treatment temperature and mass fraction of iron chloride, with the electrochemical performance in carbon vertical bar vertical bar Li metal cells. The structural investigations of the materials reveal a positive impact of an increasing heat treatment temperature and/or mass fraction of inserted activator on the degree of graphitization and the delithiation capacity. However, a saturation point regarding the maximum degree of graphitization at 2000 °C and reversible capacity by the 'catalytic' graphitization approach using iron (III) chloride has been found. A maximum degree of graphitization of approximate to 69% could be reached by applying 2000 °C and 40 wt.% $FeCl_3$ center dot $6H_2O$, resulting in a reversible capacity of 235 mAh g^{-1}.

Biopolymer-Based Films Reinforced with FexOy-Nanoparticles

Abdullah, JAA; Jiménez-Rosado, M; Benitez, JJ; Guerrero, A; Romero, A
Polymers, **14** (2022) 4487
Noviembre, 2022 | **DOI:** 10.3390/polym14214487

Nowadays, natural polymer-based films are considered potentially environmentally friendly alternatives to conventional plastic films, due to many advantageous properties, including their easy processability, high flexibility, non-toxicity, low cost, high availability, and environmental safety. However, they are limited in their application by a number of shortcomings, including their high water solubility and vapor permeability as well as their poor opacity and low mechanical resistance. Thus, nanoparticles, such as green FexOy-NPs, can be used to overcome the drawbacks associated with these materials. Therefore, the aim of this study was to develop three different polymer-based films (gelatin-based, cellulose acetate-based and chitosan-based films) containing green synthesized FexOy-NPs (1.0% w/w of the initial polymer weight) as an additive to improve film properties. This was accomplished by preparing the different films using the casting method and examining their physicochemical, mechanical, microstructural, and functional characteristics. The results show that the incorporation of FexOy-NPs into the different films significantly enhanced their physicochemical, mechanical, and morphological properties as well as their antioxidant characteristics. Consequently, it was possible to produce suitable natural polymer-based films with potential applications across a wide range of industries, including functional packaging for food, antioxidants, and antimicrobial additives for pharmaceutical and biomedical materials as well as pesticides for agriculture.

Structural analysis of mixed alpha- and beta-amyrin samples

Gomez-Pulido, LDM; González-Cano, RC; Benitez, JJ; Dominguez, E; Heredia, A
Royal Society Open Science, **9** (2022) 211787
Abril, 2022 | **DOI:** 10.1098/rsos.211787

Little is known about the structure and molecular arrangement of alpha- and beta-amyrin, a class of triterpenoids found within the cuticle of higher plants. Blends of both amyrin isomers with different ratios have been studied taking into consideration a combined methodology of density functional theory (DFT) calculations with experimental data from scanning electron microscopy, differential scanning calorimetry and Raman vibrational spectroscopy. Results indicate that trigonal trimeric aggregations of isomer mixtures are more stable, especially in the 1 : 2 (alpha : beta) ratio. A combination of Raman spectroscopy and DFT calculations has allowed to develop an equation to determine the amount of beta-amyrin in a mixed sample.

High temperature mechanical properties of polycrystalline Y_2SiO_5

Cabezas-Rodríguez, R; Ciria, D; Martínez-Fernandez, J; Dezanneau, G; Karolak, F; Ramírez-Rico, J
Boletin de la Sociedad Española de Ceramica y Vidrio, **61** (2022) S60-S68-228
Mayo, 2022 | **DOI:** 10.1016/j.bsecv.2021.09.008

The high temperature mechanical properties of polycrystalline Y_2SiO_5 were studied in compression at temperatures in the range of 1200-1400 °C, both in constant strain rate and constant stress experiments. To examine the effect of grain size on the plastic deformation, two routes were used for the synthesis and sintering of Y_2SiO_5: one of solid state reaction followed by conventional sintering in air, and one of sol-gel synthesis followed by spark-plasma sintering, resulting in starting grain sizes of 2.2 and 0.9 mu m, respectively. Ceramics obtained by these routes exhibited different high-temperature compression behavior: while the conventionally processed ceramic exhibited grain growth during mechanical testing and a stress exponent close to one, compatible with diffusional creep, the spark-plasma sintered ceramic showed no grain growth but significant cavitation, a stress exponent close to two and partially superplastic behavior. These results have implications for the design and lifetime assessment of rare earth silicate-based environmental barrier coatings.

Strength and thermal shock resistance of fiber-bonded Si-Al-C-O and Si-Ti-C-O ceramics
Vera, MC; Martínez-Fernandez, J; Singh, M; Ramírez-Rico, J
International Journal of Applied Ceramic Technology, **19** (2022) 1126-1135
Marzo, 2022 | **DOI:** 10.1111/ijac.13928

Silicon carbide-based fiber-bonded ceramics, obtained from hot pressing of woven silicon carbide fibers, are a cost-effective alternative to ceramic-matrix composites due to their ease of fabrication, involving few processing steps, and competitive thermomechanical properties. In this work, we studied the high-temperature strength and thermal shock resistance of Si-Al-C-O and Si-Ti-C-O fiber-bonded SiC ceramics obtained from hot pressing of two types of ceramic fibers, by mechanical testing in four-point bending. The bending strength of Si-Al-C-O-based fiber-bonded ceramics at room temperature is similar to 250-260 MPa and remains constant with temperature, while the bending strength of Si-Ti-C-O increases slightly from the initial 220 to similar to 250 MPa for the highest temperature. Both materials retain up to 90% of their room temperature strength after thermal shocks of 1400 ºC and show no reduction in elastic moduli. After thermal shock, failure mode is the same as in the case of as-received materials.

Congresos y Reuniones Internacionales / International Congress and Meetings

Comunicaciones / Communications

XXX International Materials Research Congress 2022
14-19 agosto [Cancún, México]

Conferencia Invitada: **Hybrid materials high charged silicate Na-2-mica and polymers: controlled delivery of fertilizers and biodegradable coatings.** S.E. Ramos Jiménez; M.C. Pazos Zarama; J.R. Chaparro Barajas; M.D. Alba; E. Pavón González; L.Tatiana Bayena Suárez; Y.L. Acero Guzmán; A.M. Montañez Velásquez; Y.J. Cruz Vera

International Congress on Separation and Purification Technology
10-14 diciembre [Online, Estados Unidos de América]

Póster: **Controlled release formulation of mcpa and paraquat from high charge synthetic micas Na-2-Mica.** L. Ruiz Bravo; M.C. Pazos; E. Pavón; M.D. Alba

Congresos y Reuniones Nacionales / National Congresses and Meetings

Participación en la Organización de Congresos y Reuniones / Participation in Organising Congresses and Meetings

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

M.D. Alba (Comité Organizador)

Comunicaciones / Communications

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

Póster: **Síntesis de bionanocomposites a partir de arcillas sintéticas y naturales para la adsorción de antibióticos.** M.D. Alba; E. Pavón; J.R. Chaparro

Póster: **Estabilidad térmica de micas frágiles de diseño.** M.D. Alba; E. Pavón; J.R. Chaparro

10th International workshop on interfaces: design for performance
4 septiembre [Santiago de Compostela, España]

Conferencia Invitada: **Biomass and wood derived materials for structural and energy applications.** J. Ramírez-Rico

FORMACION / TRAINING

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título:	**Activación de carbones derivados de biomasa para aplicaciones como adsorbente de CO_2**
Autor:	Irene Lamata Bermejo
Tutores:	Esperanza Pavón González, Joaquín Ramírez Rico, Mª Dolores Alba Carranza
Grado:	Trabajo Fin de Máster
Centro:	Universidad de Sevilla
Fecha Defensa:	15 de septiembre de 2022

DOCENCIA / TEACHING

Investigadores de esta unidad participan en el Máster en Ciencia y Tecnología de Nuevos Materiales y en titulaciones de Grado y doble Grado de la Universidad de Sevilla (ver ACTIVIDADES DIVULGATIVAS Y FORMATIVAS)

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	Dr. Luis Allan Pérez Maqueda
Catedráticos	Dr. Diego Gómez García
Investigadores Científicos	Dr. Francisco José Gotor Martínez
	Dra. Concepción Real Pérez
	Dr. Pedro José Sánchez Soto
Científicos Titulares	Dra. Rosalía Poyato Galán
	Dra. María Jesús Sayagués de Vega
Profesores Titulares	Dra. María Dolores Alcalá González
	Dra. María Regla Ayala Espinar
	Dr. Antonio Perejón Pazo
Talentia Senior CCAA	Dr. Pedro E. Sánchez Jiménez
Doctores Contratados	Dr. Juan Jesús Arcenegui Troya
	Dra. Eva Gil González
	Dr. Alejandro F. Manchón Gordón
	Dr. Sergio Martínez Martínez
Investigadores en Formación	Ldo. Nabil Mohamed Amghar
	Gda. Sandra Molina Molina
Garantía Juvenil	Gda. Andrea Vañes Vallejo

PROYECTOS DE INVESTIGACIÓN / RESEARCH PROJECTS

Materiales termoquímicos para almacenamiento de energía mejorados mediante control microestructural

Thermochemical Energy storage materials enhanced by microstructural control

MINISTERIO DE CIENCIA E INNOVACIÓN
Financiado por la Unión Europea NextGenerationEU
Plan de Recuperación, Transformación y Resiliencia
AGENCIA ESTATAL DE INVESTIGACIÓN

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 almaceamiento 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

MINISTERIO DE CIENCIA E INNOVACIÓN
Financiado por la Unión Europea NextGenerationEU
Plan de Recuperación, Transformación y Resiliencia
AGENCIA ESTATAL DE INVESTIGACIÓN

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
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RESUMEN / ABSTRACT

España es uno de los países europeos con mayor irradiación solar media y lider 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. La plantas CSP de última generación incluyen sistemas de almacenamiento en sales fundidas (calor sensible) que pesentan 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 imporvement strategies for achiving 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 achive 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.

Integración del proceso Ca-looping en centrales de energía solar concentrada para el almacenamiento termo-químico de energía

Integration of the Ca-looping process in concentrated solar power plants for thermochemical energy storage

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
CTQ2017-83602-C2-1-R	01-01-2018 30-09-2022	Ministerio de Ciencia e Innovación	145.200 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El proyecto solicitado se enmarca dentro del reto general de encontrar nuevas tecnologías de almacenamiento de energía baratas y no contaminantes que permitan superar una de las limitaciones mayores de las fuentes renovables que es la intermitencia en la generación de electricidad. En particular, en este proyecto se propone realizar una integración de la tecnología de Ca-looping en una planta termosolar de concentración. La tecnología de Ca-looping, originariamente propuesta para procesos de captura de CO_2, se basa en procesos de carbonatación-descarbonatación (o calcinación) de óxido de calcio-carbonato cálcico repetidos de forma cíclica. Nuestro grupo de investigación ha trabajado durante varios años en esta tecnología, con el objeto de comprender los mecanismos de desactivación conforme se incrementa el número de ciclos. Así, hemos estudiado los mecanismos cinéticos de estos procesos y los cambios microestructurales que tienen lugar a medida que se ciclan los compuestos. En un proyecto coordinado que concluye a finales de año (SOLARTEQH, Retos 2014) hemos realizado ya una propuesta de integración de Ca-Looping para almacenamiento de energía solar. Este proyecto ha dado lugar a una propuesta H2020 (SOCRATCES) aprobada y que comenzará a comienzos del año próximo. En el proyecto CALSOLAR que ahora presentamos se pretende avanzar más en esta idea de integración para incrementar los valores de eficiencia termoeléctrica. El subproyecto I realizará las tareas de coordinación de todo el proyecto. Además, en el subproyecto I se realizará la selección, preparación y caracterización de los compuestos a utilizar en el proyecto. En este sentido, se trabajará con empresas mineras que nos facilitarán distintas materias primas (principalmente calizas y dolomitas) con diverso grado de pureza y cristalinidad. Se prepararán compuestos con sílices nanoestructuradas obtenidas a partir de cascarilla de arroz (suministradas por arroceras del valle del Guadalquivir). Se investigarán compuestos preparados a partir de escorias de acerías (suministrados por dos empresas del sector afincadas en Andalucía) que son ricos en calcio para su aplicación en ciclos de almacenamiento termoquímico. En el subproyecto, se diseñará y construirá un equipo termogravimétrico que permita

realizar experimentos en las condiciones realistas de los ciclos de almacenamiento térmico. Así el equipo permitirá trabajar en condiciones de presión absoluta controlada de CO_2 y en vapor sobrecalentado. En dicho instrumento se realizarán los ciclos de almacenamiento y se estudiarán las condiciones óptimas de dichos ciclos. Se investigarán los mecanismos cinéticos de carbonatación y descarbonatación y se estudiarán los cambios microestructurales durante el ciclado. El equipo de investigación está compuesto por personal con gran experiencia en las tareas propuestas y se cuenta con la participación de investigadores extranjeros con gran experiencia en reacciones sólido-gas y en caracterización microestructural por microscopía de alta resolución. Además, participa una investigadora de la empresa Abengoa con extensa experiencia en almacenamiento termoquímico en plantas solares. Se trabajará en este subproyecto de forma totalmente coordinada con los investigadores del subproyecto 2 con idea de establecer conjuntamente las condiciones de proceso óptimas. Finalmente, los resultados obtenidos del proyecto podrán demostrarse en la planta piloto que se construye en el marco del proyecto H2020 SOCRATCES.

The proposal deals with the general social challenge of finding new cheap and environmentally friendly energy storage technologies to overcome the intermittency of energy generation from renewable sources. Particularly, in this project we propose integrating Ca-looping technology within a thermosolar concentration plant. Ca-Looping technology was originally proposed for CO_2 capture and it is based on cycled carbonation-calcination of calcium oxide-calcium carbonate. Our research group has been working on this technology for several years with the objective of understanding the deactivation mechanisms as the number of cycles increases. Thus, we have studied the kinetic mechanisms of these processes and the microstructural changes that takes place during cycling. In a coordinated project that is about to finish this year (SOLARTEQH, Retos 2014) where we already proposed the integration of Ca-Looping for thermosolar energy storage. This project was the basis of a H2020 proposal (SOCRATCES) that has been recently approved and that will start by the beginning of 2018. The project CALSOLAR is a step forward in the integration to increase the efficiency of the plant. Subproject 1 will coordinate the new project. Moreover, subproject 1 will select, prepare and characterize all compounds investigated in the project. We will work with mining companies that will provide the raw materials (mainly limestone and dolomite) with different purities and crystallinity. Composite materials with nanostructured silica obtained from rice husk (provided by rice mills from the Guadalquivir area) will be prepared. Compounds obtained from steel slags (supplied by nearby steel mills) rich in calcium will be prepared. Within subproject 1, a new thermogravimetric instrument to perform thermal storage cycles under realistic conditions will be designed and constructed in our laboratories. This instrument should work under different controlled CO_2 pressures and under superheated steam. The kinetic mechanisms of carbonation and decarbonation and the microstructural changes will be investigated during cycling. The working team is experienced in the tasks of the project while some additional external scientists will participate. Thus, two foreign professors with solid backgrounds in solid-gas reactions and high resolution TEM are collaborating with us. Moreover, an industrial scientist from Abengoa with a very broad experience in thermal storage and thermosolar power plants is also included in the team. Both subprojects will work in a coordinated way with the aim of setting the optimum conditions for the final application. Finally, the results of the project will be directly applied to the pilot plant constructed within the H2020 SOCRATCES project.

Procesado y Caracterización de Composites Cerámicos con Nanomateriales Laminados Bidimensionales **Processing and Characterization of ceramic composites with two-dimensional laminar nanomaterials**

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PGC2018-101377-B-I00	01-01-2019 31-12-2022	Ministerio de Ciencia e Innovación	121.000 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

La incorporación de nanomateriales bidimensionales en materiales compuestos de matriz cerámica está aumentando en un esfuerzo para superar la inherente fragilidad de las cerámicas y para conferirles nuevas funcionalidades. Aún existen cuestiones abiertas en este campo en cuanto a resistencia mecánica, tenacidad a la fractura, cinética de crecimiento de fisuras, comportamiento tribológico, papel de fases interfaciales o idoneidad para el electromecanizado, entre otras. Aunque las nanoláminas de grafeno (NLG) se han mostrado como una segunda fase muy adecuada, los nanomateriales inorgánicos análogos al grafeno podrían extender el rango de aplicabilidad de los materiales con grafeno. El uso de nanoláminas de nitruro de boro (NLNB) en estos compuestos es muy prometedor y está prácticamente inexplorado.

Este proyecto propone un estudio sistemático de materiales compuestos con usos en aplicaciones estructurales y funcionales, con dos matrices de circona estabilizada con itria y dos tipos diferentes de nanomateriales 2D -nanoláminas de grafeno o de nitruro de boro- para profundizar en la comprensión de sus comportamientos mecánico y eléctrico. Con este fin, se fabricarán materiales con matrices de circona tetragonal dopada con 3 %mol de itria y circona cúbica dopada con itria, persiguiendo una microestuctura óptima con una distribución homogénea de los nanomateriales 2D en ambas matrices cerámicas. Se investigarán en profundidad materiales con NLG para dar respuesta a cuestiones abiertas en el conocimiento de estos materiales. La distribución, tamaño e integridad estructural de las NLG se caracterizarán mediante difracción de rayos X, microscopía electrónica de barrido y espectroscopía Raman, y las intercaras entre las NLG y la matriz se caracterizarán mediante microscopía electrónica de transmisión. La resistencia mecánica, resistencia a la rotura, mecanismos de refuerzo y cinética de crecimiento de grano en estos materiales se examinará en profundidad, y se establecerá la mejor combinación de ruta de procesado y contenido de NLG en términos de refuerzo a la matriz. Se realizarán medidas de conductividad eléctrica en materiales con diferentes contenidos de

NLG y se evaluará la respuesta al electromecanizado de los materiales eléctricamente conductores. Se realizarán también medidas de conductividad eléctrica en función de la temperatura para describir las posibles variaciones en el tipo de conducción al aumentar el contenido en NLG. Por otra parte, se investigarán materiales con NLNB con el objetivo de obtener una primera aproximación a la comprensión de este sistema. Con este fin, tras la síntesis de las NLNB usando una estrategia de mezcla de disolventes para la exfoliación en fase líquida de nanoláminas a partir de polvo de BN hexagonal, se prepararán polvos con diferentes contenidos de NLNB usando técnicas de procesado de polvo en medio húmedo. La caracterización microestructural de los materiales sinterizados mediante "Spark Plasma Sintering" se realizará mediante microscopía electrónica de barrido y de transmisión, difracción de rayos X y espectroscopía Raman. Se estudiarán propiedades como dureza, resistencia a la flexión y resistencia al desgaste, y se realizarán ensayos mecánicos a alta temperatura. Se analizará la conductividad eléctrica en función de la temperatura para esclarecer el efecto de la incorporación de una segunda fase aislante en las fronteras de grano sobre el comportamiento eléctrico de un conductor iónico.

Two-dimensional nanomaterials are being increasingly used as fillers in ceramic composites in an effort to overcome the inherent fragility of ceramics and to provide them with new functionalities. There are open issues in the field of these composites regarding their strength and fracture toughness mechanisms, crack growth kinetics, tribological behavior, role of interfacial phases or suitability for electrical discharge machining, among others. Although graphene nanosheets (GNS) are excellent fillers, inorganic graphene analogues could extend the range of applicability of graphene ceramic composites. The use of boron nitride nanosheets (BNNS) as fillers in ceramic composites is promising and practically unexplored.

This proposal outlines a systematic study of composites intended for use in structural and functional applications, with two different ceramic matrices from the yttria-stabilized zirconia system incorporating two different 2D laminar nanomaterials -graphene or boron nitride nanosheets-, to deepen in the understanding of their mechanical and electrical behavior. To that end, composites with 3 mol% yttria tetragonal zirconia and 8 mol% yttria cubic zirconia matrices will be fabricated, pursuing an optimum microstructure with a homogeneous distribution of the 2D nanomaterials throughout both ceramic matrices. On the one hand, ceramic composites with graphene nanosheets will be investigated in depth to complete the gaps in the current knowledge of these materials. The distribution, size and structural integrity of the GNS will be characterized by X-ray diffraction, scanning electron microscopy and Raman spectroscopy while the interfaces between the GNS and the matrix will be characterized by transmission electron microscopy. The strength, failure resistance, reinforcement mechanisms and crack growth kinetics of these composites will be thoroughly examined, and the best combination of processing route and GNS content in terms of reinforcement will be established. Electrical conductivity measurements of composites with different GNS contents will be carried out at room temperature and the response to electrical discharge machining of the electrically conductive composites will be evaluated. Conductivity measurements will be carried out also as a function of temperature in order to describe the possible variations of conduction type when increasing the GNS content. On the other hand, ceramic composites with boron nitride nanosheets will be investigated in order to get a first approach to the understanding of this system. For this purpose, after the synthesis of the BN nanosheets using a mixed-solvent strategy for liquid exfoliation of BNNS from h-BN powder, composites with different contents of BNNS will be prepared using wet powder processing techniques. The microstructural characterization of the spark plasma sintered composites will be carried out by scanning and transmission electron microscopy, X-ray diffraction and Raman spectroscopy. Mechanical properties as hardness, flexural strength and wear resistance will be studied at room temperature, whereas deformation tests at high temperatures will be also performed. The electrical conductivity as a function of temperature will be analyzed in order to clarify the effect of incorporating an insulating second phase at the grain boundaries on the electrical performance of an ionic conductor.

Cerámicas en un Flash: La nueva ruta para un procesado energética y medioambientalmente eficiente

Ceramics in a FLASH: The new route for environmentally efficient ceramic processing

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P18-FR-1087	01-01-2021 31-12-2022	Junta de Andalucía	99.700 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El proyecto CeramFLASH propone la utilización de las novedosas técnicas de Sinterizado Flash (FS) y Sinterizado Flash Reactivo (SFR) para la síntesis y preparación de cerámicas con interés tecnológico tales como electrolitos sólidos, piezoeléctricos o cerámicas duras electromecanizables. Estas técnicas permiten preparar materiales cerámicos en segundos a temperaturas significativamente más bajas que las requeridas por las técnicas de sinterizado convencional simplemente haciendo circular por la pieza una muy pequeña intensidad de corriente eléctrica (de unos pocos miliamperios). Esta ventaja permite reducir de forma significativa el elevado consumo energético necesario en el procesado de materiales cerámicos.

Adicionalmente, se posibilita la preparación en forma densa y nanoestructurada de cerámicas muy difíciles de preparar mediante métodos convencionales, tales como compuestos de baja estabilidad térmica o compuestos que requieren temperaturas de sinterizado muy elevadas.

Finalmente, CeramFLASH pretende utilizar campos alternos con frecuencia de oscilación variable y métodos de control inteligente basados en la respuesta de la muestra al campo para conseguir un mejor control de las características microestructurales en las cerámicas resultantes. A pesar de que la técnica de FS se propuso por vez primera hace solo 8 años, y la SFR fue introducida en 2018 por nuestro grupo, el interés por este proceso está creciendo de forma importante por su gran potencial científico y tecnológico. CeramFLASH cuenta con la implicación de personal con experiencia en la técnica y la colaboración activa del investigador pionero en su propuesta, por lo que su financiación permitirá establecer una línea de investigación a largo plazo que permita consolidar en Andalucía un grupo de referencia a nivel internacional en este ámbito.

The CeramFLASH project proposes the novel ceramic processing techniques Flash Sintering (FS) and Reaction Flash Sintering (RFS) for the synthesis and preparation of ceramics with technological interest such as solid electrolytes, piezoelectric or hard ceramics. These techniques allow the preparation of ceramic materials in mere seconds at significantly lower temperatures than required by conventional sintering techniques simply by circulating a small electric current under moderate electric fields. This advantage makes it possible to reduce the considerable energy consumption required current ceramic processing techniques. Additionally, it facilitates the preparation of ceramics difficult to obtain in dense and nanostructured form by conventional methods, such as compounds of low thermal stability or compounds that require very high sintering temperatures.

Finally, CeramFLASH aims to use alternating fields with oscillation frequency as well as intelligent control methods based on the sample response to improve the control of microstructural characteristics of resulting ceramics. Although the FS technique was first discovered only 8 years ago, and the RFS was first proposed in 2018 by our group, there is rising interest in this process due to its great scientific and technological potential.

Nuevos materiales para el almacenamiento de Energía Solar Concentrada mediante Calcium-Looping (SOLACAL

New materials for energy storage of Concentrated Solar Power using Calcium-Looping (SOLACAL) processes

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
US-1262507	01-02-2020 30-04-2022	Junta de Andalucía	76.700 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

En este proyecto se estudia el comportamiento de nuevos materiales basados en CaO durante ciclos de calcinación/carbonatación (Ca-Looping) en condiciones realistas de almacenamiento de energía en centrales de energía solar concentrada (CSP).

Para simular las condiciones realistas se utilizan equipos termogravimétricos capaces de emplear elevadas velocidades de calentamiento y enfriamiento y diferentes atmósferas de gases. De esta forma,

los resultados obtenidos son realmente representativos y podrán ser extrapolados a las condiciones prácticas de operación en plantas CSP.

Se estudia la reactividad multicíclica de muestras de caliza y dolomita, a las que se les realizan tratamientos mecánicos y con ácido acético que pueden mejorar su actividad. Además, se ha demostrado que la presencia de MgO en la dolomita calcinada estabiliza térmicamente el CaO, por lo que se preparan dolomitas sintéticas con distinto contenido en MgO mediante tratamientos mecánicos y coprecipitación con el objeto de encontrar la cantidad óptima de MgO que mejore la actividad multicíclica del CaO. Se estudian asimismo otros materiales con los que se pueda aumentar la temperatura de carbonatación, como el $SrCO_3$ y el $BaCO_3$, lo que permitiría incrementar aún más la eficiencia termoeléctrica de las plantas CSP con almacenamiento termoquímico.

Un aspecto relevante de SOLACAL es que los resultados obtenidos serán transferidos de manera directa a la planta CSP-CaL de demostración que se está construyendo en Sevilla dentro del proyecto H2020 SOCRATCES iniciado en 2018 y coordinado por la Universidad de Sevilla.

This project is focused on the performance of new CaO-based materials during calcination/carbonation cycles (Ca-Looping) under realistic energy storage conditions in concentrated solar power plants (CSP).

In order to simulate realistic conditions, thermogravimetric instruments are used, which are able of employing high heating and cooling rates and different atmospheres of gases. In this way, the results obtained are truly representative and can be extrapolated to practical operating conditions in CSP plants. The multicycle reactivity of limestone and dolomite samples is studied. These samples are modified by mechanical and acetic acid treatments that can improve their reactivity. Moreover, it has been shown that the presence of MgO in calcined dolomite thermally stabilizes CaO. Synthetic dolomites with different MgO content are prepared by mechanical treatments and co-precipitation in order to find the optimal amount of MgO that improves the multicycle activity of CaO. Other materials in which the carbonation temperature can be increased, such as SrCO3 and BaCO3, are also studied, which would further increase the thermoelectric efficiency of CSP plants with thermochemical energy storage.

A relevant aspect of SOLACAL is that the results obtained will be transferred directly to the CSP-CaL demonstration plant that is being built in Seville within the H2020 SOCRATCES project, started in 2018 and coordinated by the University of Seville.

Otros Proyectos / Other Projects

Desarrollo de Cerámicas Avanzadas con Nanomateriales 2D para su Aplicación en Sistemas de Propulsión y Frenado en la Industria Aeroespacial (AEROCER-2D)

Código/Code:	PY20_01024
Periodo/Period:	05-10-2021 / 31-12-2022
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	60.125 €
Investigador responsable/Research head:	Ángela Gallardo López (US)
Participante del ICMS como investigador:	Rosalía Poyato Galán

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

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 de Vega

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)

Ayudas extraordinarias para la preparación de proyectos: CTQ2017-83602-C2-1-R

Código/Code:	2021AEP127
Periodo/Period:	01-01-2022 / 31-08-2022
Organismo Financiador/Financial source:	CSIC
Importe total/Total amount:	30.000 €
Investigador responsable/Research head:	Luis A. Pérez Maqueda

Diseño y selección de materiales novedosos para fabricar pilas de combustible de óxido sólido de alto rendimiento

Código/Code:	US-15382
Periodo/Period:	01-02-2020 / 31-01-2022
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	23.000 €
Investigador responsable/Research head:	Francisco J. García García (US)
Participante del ICMS como investigador:	Francisco J. Gotor Martínez

Fabricación y caracterización de cilindros con gradiente de porosidad longitudinal mediante congelación dirigida, modificación superficial e infiltración con un compuesto de quitosano y bio-vidrios para sustitución de tejido óseo

Código/Code:	P20_00671
Periodo/Period:	05-10-2021 / 31-12-2022
Organismo Financiador/Financial source:	Junta de Andalucía
Importe total/Total amount:	43.500 €
Investigador responsable/Research head:	Yadir Torres Hernández (US)
Participante del ICMS como investigador:	Francisco J. Gotor Martínez

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

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

Sinterización FLASH Reactiva para la preparación de compuestos inestables y resistentes a la densificación

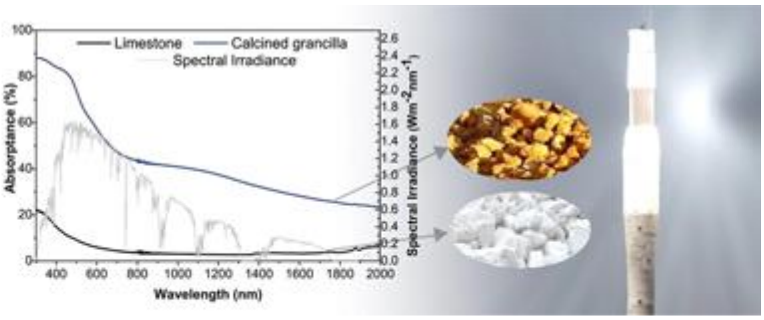
Código/Code:	201960E092
Periodo/Period:	01-10-2019 / 30-09-2022
Organismo Financiador/Financial source:	CSIC (Intramural)
Importe total/Total amount:	350.000 €
Investigador responsable/Research head:	Luis Allan Pérez Maqueda

Artículos Publicados en Revistas SCI / Papers In SCI Journals

Albero: An alternative natural material for solar energy storage by the calcium-looping process

Moreno, V; Arcenegui-Troya, J; Sánchez-Jiménez, P; Perejón, A; Chacartegui, R; Valverde, JM; Pérez-Maqueda, LA

Chemical Engineering Journal, **440** (2022) 135707
Julio, 2022 | **DOI:** 10.1016/j.cej.2022.135707



Large-scale thermochemical energy storage (TCES) is gaining relevance as an alternative to current thermal energy storage systems in Concentrated Solar Power plants. Among the different systems, the reversible reaction between CaO and CO_2 stands out due to the wide availability and low cost of the raw material: limestone. Direct solar absorption of the storage media would improve the efficiency of solar-to-thermal energy storage due to reduced thermal transfer barriers, but the solar optical absorption of $CaCO_3$ is poor. In this work, we propose the use of a Ca-rich calcarenite sedimentary rock so-called albem as an alternative to limestone. We demonstrate that this reddish material exhibits an average solar absorptance that is approximately ten times larger than limestone. Moreover, the multicycle carbonation/calcination performance under different experimental conditions has been studied by thermogravimetry, and similar values to those exhibited for limestone have been obtained. Besides, the material is cheap (6 €/ton), and simulations showed that the use of this material would significantly improve the overall CaL-CSP efficiency at the industrial level.

Low-pressure calcination to enhance the calcium looping process for thermochemical energy storage

Ortiz, C; Carro, A; Chacartegui, R; Valverde, JM; Perejón, A; Sánchez-Jiménez, PE; Pérez-Maqueda, LA

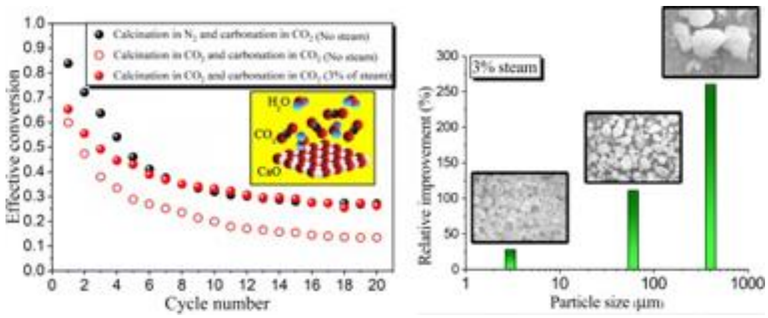
Journal of Cleaner Production, **363** (2022) 132295
Agosto, 2022 | **DOI:** 10.1016/j.jclepro.2022.132295

The Calcium-Looping (CaL) process, based on the multicyclic calcination-carbonation of $CaCO_3$/CaO, is considered a promising Thermochemical Energy Storage (TCES) technology to be integrated into Concentrating Solar Power (CSP) plants. This work proposes a novel CaL integration that operates at low-pressure calcination under pure CO_2 and a moderated temperature. Low-pressure calcination (0.01 bar) provides a suitable solution to mitigate CaO sintering and its consequent loss of reactivity in the carbonation stage. Since the temperature for quick calcination in a pure CO_2 atmosphere is decreased (from around 950 °C at 1 bar to 765 °C at 0.01 bar), the energy losses at the receiver are minimised. In addition, a reduced calcination temperature allows for the use of metallic receivers already tested at the MW-scale, which significantly increases the CSP-CaL integration reliability. Moreover, multicycle CaO reactivity is promoted in short residence times, allowing the use of a simpler reactor design. Furthermore, there is an increase of 85% in the energy storage density of the system. The proposed plant proposes a smooth integration of the CaL process in CSP plants, with a moderate storage level and supported by a natural gas backup system (solar share higher than 50%). The results show that the solar thermal-to electric efficiency is above 30%.

Steam-enhanced calcium-looping performance of limestone for thermochemical energy storage: The role of particle size

Arcenegui-Troya, J.; Sánchez-Jiménez, PE; Perejón, A; Valverde, JM; Pérez-Maqueda, LA

Journal of Energy Storage, **51** (2022) 104305
Julio, 2022 | **DOI:** 10.1016/j.est.2022.104305



Steam injection has been proposed to attenuate the decay of CaO reactivity during calcium looping (CaL) under operating conditions compatible with carbon capture and storage. However, it is yet unknown whether the perceived advantages granted by steam hold under the distinct operating conditions required for the integration of the CaL process as a thermochemical energy storage system in Concentrating Solar Power Plants (CaL-CSP). Here, we study the influence of steam in conditions compatible with a CaL-CSP scheme and assess its impact when injected only during one stage; either calcination or carbonation, and also when it is present throughout the entire loop. The results presented here demonstrate that steam boosts the CaO multicycle performance in a CO_2 closed loop to attain residual conversion values similar to those achieved at moderate temperatures under inert gas. Moreover, it is found that the enhancement in multicycle activity is more pronounced for larger particles.

Supercooled sodium acetate aqueous solution for long-term heat storage to support heating decarbonisation

Lizana, J; Sánchez-Jiménez, PE; Chacartegui, R; Becerra, JA; Pérez-Maqueda, LA
Journal of Energy Storage, **55** (2022) 105584
Noviembre, 2022 | **DOI:** 10.1016/j.est.2022.105584

Heating decarbonisation through electrification requires the development of novel heat batteries. They should be suitable for the specific application and match the operation conditions of domestic renewable energy sources. Supercooled liquids, often considered a drawback of phase change materials, are among the most promising technologies supporting heating decarbonisation. Although some studies have shed light on stable supercooling, the fundamentals and stability remain open problems not always accompanied by relevant experimental in-vestigations. This research critically analyses the physic and chemistry of sodium acetate (*SA,* $NaCH_3COO$) aqueous solution, a low-cost, non-toxic, and abundant compound with stable supercooling for long-term heat storage. It has an appropriate phase change temperature for high-density heat storage using heat pumps or solar thermal technologies in residential applications. The existing discrepancies in literature are critically discussed through a systematic experimental evaluation, providing novel insights into efficient material design and appropriate boundary conditions for reliable material use in long-term heat batteries. Despite previous studies showing that the thermal reliability and stability of sodium acetate aqueous solution as a supercooled liquid for heat storage cannot be guaranteed, this study demonstrates that through an appropriate encapsulation and sealing method, the peritectic composition of sodium acetate solution (p-SA 58 wt%) can be used as a super-cooled liquid for long-term heat storage with a stable melting temperature of 57 °C, appropriate for domestic heat technologies. It is demonstrated that energy storage efficiency can be maintained under cycling, with a constant latent heat storage capacity of 245 kJ/kg and a volumetric storage density of 314 MJ/m^3. It was confirmed that the material should achieve a fully-melted state for stable supercooling. Finally, local cooling and retaining seed crystals through high pressure were highlighted as the most suitable basic principles for successful crystallization and heat release. This promising material can store energy for long periods without latent heat losses due to its stable subcooling. Latent heat can be released when required at any selected time and tem-perature just by a simple activation process.

Oxygen production routes assessment for oxy-fuel combustion

García-Luna, S; Ortiz, C; Carro, A; Chacartegui, R; Pérez-Maqueda, LA
Energy, **254** (2022) 124303
Septiembre, 2022 | **DOI:** 10.1016/j.energy.2022.124303

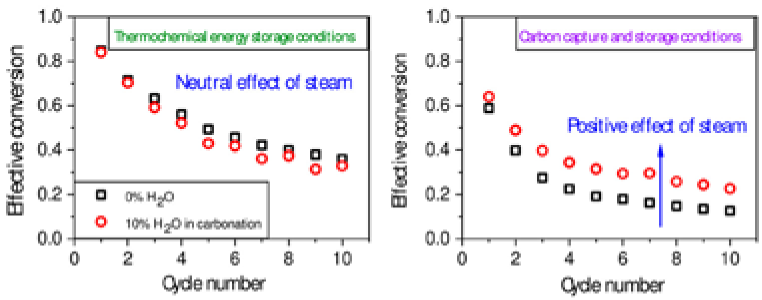
Oxyfuel combustion is a promising alternative to decarbonize the power sector. However, the main barrier to commercial deployment of the technology is the high energy consumption associated with oxygen production (~200-300 kWh per ton of O_2), which penalizes the thermal-to-electric efficiency of 8.5-12% compared to traditional air combustion plants. Typically, oxygen is obtained from a cryogenic air separation process. However, other technologies have been gaining momentum in recent years, such as membrane technologies, chemical looping air separation, and renewable-driven electrolysis. The present work evaluates all these options for O_2 production to retrofit a 550 MWe coal-

fired power plant with oxyfuel combustion. A techno-economic assessment is carried out to estimate the energy penalty, the O_2 production cost (V/ton) and the Levelized Cost of Electricity. The best results are obtained by combining oxygen transport membranes and electrolysis since the energy consumption has been reduced to 98.56 kWh/ton of O_2, decreasing by 59.31% the cryogenic distillation energy consumption (242.24 kWh/ ton O_2), reducing the overall energy penalty compared to cryogenic air separation from 8.88% points to 7.56%points. The oxygen transport membrane presents the lowest cost of electricity in retrofitting cases, 51.48 $/MWh, while cryogenic distillation estimated cost is 52.7 $/MWh. Their costs of avoided CO_2 are 31.79 $/ton CO_2 and 34.15 $/ton CO_2 respectively.

Effect of Steam Injection during Carbonation on the Multicyclic Performance of Limestone ($CaCO_3$) under Different Calcium Looping Conditions: A Comparative Study

Troya, JJA; Moreno, V; Sánchez-Jiménez, PE; Perejón, A; Valverde, JM; Pérez-Maqueda, LA

ACS Sustanaible Chemistry & Engineering, **10** (2022) 850-859
Enero, 2022 | **DOI:** 10.1021/acssuschemeng.1c06314

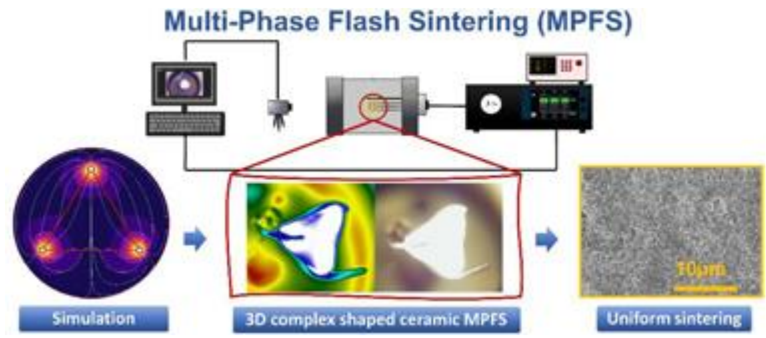


This study explores the effect of steam addition during carbonation on the multicyclic performance of limestone under calcium looping conditions compatible with (i) CO_2 capture from postcombustion gases (CCS) and with (ii) thermochemical energy storage (TCES). Steam injection has been proposed to improve the CO_2 uptake capacity of CaO-based sorbents when the calcination and carbonation loops are carried out in CCS conditions: at moderate carbonation temperatures (similar to 650 °C) under low CO_2 concentration (typically similar to 15% at atmospheric pressure). However, the recent proposal of calcium-looping as a TCES system for integration into concentrated solar power (CSP) plants has aroused interest in higher carbonation temperatures (similar to 800-850 °C) in pure CO_2. Here, we show that steam benefits the multicyclic behavior in the milder conditions required for CCS. However, at the more aggressive conditions required in TCES, steam essentially has a neutral net effect as the CO_2 uptake promoted by the reduced CO_2 partial pressure but also is offset by the substantial steam-promoted mineralization in the high temperature range. Finally, we also demonstrate that the carbonation rate depends exclusively on the partial pressure of CO_2, regardless of the diluting gas employed.

A novel Multi-Phase Flash Sintering (MPFS) technique for 3D complex-shaped ceramics

Molina-Molina, S; Gil-González, E; Duran-Olivencia, FJ; Valverde, JM; Perejón, A; Sánchez-Jiménez, PE; Pérez-Maqueda, LA

Applied Materials Today, **26** (2022) 101274
Marzo, 2022 | **DOI:** 10.1016/j.apmt.2021.101274

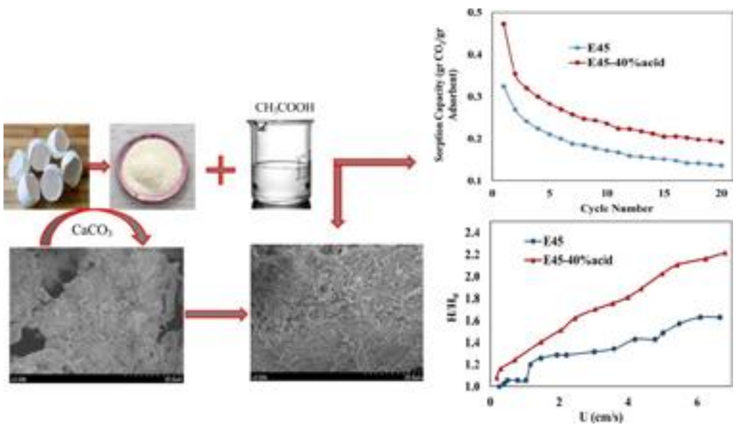


This work demonstrates the first proof-of-concept of Multi-Phase Flash Sintering (MPFS). This novel technique essentially consists of applying a rotating electric field to the sample by means of a multi-phase voltage source as furnace temperature increases. Several ceramic materials with different types of electrical conductivities are sintered within seconds at furnace temperatures much lower than those used for traditional DC flash sintering due to the higher power densities administered by a multi-phase power supply. Thus, ceramic materials are flashed at relatively lower applied voltages which minimizes undesired phenomena such as localization and preferential current pathways. Furthermore, MPFS allows diverse electrode configurations to promote a more uniform electric field distribution, enhancing the sintering of 3D complex-shaped specimens. MPFS could be a true breakthrough in materials processing, as 3D complex-shaped specimens are homogeneously sintered at reduced temperatures, while keeping all the advantages of conventional flash sintering.

Improvement in cyclic CO_2 capture performance and fluidization behavior of eggshell-derived $CaCO_3$ particles modified with acetic acid used in calcium looping process

Imani, M; Tahmasebpoor, M; Sánchez-Jiménez, PE; Valverde, JM; Moreno, V

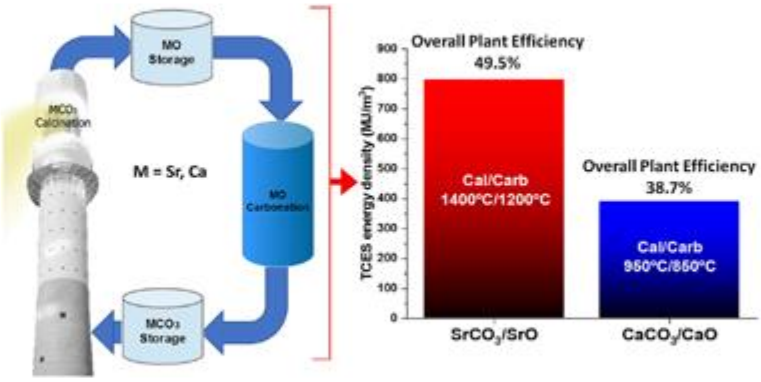
Journal of CO2 Utilization, **65** (2022) 102207
Noviembre, 2022 | **DOI:** 10.1016/j.jcou.2022.102207



Although calcium-based materials are the most promising adsorbents used in calcium looping process for carbon dioxide removing, their CO_2 capture capacity decaying besides poor fluidization, still are the important challenges. In the present investigation, eggshell as a cheap, easily available and unpolluted source of calcium carbonate was used for CO_2 capturing in calcium looping process. Eggshell particles were treated with various volume concentrations of acetic acid to improve its sorption capacity. According to the TGA results after 20 carbonation/calcination cycles, the effective carbonation conversion of modified eggshell with 5%, 20%, 30% and 40%. v/v acetic acid was 21.33%, 24.26%, 25.97% and 28.97%, respectively, which is considerable compared to 20.54% for untreated eggshell. The effect of initial eggshell particle size on the adsorption behavior of final adsorbent was also investigated by using two different sizes including dp< 45 μm and dp> 320 μm. The results showed that the effective conversion of the adsorbent containing 40%. v/v acetic acid derived from small particle size eggshells was 9.32% higher than that from larger particle size eggshells. In terms of fluidization behavior, surprisingly the addition of acetic acid to the eggshell particles also increased the bed expansion ratio as 8% and 36.2% at gas velocities of 0.27 and 6.67 cm/s, respectively. Further improvement in the fluidity of eggshell modified with 40% acid was performed by manually mixing of SiO_2 nanoparticles at different weight percentages. According to the results, adding 7.5 wt% SiO_2 leaded to the homogeneous and agglomerate particulate fluidization.

The $SrCO_3$/SrO system for thermochemical energy storage at ultra-high temperature

Amghar, N; Ortiz, C; Perejón, A; Valverde, JM; Maqueda, LP; Jiménez, PES
Solar Energy Materials and Solar Cells, **238** (2022) 111632
Mayo, 2022 | **DOI:** 10.1016/j.solmat.2022.111632



Thermochemical energy storage (TCES) has attracted interest in the last years due to the possibility of attaining high energy densities, seasonal storage capacity and greater efficiencies than currently commercial thermal energy storage systems using molten salts. This work analyses the potential of an ultra-high temperature TCES system based on the $SrCO_3$/SrO system. The process relies upon the reversible decomposition of $SrCO_3$ into SrO and CO_2. As proposed in previous works for the integration of the Ca-Looping process to store energy in CSP plants, both the calcination (endothermic) and carbonation (exothermic) reactions are carried out in a closed CO_2 loop. At these conditions, the required temperature to attain full calcination in short residence times is around 1400 °C whereas carbonation takes place at about 1200 °C. Using this process, the energy density potentially achievable by the storage material is very high (around 2000 MJ/m^3) while the ultra-high carbonation temperature would improve thermoelectric efficiency. The enhancement of the multicycle performance of the $SrCO_3$/SrO system using refractory additives is also explored. Even though current commercial CSP plants with tower technology cannot yet operate at these ultra-high temperatures, recent advances in the development of high-temperature solar receivers could allow operation at 1400 °C in the medium term. Finally, a conceptual model of the integration of the $SrCO_3$/SrO system in a CSP plant supports higher overall efficiency and energy density, but lower solar-to-electric efficiency due to thermal losses.

Overlooked pitfalls in CaO carbonation kinetics studies nearby equilibrium: Instrumental effects on calculated kinetic rate constants

Arcenegui-Troya, J; Duran-Martín, JD; Perejón, A; Valverde, JM; Maqueda, LAP; Jiménez, PES
Alexandria Engineering Journal, **61** (2022) 6129-6138
Agosto, 2022 | **DOI:** 10.1016/j.aej.2021.11.043

Due to its technological applications, such as CO_2 capture, CaO carbonation kinetics has been extensively studied using a wide array of methods and experimental conditions. A complete understanding of carbonation kinetics is key to optimizing the operating conditions as well as to correctly design the carbonation reactor. However, there is yet no consensus on the reaction model and kinetic parameters that can best describe the CaO carbonation reaction. For instance, the value of the activation energy proposed in different works can vary up to 300%. In this work, we demonstrate that the strong influence of the thermodynamic equilibrium on CaO carbonation kinetics demands careful control of the experimental conditions to obtain meaningful kinetic parameters. Specifically, we explore the influence of three experimental parameters on carbonation kinetics: the gas flow rate, the CO_2 partial pressure and the time required to fill the reactor after a gas change. We demonstrate that disregarding these aspects may lead to bogus conclusions on reaction kinetics, which could partly explain the considerable discrepancies found in the literature. The conclusions of this work are not only applicable to the process and experimental setup studied here but also to any study that involves the use of gas flow to drive a reaction.

Reactive flash sintering of $SrFe_{12}O_{19}$ ceramic permanent magnets

Manchon-Gordon, AF; Sánchez-Jiménez, PE; Blazquez, JS; Perejón, A; Pérez-Maqueda, LA
Journal of Alloys and Compounds, **922** (2022) 166203
Noviembre, 2022 | **DOI:** 10.1016/j.jallcom.2022.166203

Reactive flash-sintering technique has been used in order to obtain strontium ferrite magnets from a mixture of $SrCO_3$ and Fe_2O_3 commercial powders. This technique allows preparing sintered $SrFe_{12}O_{19}$ at a furnace temperature of just 973 K during just 2 min by applying a modest field of 40 V cm^{-1}, instead of the conventional sintering process employed in ferrite magnet manufacturing that demands high temperature and long dwell times. Analysis of structural and magnetic properties were performed as a function of time in which the flash event was held. Mossbauer spectra show the existence of five different kinds of local environments, confirming the formation of strontium hexaferrite. The resulting samples exhibit comparable magnetic properties to the state-of-the-art ferrite magnets. In particular, produced samples reach a coercivity of 0.4 T and a specific saturation magnetization of 70 $Am^2\ kg^{-1}$.

Ageing-resistant zirconia/graphene-based nanostructures composites for use as biomaterials

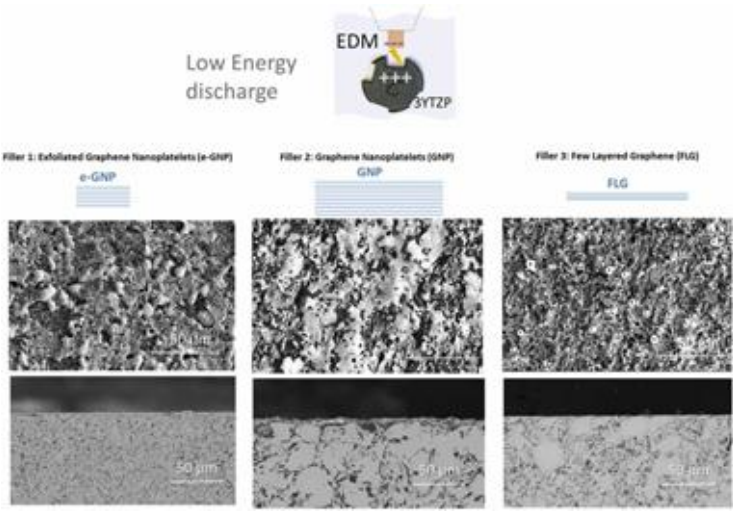
Morales-Rodríguez, A; González-Orellana, C; Pérez-García, AA; López-Pernia, C; Muñoz-Ferreiro, C; Poyato, R; Gallardo-López, A
Journal of the European Ceramic Society, **42** (2022) 1784-1795
Abril, 2022 | **DOI:** 10.1016/j.jeurceramsoc.2021.11.060

This work explores the incorporation of graphene-based two-dimensional nanostructures as moisture barriers to delay hydrothermal ageing of yttria-stabilized zirconia and strengthen its use in biomedical applications. Two sets of highly dense zirconia composites incorporating multilayered graphene with very different lateral dimensions, few layer graphene and exfoliated graphene nanoplatelets, were prepared. The effect of the addition of graphene nanostructures on zirconia ageing was investigated by conducting accelerated hydrothermal degradation experiments in an autoclave. An improved resistance to low-temperature degradation and a high tolerance to damage were achieved in the composites compared to those of monolithic zirconia. The incorporation of 1 vol% multilayered graphene was very effective in restricting the hydrothermal degradation. In particular, the composite incorporating exfoliated graphene nanosheets exhibited outstanding resistance to ageing because of their fine dispersion throughout the matrix, which effectively seemed to restrict grain growth and slow the propagation of the transformation front to the ceramic bulk.

Highly efficient electrical discharge machining of yttria-stabilized zirconia ceramics with graphene nanostructures as fillers

Muñoz-Ferreiro, C; López-Pernia, C; Moriche, R; Gommeringer, A; Kern, F; Poyato, R; Gallardo-López, A

Journal of the European Ceramic Society, **42** (2022) 5943-5952
Octubre, 2022 | **DOI:** 10.1016/j.jeurceramsoc.2022.06.037



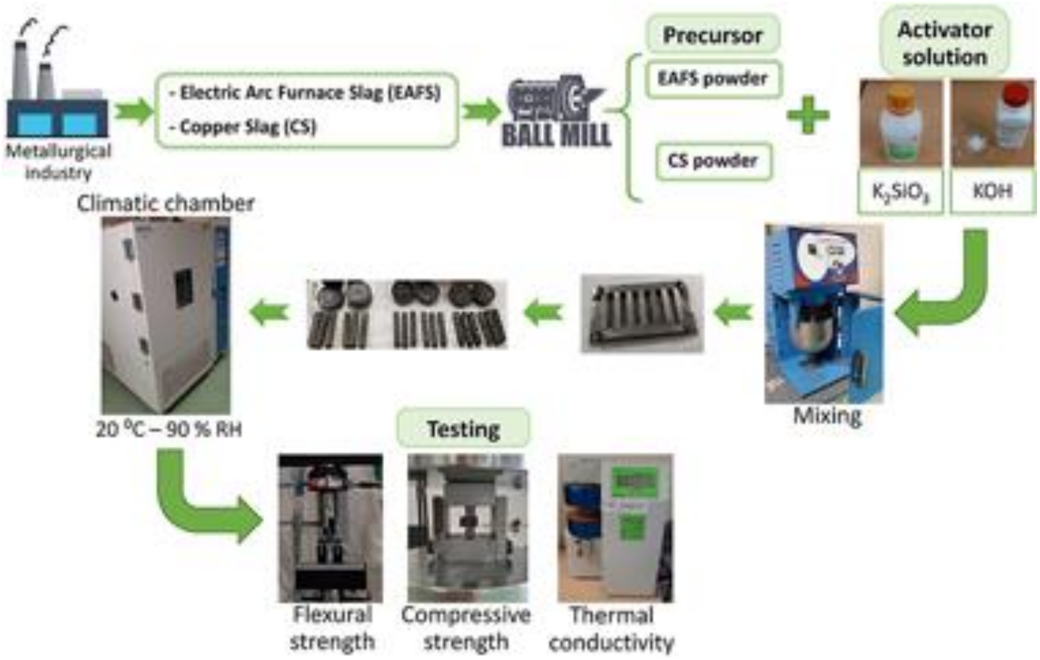
Electrical-discharge machining (EDM) of advanced ceramics allows the miniaturization of parts with complex shapes. Since electrical conductivity is required, non-conductive ceramics need a conductive second phase. This work assesses the feasibility of industrial EDM in advanced yttria-stabilized tetragonal zirconia (3YTZP) composites with 20 vol% graphene nanostructures with different morphology using different EDM energies. The structural integrity of the graphene nanostructures, the roughness of the machined surfaces and the geometrical tolerances have been evaluated by Raman spectroscopy, confocal microscopy and scanning electron microscopy, showing that it is possible to obtain a stable and efficient EDM process in these composites using low electrode energies. The use of the largest and thickest graphene nanostructures led to the best performance in terms of EDM machinability, the smallest nanostructures produced the best surface finish for low electrode energy and the thinnest nanostructures allowed the highest material removal rate at medium energy in the composites.

Comparative study of alkali activated cements based on metallurgical slags, in terms of technological properties developed

Gómez-Casero, MA; Pérez-Villarejo, L; Sánchez-Soto, PJ; Eliche-Quesada, D

Sustainable Chemistry and Pharmacy, **29** (2022) 100746
Octubre, 2022 | **DOI:** 10.1016/j.scp.2022.100746

In this work, an investigation on the use of two slags from different origins (electric arc furnace slag (EAFS) and copper slag (CS)) as raw materials in the manufacture of alkali-activated cements has been carried out. A comparison of the different mechanical properties developed by the alkaline activation of each raw material has been studied. Combination of 35 wt% potassium hydroxide (KOH) solution with different concentration (5, 8, 12 and 15 M) and 65 wt% potassium silicate (K_2SiO_3) solution was used as activating solution to manufacture alkali activated cements. The pastes were cured 24 h in a climatic chamber at 20 °C at 90% of relative humidity, subsequently demoulded and cured at same condition during 1, 7, 28 and 90 days. Alkali activated materials have been characterized using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and scanning electron microscopy (SEM). The physical properties: bulk density, water absorption and apparent porosity, mechanical properties,



flexural strength and compressive strength and thermal properties: thermal conductivity have been determined. The results indicate that two types of slags studied are a suitable source of aluminosilicates that can be activated for the manufacture of alkali-activated materials. These precursors are capable of developing high values of flexural and compressive strength and low values of thermal conductivity when optimal concentration of KOH was used. The optimal composition was developed when CS was utilized. Binders with CS and 12 M M ratio achieved compressive strength values up to 70 MPa.

Theoretical Analysis of Polynuclear Zinc Complexes Isolobally Related to Hydrocarbons

Ayala, R; Galindo, A

International Journal of Molecular Sciences, **23** (2022) 14858
Diciembre, 2022 | **DOI:** 10.3390/ijms232314858

Based on the isolobal analogy of ZnCp (Cp = η^5-C_5H_5) and ZnR (R = alkyl or aryl group) fragments with hydrogen atom and fragment [Zn(CO)$_2$] with a CH_2 carbene, the following complexes [(ZnCp)$_2${μ-Zn(CO)$_2$}], **1**, [(ZnPh)$_2${μ-Zn(CO)$_2$}], **2**, [(ZnPh){μ-Zn(CO)$_2$}(ZnCp)], **3**, [(ZnCp)$_2${μ-Zn$_2$(CO)$_4$}], **4**, [(ZnPh)$_2${μ-Zn$_2$(CO)$_4$}], **5**, [(ZnPh){μ-Zn(CO)$_2$}$_2$(ZnCp)], **6**, [Zn$_3$(CO)$_6$], **7** and [Zn$_5$(CO)$_{10}$], **8**, were built. These polynuclear zinc compounds are isolobally related to simple hydrocarbons (methane, ethane, cyclopropane and cyclopentane). They have been studied by density functional theory (DFT) and quantum theory of atoms in molecules (QTAIM) to compare the nature and topology of the Zn–Zn bond with previous studies. There are bond critical points (BCPs) between each pair of adjacent Zn centers in complexes **1**–**8** with Zn–Zn distances within the range 2.37–2.50 Å. The nature of the Zn–Zn bond in these complexes can be described as polar rather than pure covalent bonds. Although in a subtle way, the presence of different ligands and zinc oxidation states introduces asymmetry and polarity in the Zn–Zn bond. In addition, the Zn–Zn bond is delocalized in nature in complex **7** whereas it can be described as a localized bond for the remaining zinc complexes here studied.

Vitrification rate and estimation of the optimum firing conditions of ceramic materials from raw clays: A review

Garzon, E; Pérez-Villarejo, L; Eliche-Quesada, D; Martínez-Martínez, S; Sánchez-Soto, PJ
Ceramics International, **48** (2022) 15889-15898
Junio, 2022 | **DOI:** 10.1016/j.ceramint.2022.02.129

The present work is a review concerning the previous investigations on the vitrification behaviour of clays containing kaolinite, feldspars, muscovite (illite/sericite) and pyrophyllite. These clays are silico-aluminous and have interesting properties as raw materials for structural ceramics. The mineralogical and chemical composition were determined. Then, the vitrification in these clay samples using pressed bodies was investigated by few researchers in the temperature range 800-1350 °C with 0.5-5.5 h of soaking times. The effect of heat treatments on the degree of vitrification in these clays was characterized by bulk densities of the ceramic bodies at the fired stage. It was found some variations of bulk density values for all these clays fired in the range 1000-1150 °C, with marked decreases of the values obtained at 1200 °C and 1300 °C. A first order reaction kinetics was applied to the analysis of vitrification of the ceramic bodies under isothermal heating. The method is based on experi-mental data of bulk densities, being proposed for the estimation of the relative degree of vitrification resulting from different firing schedules. The analysis considered the temperature dependence of the rate of vitrification following Arrhenius behaviour. Thus, the vitrification activation energy can be obtained. The activation energies for the physical process of vitrification in these clays ranged from 45 to 151 kJ/mol. The relative rates of vitrification or degree of vitrification attained during heating and soaking were calculated. The results suggested that the contribution of vitrification due to heating in all these clays was relatively small compared to the vitrification during soaking. However, it was evidenced that the influence of the particle sizes in the thermal behaviour of these clays cannot be neglected. The vitrification rate equations, as deduced in these previous studies, can be useful tools to estimate the optimum firing conditions of these clays, allowing the extension of this method to other clay types.

Predictions of polymer thermal degradation: relevance of selecting the proper kinetic model

Sánchez-Jiménez, PE; Perejón, A; Arcenegui-Troya, J; Pérez-Maqueda, LA
Journal of Thermal Analysis and Calorimetry, **147** (2022) 2335-2341
Febrero, 2022 | **DOI:** 10.1007/s10973-021-10649-x

Making predictions, such as lifetime estimations, is one of the main objectives of kinetic studies. Thus, from conventional thermal analysis experiments, the behavior of polymeric materials under processing or application conditions, usually far away from those used in the laboratory experiments, could be estimated. Conventional prediction procedures usually make use of oversimplified equations based on simple approaches. One of the most common approaches is the assumption of a first, or n-order, kinetic model for the process. However, recent studies have shown, for a number of polymers, that random scission kinetic models are not only physically sound, but more reliable in terms of describing the degradation kinetics. In this paper, the consequences of selecting an erroneous kinetic model on lifetime predictions is discussed. It is demonstrated, using both simulated and experimental data, that any kinetic analysis of a chain scission driven reaction performed assuming a first-order model entails enormous deviations in predictions. This occurs despite the fact that the first-order kinetic model can fit experimental data from chain scission driven reactions with significant correlation coefficients, and even lead to a reasonably good reconstruction of the original experimental curves.

Synthesis and characterization of alkali-activated materials containing biomass fly ash and metakaolin: effect of the soluble salt content of the residue

Jurado-Contreras, S; Bonet-Martínez, E; Sánchez-Soto, PJ; Gencel, O; Eliche-Quesada, D
Archives of Civil and Mechanical Engineering, **22** (2022) 121
Mayo, 2022 | **DOI:** 10.1007/s43452-022-00444-2

The present study investigates the production and characterization of alkali-activated bricks prepared with mixing metakaolin (MK) and biomass fly ash from the combustion of a mix of pine pruning, forest residues and energy crops (BFA). To use this low cost and high availability waste, different specimens were prepared by mixing MK with different proportions of BFA (25, 50 and 75 wt%). Specimens containing only metakaolin and biomass fly ash were produced for the purpose of comparison. Effects of the alkali content of biomass fly ash, after a washing pretreatment (WBFA), as well as the concentration of NaOH solution on the physical, mechanical and microstructural properties of the alkali-activated bricks were studied. It was observed that up to 50 wt% addition of the residue increases compressive strength of alkali-activated bricks. Alkalinity and soluble salts in fly ash have a positive effect, leading materials with the improved mechanical properties. Concentration of NaOH 8 M or higher is required to obtain optimum mechanical properties. The compressive strength increases from 23.0 MPa for the control bricks to 44.0 and 37.2 MPa with the addition of 50 wt% BFA and WBFA, respectively, indicating an increase of more than 60%. Therefore, the use of biomass fly ash provides additional alkali (K) sources that could improve the dissolution of MK resulting in high polycondensation. However, to obtain optimum mechanical properties, the amount of BFA cannot be above 50 wt%.

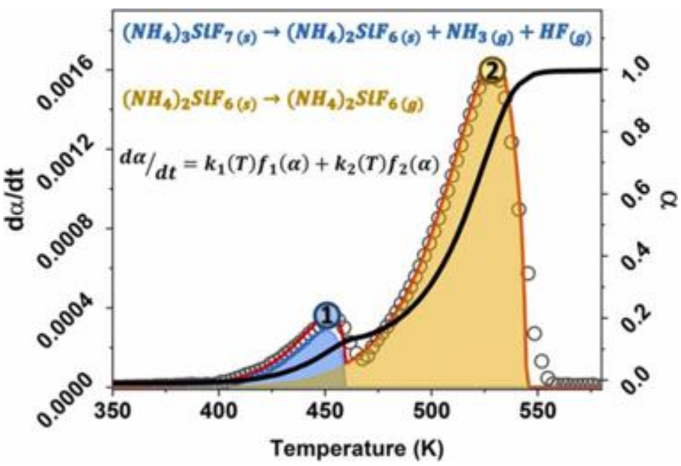
Thermal behaviour of the different parts of almond shells as waste biomass

Garzon, E; Arce, C; Callejon-Ferre, AJ; Pérez-Falcon, JM; Sánchez-Soto, PJ
Journal of Thermal Analysis and Calorimetry, **147** (2022) 5023-5035
Junio, 2022 | **DOI:** 10.1007/s10973-021-10940-x

The main aim of this study is to investigate the thermal behaviour of the different parts of almond shells produced in an almond industry as a waste biomass. For this purpose, several experiments have been conducted under laboratory conditions. After removing the mature almonds, the waste raw materials subject of this study were treated with distilled water (10 min) and separated in several parts. Taking into account their physical characteristics, they were: (a) complete shells: exocarp, mesocarp and endocarp without grinding (Sample C); (b) ground samples of complete shells, sieved under 0.2 mm (Sample M); (c) hard layers of the endocarp (Sample E); (d) internal layers of the endocarp (Sample I); and (e) mature drupes (Sample P) or skin, being constituted by the flexible part of green colour (fresh form) or yellow (after drying). The thermal behaviour of all these sample materials has been investigated using a laboratory furnace, with determination of ash contents and mass loss by progressive heating (120 min of holding time). Elemental and DTA-TG/DTG analyses of selected sample materials have been carried out. Although a complete study can be very complex, a first approach has been performed in this investigation. Results on thermal decomposition of this biomass waste have been presented to emphasize the main differences between sample materials of almond shells. These results have demonstrated the influence of several parameters, such as the particle size, and previous treatments in the thermal behaviour of the different parts of the almond shells, as showed in this investigation. Structural analysis of almond shells allowed to determine lignin, cellulose and hemicellulose. From the lignin content, it has been predicted the higher heating value (18.24 $MJkg^{-1}$) of this waste as by-product of industrial interest. Other linear correlations to calculate this parameter have been applied with similar results in all these samples.

Thermal behavior of ammonium fluorosilicates complexes: Obtaining and kinetic analysis

Resentera, AC; Perejón, A; Esquivel, MR; Pérez-Maqueda, LA; Rodríguez, MH
Chemical Engineering Research and Design, **182** (2022) 490-501
Junio, 2022 | **DOI:** 10.1016/j.cherd.2022.04.021



In this work, a mixture of $(NH_4)_3SiF_7/(NH_4)_2SiF_6$ powders was obtained as a by-product of the Li extraction process from alpha-spodumene aluminosilicate with NH_4HF_2. The thermal behavior of the powders was analyzed by non-isothermal thermogravimetric experiments. The kinetic parameters that describe the processes involved were obtained using mathematical deconvolution, Friedman's method, combined kinetic analysis, and nonlinear regression optimization. The results show that the process occurs in two partially overlapping steps, the thermal decomposition of $(NH_4)_3SiF_7$ into $(NH_4)_2SiF_6$ and the subsequent sublimation of $(NH_4)_2SiF_6$. The apparent activation energies were 72.6 and 79.8 kJ/ mol for steps 1 and 2, respectively. The apparent pre-exponential factors were 1.19×10^6 and 2.50×10^5 s^{-1}, respectively. The kinetic models indicated that Step 1 follows an A2 model, while Step 2 follows an F0 model. Finally, the resulting kinetic parameters allowed the reconstruction of the original experimental curves and obtaining predictions of curves recorded under other heating programs.

Chemical, Radiometric and Mechanical Characterization of Commercial Polymeric Films for Greenhouse Applications

Franco, JE; Rodríguez-Arroyo, JA; Ortiz, IM; Sánchez-Soto, PJ; Garzón, E; Lao, MT
Materials, **15** (2022) 5532
Agosto, 2022 | **DOI:** 10.3390/ma15165532

In the agricultural sector, companies involved in the production of plastic greenhouses are currently searching for a suitable covering adapted for every climate in the world. For this purpose, this research work has determined the chemical, radiometric and mechanical properties of 53 polymeric films samples from Europe and South America. The chemical tests carried out with these samples were elemental analysis (C, H and N) and FT-IR spectrometry. The radiometric properties here studied were the transmission, absorption and reflection coefficients along the spectrum between 300 and 1100 nm. For the mechanical properties, tensile strength, tear strength and dart impact strength, tests were carried out. Finally, all these data were collected, and a multivariate statistical analysis was carried out using the SPSS statistical to group the samples into statistical groups adapted to specific climatic regions. The elemental analysis and FT-IR spectrometry allowed group the samples into nine groups. The samples were grouped according to their chemical (elemental analysis), radiometric and mechanical properties by multivariate analysis. The dendrogram separated five very different groups in terms of number of samples. These groups have specific chemical, radiometric and mechanical characteristics that separate them from the rest. These groups make it possible to narrow down the applications and

correlate with the radiometric properties to see in which geographical area of the world they are most effective in increasing yields and achieving higher quality production.

Effect of the Processing Parameters on the Porosity and Mechanical Behavior of Titanium Samples with Bimodal Microstructure Produced via Hot Pressing

Chavez-Vasconez, R; Lascano, S; Sauceda, S; Reyes-Valenzuela, M; Salvo, C; Mangalaraja, RV; Gotor, FJ; Arevalo, C; Torres, Y
Materials, **15** (2022) 136
Enero, 2022 | **DOI:** 10.3390/ma15010136

Commercially pure (c.p.) titanium grade IV with a bimodal microstructure is a promising material for biomedical implants. The influence of the processing parameters on the physical, microstructural, and mechanical properties was investigated. The bimodal microstructure was achieved from the blends of powder particles with different sizes, while the porous structure was obtained using the space-holder technique (50 vol.% of ammonium bicarbonate). Mechanically milled powders (10 and 20 h) were mixed in 50 wt.% or 75 wt.% with c.p. titanium. Four different mixtures of powders were precompacted via uniaxial cold pressing at 400 MPa. Then, the specimens were sintered at 750 °C via hot pressing in an argon gas atmosphere. The presence of a bimodal microstructure, comprised of small-grain regions separated by coarse-grain ones, was confirmed by optical and scanning electron microscopies. The samples with a bimodal microstructure exhibited an increase in the porosity compared with the commercially available pure Ti. In addition, the hardness was increased while the Young's modulus was decreased in the specimens with 75 wt.% of the milled powders (20 h).

Flash Sintering Research Perspective: A Bibliometric Analysis

Gil-González, E; Pérez-Maqueda, LA; Sánchez-Jiménez, PE; Perejón, A
Materials, **15** (2022) 416
Enero, 2022 | **DOI:** 10.3390/ma15020416

Flash Sintering (FS), a relatively new Field-Assisted Sintering Technique (FAST) for ceramic processing, was proposed for the first time in 2010 by Prof. Rishi Raj's group from the University of Colorado at Boulder. It quickly grabbed the attention of the scientific community and since then, the field has rapidly evolved, constituting a true milestone in materials processing with the number of publications growing year by year. Moreover, nowadays, there is already a scientific community devoted to FS. In this work, a general picture of the scientific landscape of FS is drawn by bibliometric analysis. The target sources, the most relevant documents, hot and trending topics as well as the social networking of FS are unveiled. A separate bibliometric analysis is also provided for Reaction or Reactive Flash Sintering (RFS), where not only the sintering, but also the synthesis is merged into a single step. To the best of our knowledge, this is the first study of this nature carried out in this field of research and it can constitute a useful tool for researchers to be quickly updated with FS as well as to strategize future research and publishing approaches.

Pre-Roman and Republican amphorae (III-I centuries b.C.) from production contexts of the Guadalquivir Basin: technical and compositional characterization

Moreno-Megías, V; García-Fernández, FJ; Martín-del-Río, JJ; Borreguero-Cid, M; Sánchez-Soto, PJ
Boletín de la Sociedad Española de Cerámica y Vidrio, **61** (2022) 498-515
Septiembre, 2022 | **DOI:** 10.1016/j.bsecv.2021.03.008

The present work consists of an archaeometric investigation concerning ceramic samples, mostly unpublished, of the III-I centuries b.C. They were found in connection with kilns of the city of Sevilla (Archbishop's Palace) and the countryside (Arrabal zone, Carmona). They are identified with evolved variations of Iron Age amphorae of Punic and Turdetanian tradition, or already Roman typologies. The main objectives of this research include their technological and compositional characterization as well as the comparison of the characteristics of each manufacture tradition.
An assemblage of 13 samples has been studied through petrographic analysis of thin sections, chemical analysis (X-ray fluorescence) and mineralogical analysis (X-ray diffraction). The chemical results showed the silico-aluminous and calcitic character of the samples, with variable contents of iron oxide as well as other minor elements and traces. The statistical treatment of the data by multivariant analysis has differentiated 3 conglomerates and one sample as an outsider. The mineralogical analysis has identified 8 crystalline phases, several of them already present in the raw materials and others formed by thermal treatment. It is interesting to note the illite, identified as dehydroxylated phase, anorthite, diopside and gehlenite. The petrographical analysis has identified 3 different petro-groups, which are correlated by a compositional point of view with the original context of the samples. Thus, according to these results, it has been possible to distinguish the manufactures of Sevilla from the Roman shapes, the common ware and the imitation types of Carmona.
It has been discussed the possible solid-state reactions which yielded the crystalline phases identified by X-ray diffraction, besides an estimation of firing temperatures between 820-850 °C in an oxidant atmosphere. Finally, the possible sources for the raw materials used in the fabrication of these amphorae have been proposed in the Guadalquivir River valley, considering their illitic-calcitic characteristics.

Study of a Waste Kaolin as Raw Material for Mullite Ceramics and Mullite Refractories by Reaction Sintering

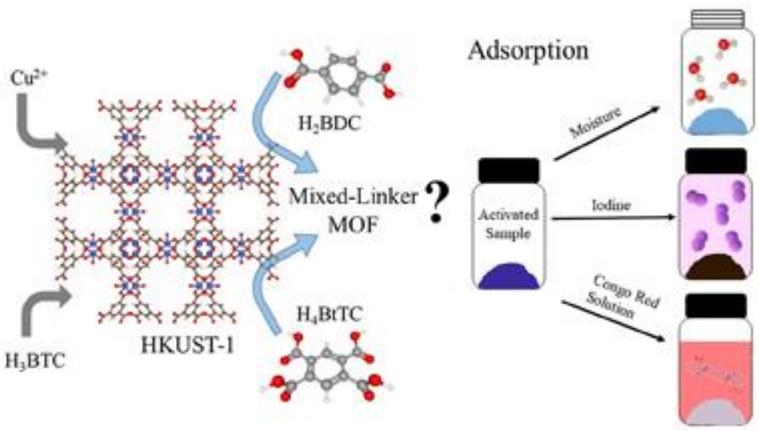
Sánchez-Soto, PJ; Eliche-Quesada, D; Martínez-Martínez, S; Pérez-Villarejo, L; Garzon, E
Materials, **15** (2022) 583
Enero, 2022 | **DOI:** 10.3390/ma15020583

A deposit of raw kaolin, located in West Andalusia (Spain), was studied in this work using a representative sample. The methods of characterization were X-ray diffraction (XRD), X-ray fluorescence (XRF), particle size analysis by sieving and sedimentation, and thermal analysis. The ceramic properties were determined. A sample of commercial kaolin from Burela (Lugo, Spain), with applications in the ceramic industry, was used in some determinations for comparison purposes. The kaolin deposit has been produced by alteration of feldspar-rich rocks. This raw kaolin was applied as an additive in local manufactures of ceramics and refractories. However, there is not previous studies concerning its characteristics and firing properties. Thus, the meaning of this investigation was to conduct a scientific study on this subject and to evaluate the possibilities of application. The raw kaolin was washed for the beneficiation of the rock using water to increase the kaolinite content of the resultant material. The results indicated that the kaolinite content of the raw material was 20 wt % as determined by XRD, showing ~23 wt % of particles lower than 63 μm. The kaolinite content of the fraction lower than 63 μm was 50 wt %. Thus, an improvement of the kaolinite content of this raw

kaolin was produced by wet separation. However, the kaolin was considered as a waste kaolin, with microcline, muscovite and quartz identified by XRD. Thermal analyses by Thermo-Dilatometry (TD), Differential Thermal Analysis (DTA) and Thermo-Gravimetry (TG) allowed observe kaolinite thermal decomposition, quartz phase transition and sintering effects. Pressed samples of this raw kaolin, the fraction lower than 63 μm obtained by water washing and the raw kaolin ground using a hammer mill were fired at several temperatures in the range 1000–1500 °C for 2 h. The ceramic properties of all these samples were determined and compared. The results showed the progressive linear firing shrinkage by sintering in these samples, with a maximum value of ~9% in the fraction lower than 63 μm. In general, water absorption capacity of the fired samples showed a decrease from ~18–20% at 1050 °C up to almost zero after firing at 1300 °C, followed by an increase of the experimental values. The open porosity was almost zero after firing at 1350 °C for 2 h and the bulk density reached a maximum value of 2.40 g/cm^3 as observed in the ground raw kaolin sample. The XRD examination of fired samples indicated that they are composed by mullite, from kaolinite thermal decomposition, and quartz, present in the raw sample, as main crystalline phases besides a vitreous phase. Fully-densified or vitrified materials were obtained by firing at 1300–1350 °C for 2 h. In a second step of this research, it was examined the promising application of the previous study to increase the amount of mullite by incorporation of alumina (α-alumina) to this kaolin sample. Firing of mixtures, prepared using this kaolin and α-alumina under wet processing conditions, produced the increase of mullite in relative proportion by reaction sintering at temperatures higher than 1500 °C for 2 h. Consequently, a mullite refractory can be prepared using this kaolin. This processing of high-alumina refractories is favoured by a previous size separation, which increases the kaolinite content, or better a grinding treatment of the raw kaolin.

On the adsorption properties and applications of mixed-linker MOFs based on HKUST-1

Puerto-Rodríguez, M; López-Cartes, C; Ayala, R
Journal of Solid State Chemistry, **312** (2022) 123260
Agosto, 2022 | **DOI:** 10.1016/j.jssc.2022.123260



Different mixed-linker MOFs based on HKUST-1 have been successfully synthesized using BtTC (1,2,4,5-benzenetetracarboxylate) and BDC (1,4-benzenedicarboxylate) as modulator ligands. These MOFs maintain the HKUST-1 structure up to 25% and 50% of trimesic acid replacing with BtTC and BDC ligands, respectively. A low percentage of modulator ligand provokes an increasing of the MOF surface area keeping its microporosity whereas a higher content of BtTC induces mesoposority in the samples. The adsorption of moisture ambient or vapour iodine reveals that there is a relation between the surface area and the capacity of adsorption of the samples. However, this relation is not found in the experiments of Congo Red removal from aqueous and ethanol solutions. The pH of the solutions has a significant effect on the adsorption capacity of the samples.

Assessment of construction and demolition wastes (CDWs) as raw materials for the manufacture of low-strength concrete and bases and sub-bases of roads
Garzon, E; Martínez-Martínez, S; Pérez-Villarrejo, L; Sánchez-Soto, PJ
Materials Letters, **320** (2022) 132343
Agosto, 2022 | **DOI:** 10.1016/j.matlet.2022.132343

A chemical (XRF) and mineralogical (XRD) characterisation has been carried out, as well as the determination of the main properties, of construction and demolition wastes (CDWs). This waste has been applied as recycled aggregate. The objective was to search for its reuse for the manufacture of concrete and road bases and sub-bases. Chemical analysis revealed the presence of SiO_2 (39.13 wt%) and Al_2O_3 (9.55 wt%) from quartz and some silicates, and gypsum. The content of CaO (21.42 wt%) was associated with calcite and dolomite. The materials' properties have suggested that the particle sizes are not inside the typical interval fixed in the Spanish normative. It can be reused as esplanades or sub-bases of roads and highways, since it is a granular material with a very high California Bearing Ratio (CBR value is 36). It was concluded that the use of CDWs as a substitute of sand for the manufacture of concrete can only be used in percentages lower than 10 wt% producing low-strength concrete.

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

IX Premios Joven a la Cultura Científica
P.J. Sánchez-Soto
Revista QUÍMICOS DEL SUR, 114 (2022) 52-55

Tomás Ramírez Reina, laureado en 2022
P.J. Sánchez-Soto
Revista QUÍMICOS DEL SUR, 114 (2022) 83

Los residuos de la industria siderúrgica y metalúrgica del aluminio
E. Bonet, S. Martínez-Martínez, D. Eliche-Quesada, L. Pérez-Villarejo, P.J. Sánchez-Soto
Acta Científica y Tecnológica, 31 (2022) 15-21

“Chemistry and Biochemistry of Food”. Recensión
P.J. Sánchez-Soto
Acta Científica y Tecnológica, 31 (2022) 31

Alkali Activated Cements Based on Slags from Different Industries
M.A. Gómez-Casero, L. Pérez-Villarejo, P.J. Sánchez-Soto, D. Eliche-Quesada
Materials Proceedings, 8 (2022) 123

Congresos y Reuniones Internacionales / International Congress and Meetings

Comunicaciones / Communications

IX International Symposium on Materials, II Iberian Meeting on Materials Science, 'Materiais 2022'
10-13 abril [Marinha Grande, Portugal]

Comunicación Oral: **Alkali Activated Cements Based on Slags from Different Industries.** M.A. Gómez-Casero, L. Pérez-Villarejo, P.J. Sánchez-Soto, D. Eliche-Quesada

15th International Ceramics Congress
20-24 junio [Perugia, Italia]

Comunicación Oral: **Creep behaviour of Zirconia composites with different amounts of reduced Graphene-oxide Sintered by Spark Plasma Sintering.** R.Cano-Crespo; P. Rivero-Antúnez; R. Moreno; D. Gómez-García; A. Domínguez-Rodríguez

Ceramics in Europe 2022
10-14 julio [Cracovia, Polonia]

Comunicación Oral: **Densification behaviour and optical properties of nano-Y_2O_3 ceramics doped with bivalent transition metals.** A. Najafzadeh; A. Talimian; V. Pouchlý; Á. Gallardo-López; R. Poyato; R. Klement; K. Maca;F. Gutiérrez-Mora; D. Galusek

Comunicación Oral: **Dependence of the tribological behaviour of graphene-based ceramic composites on the graphene structure.** F. Gutiérrez Mora; C. Muñoz-Ferreiro; R. Moriche; A. Morales-Rodríguez; A. Gallardo-López; R. Poyato

Comunicación Oral: **Zirconia- Few-Layer Graphene multifunctional composites: a compromise between mechanical and electrical properties.** C. Muñoz-Ferreiro; H. Reveron; J. Chevalier; A. Morales-Rodríguez; R. Poyato; Á. Gallardo-López

IX Jornadas de I+D+i & 1st International Workshop on STEM
3 – 4 octubre [Sevilla, España]

Comunicación Oral: **New β-Ti alloy substrates for bone replacements: manufacture and microstructural and tribomechanical characterization.** J.E. de la Rosa-Melian, L.M. Rodríguez-Albelo, P. Navaro, F.J. Gotor, E. Delgado, F.J. García-García, A. Beltrán, D. Mena, A. Alcudia, P. Trueba, B. Begines, Y. Torres

Czech and Slovak Conference on Glass 2022
9-11 noviembre [Praga, República Checa]

Póster: **Fabrication of Al_2O_3-$Y_3Al_5O_{12}$-ZrO_2 eutectic ceramic using spark plasma sintering.** M. Vakhshouri, A. Najafzadeh, A. Talimian, A. Gallardo-López, R. Poyato, F. Gutiérrez-Mora, A. Prnová, D. Galusek

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

Comunicación Oral: **A novel multi-phase flash sintering (MPFS) technique for 3D complex-shaped ceramics.** S. Molina-Molina, E. Gil-González, A. Taibi, F.J. Durán-Olivencia, J.M. Valverde, A. Perejón, P.E. Sánchez-Jiménez, L.A. Pérez-Maqueda

Comunicación Oral: **Ca-Looping for thermochemical energy storage.** N. Amghar, A. Carro, P.E. Sánchez-Jiménez, A. Perejón, C. Ortiz, R. Chacartegui, L.A. Maqueda

Póster: **Thermochemical storage based on sodium acetate for heating in buildings.** N. Amghar, J. Lizana, P.E. Sánchez-Jiménez, A. Perejón, L.A. Maqueda

Póster: **Rapid densification of BiFeO3-BaTiO3 piezoelectric ceramics b y flash sintering from mechanically activated powders.** A. Taibi, S. Molina-Molina, E. Gil-González, P.E. Sánchez-Jiménez, A. Perejón, J.E. García, L.A. Pérez-Maqueda

LVIII Congreso de la Sociedad Española de Cerámica y Vidrio
3 – 6 mayo [Madrid, España]

Comunicación Oral: **Diseño de compuestos cerámica-grafeno con conductividad eléctrica "a la carta".** R. Poyato; C. López-Pernía; C. Muñoz-Ferreiro; R. Moriche; A. Morales-Rodríguez; A. Gallardo-López

Comunicación Oral: **Tailoring the properties of zirconia composites with 2D nanomaterials.** C. Muñoz-Ferreiro; H. Reveron; J. Chevalier; A. Morales-Rodríguez; R. Poyato; A. Gallardo-López

Póster: **Arcillas cerámicas de Alhabia (Almería).** P.J. Sánchez-Soto; S. Martínez-Martínez; L. Pérez-Villarejo; J.A. Sánchez-Garrido; E. Garzón

Póster: **Proyecto Reliqua. Una nueva herramienta para el desarrollo de la Economía Circular.** S. Martínez-Martínez; D. Eliche-Quesada; L. Pérez-Villarejo; P.J. Sánchez-Soto

XVI Congreso Nacional de Materiales | CNMAT2022
28 junio – 1 julio [Ciudad Real, España]

Comunicación Oral: **Fabricación y caracterización de piezas de Ti35Nb7Zr5Ta porosas para sustituciones óseas: límites de la PM convencional vs la técnica de espaciadores.** L.M. Rodriguez-Albelo, P. Navarro, F.J. Gotor, E.J. Delgado-Pujol, F.J. García-García, A.M. Beltrán, J.E. de la Rosa, D. Mena, A. Alcudia, P. Trueba, B. Begines, Y. Torres

FORMACION / TRAINING

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título:	**Procesado y sinterización de matrices de circona cúbica con nanoestructuras de grafeno**
Autor:	Tomás Espuny Plaza
Directoras:	Rosalía Poyato Galán y Rocío Moriche Tirado
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	12 de enero de 2022

Título:	**Fabrication and microstructural characterisation of titanium matrixes reinforced with graphene nanoplatelets**
Autor:	Irene Neri Beaus
Directoras:	Rosalía Poyato Galán y Cristina Arévalo Mora (US)
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	21 de julio de 2022

Título:	**Envejecimiento hidrotermal de circona reforzada con nanoláminas de nitruro de carbono**
Autor:	Palma García Sanz
Directoras:	Rosalía Poyato Galán y Ana Morales Rodríguez
Grado:	Trabajo Fin de Grado
Centro:	Universidad de Sevilla
Fecha Defensa:	5 de septiembre de 2022

Título:	**Procesado y degradación hidrotermal de composites de circona con refuerzo de nitruro de boro 2D**
Autor:	Sixto Sánchez Moreno
Directoras:	Rosalía Poyato Galán y Ana Morales Rodríguez
Grado:	Trabajo Fin de Máster
Centro:	Universidad de Sevilla
Fecha Defensa:	7 de julio de 2022

DOCENCIA / TEACHING

Investigadores de esta unidad participan en el Máster en Ciencia y Tecnología de Nuevos Materiales y en titulaciones de Grado y doble Grado de la Universidad de Sevilla (ver ACTIVIDADES DIVULGATIVAS Y FORMATIVAS)

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)
- Horno horizontal alta temperatura 1800 °C AGNI
- Horno horizontal alta temperatura 1600 °C Carbolite
- Horno horizontal 1200 °C 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 °C Hobersal
- Impedancímetro Agilent 4294ª
- Multímetro Keysight B2901A
- Equipo de Hot-Press TERMOLAB

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

Profesores de Investigación	Dr. Juan Pedro Espinós Manzorro
	Dra. Asunción Fernández Camacho
Catedráticos	Dr. José Cotrino Bautista
Investigadores Científicos	Dr. Ángel Barranco Quero
	Dr. Juan Carlos Sánchez López
	Dr. Francisco Yubero Valencia
Científicos Titulares	Dra. Ana Isabel Borrás Martos
	Dra. María Aránzazu Díaz Cuenca
	Dr. Alberto Palmero Acebedo
	Dra. T. Cristina Rojas Ruiz
	Dr. Juan Ramón Sánchez Valencia
Profesores Titulares	Dr. Rafael Álvarez Molina
	Dra. Ana María Gómez Ramírez
Profesores "Ad Honorem"	Dr. Agustín Rodríguez González-Elipe
Doctores (Laboral Fijo)	Dra. Vanda Cristina Fortio Godinho
	Dr. Jorge Gil Rostra
Doctores Contratados	Dr. Francisco J. Aparicio Rebollo
	Dr. Jorge A. Budagosky Marcilla
	Dra. Lidia Contreras Bernal
	Dr. Daniel Fernández de los Reyes
	Dr. Víctor López Flores
	Dra. Carmen López Santos
	Dr. Manuel Oliva Ramírez
	Dr. Guillermo F. Regodón Harkness
Investigadores en Formación	Ldo. Javier Castillo Seoane
	Gda. Triana Czermak Álvarez
	Gdo. Jaime Del Moral Jalón
	Gdo. Juan Delgado Álvarez
	Ldo. Xabier García Casas
	Gdo. Darío Jumilla Núñez
	Gdo. Pedro Javier Lloreda Jurado
	Gdo. Servando Marín Meana
	Gdo. Adrián Megías Sánchez
	Gda. Laura Montes Montañez
	Gda. Gloria Patricia Moreno Martínez
	Gdo. Fernando Núñez Gálvez
	Ldo. José Manuel Obrero Pérez
	Ldo. Noel Orozco Corrales
	Lda. Claudia Ibeth Parra Montero
	Lda. Xiaozhe Song
Técnicos Superiores Especializados	Dr. Víctor J. Rico Gavira

Técnicos Contratados	Ldo. Dirk Hufschmidt
	Ldo. Álvaro Perea Brenes
	Lda. Miriam Sánchez Pérez
	Lda. Iru Nerea Tena Álvarez
Garantía Juvenil	Gdo. José Manuel Moreno de la Vega
	D. Juan Miguel Ojeda Bobo

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.

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 revaloritazion 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
Ana María Gómez Ramírez Manuel Oliva Rodríguez	Rafael Álvarez Molina José Cotrino Bautista María del Carmen García Martínez (US) Alberto Palmero Acebedo Agustín R. González-Elipe

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 procesos 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 renovably 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

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
TED2021-130916B-100	01-12-2022 30-11-2024	Ministerio de Ciencia e Innovación	253.000 €

Investigador Principal Research Head	Componentes Research Group
Ana Isabel Borrás Martos María del Carmen López Santos	Ángel Barranco Quero José Cotrino Bautista Juan Pedro Espinós Manzorro Luis Alberto Angurel Lamban (INMA) Germán de la Fuente Leis (INMA) Jorge Gil Rostra Antonio José Ginés Arteaga (IMSE) Gildas Leger (IMSE) Ricardo Molina Mansilla (IQAC) Víctor J. Rico Gavira Agustín R. González-Elipe Juan Ramón Sánchez Valencia

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
Ana María Gómez Ramírez	José Javier Brey Sánchez (US) José Cotrino Bautista María del Carmen García Martínez (US) Antonio Rodero Serrano (US) Paula de Navascués Garvín Manuel Oliva Ramírez

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
Rafel Álvarez Molina Alberto Palmero Acebedo	Víctor J. Rico Gavira Agustín R. González-Elipe

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

MINISTERIO DE CIENCIA E INNOVACIÓN

AGENCIA ESTATAL DE INVESTIGACIÓN

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

MINISTERIO DE CIENCIA E INNOVACIÓN

AGENCIA ESTATAL DE INVESTIGACIÓN

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 €

Investigador Principal Research Head	Componentes Research Group
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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.

Desarrollo de catalizadores y soportes para procesos de almacenamiento químico de energía neutros en CO_2 basados en líquidos orgánicos portadores de hidrógeno
Development of catalysts and supports for CO_2 neutral chemical energy storage processes based on liquid organic hydrogen carriers

MINISTERIO DE CIENCIA E INNOVACIÓN
UNIÓN EUROPEA
FONDO EUROPEO DE DESARROLLO REGIONAL
"Una manera de hacer Europa"
AGENCIA ESTATAL DE INVESTIGACIÓN

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
RTI2018-093871-B-I00	01-01-2019 30-09-2022	Ministerio de Ciencia e Innovación	176.176 €

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

RESUMEN / ABSTRACT

El agotamiento de los combustibles fósiles (a corto y largo plazo) y el calentamiento global derivado del efecto invernadero son consecuencias del uso extensivo de estos combustibles. Por lo tanto, es muy conveniente utilizar y desarrollar energías renovables y así eliminar nuestra dependencia de los combustibles fósiles. Esto hace que el almacenamiento de energía producida por fuentes renovables (que son intermitentes) sea un objetivo importante de investigación. En proyectos anteriores, hemos trabajado en el estudio de nanomateriales y catalizadores para el almacenamiento de hidrógeno como vector de transporte y almacenamiento de energía (ciclo del H_2). En este nuevo proyecto, el grupo de investigación propone avanzar en la Implementación de líquidos orgánicos como portadores de hidrógeno (LOHC) como una forma prometedora de combinar los ciclos del CO_2 y del H_2 que conduzca a un almacenamiento de energía sostenible en un ciclo neutro en carbono. Pequeñas moléculas orgánicas, como el ácido fórmico o el metanol, se pueden usar para almacenar el H_2 (y la energía) proveniente de fuentes renovables. Estos combustibles alternativos se pueden quemar o usarse para generar H_2 que alimente directamente a una pila de combustible.

En este proyecto se llevarán a cabo investigaciones para la implementación de dos procesos relacionados con las tecnologías LOHC:

i) La descomposición térmica selectiva del ácido fórmico por catálisis heterogénea para la producción bajo demanda de hidrógeno exento de monóxido de carbono.

ii) La producción de hidrógeno por reformado de alcoholes (biometanol) en procesos fotocatalíticos heterogéneos. La catálisis desempeña un papel clave en la implementación de estos dos

procesos. Por lo tanto, los principales objetivos y actividades del proyecto son el diseño racional y la preparación de catalizadores y soportes para estudiar las relaciones composición-estructura desempeño en los dos procesos mencionados anteriormente. El enfoque innovador es la aplicación de técnicas asistidas por plasma, como la pulverización catódica para el crecimiento de películas delgadas, y los tratamientos con plasmas de oxidación, reducción y grabado, para el desarrollo de recubrimientos catalíticos nanoestructurados y nanopartículas soportadas. Se desarrollarán espumas de carbono poroso y catalizadores basados en Pd que incluyen Pd, Pd-C, Pd-B o Pd-Cu para el estudio de la reacción de descomposición de ácido fórmico. Se investigarán películas fotocatalíticas de TiO_2-TiO_x con Pt (y/o Au) como co-catalizadores para el foto-reformado de metanol.

The depletion of fossil fuels (in short and long term) and the global warming derived from greenhouse effect are consequences of the extensive use of these fuels. It is therefore highly desirable to use and develop renewable energies and so eliminate our dependence on fossil fuels. This makes the storage of energy produced by renewable sources (which are intermittent) an important target. In previous projects we have been working in the study of nanomaterials and catalysts for the storage of hydrogen as a vector of energy transport and storage (H_2 cycle). In this new project the research group propose to move into the implementation of the liquid organic hydrogen carriers (LOHC) as a promising way of combining the CO_2 and de H_2 cycles leading to a sustainable energy storage in a carbon neutral cycle.

Small organic molecules, like formic acid or methanol, can be used to store the H_2 (and energy) coming from renewable sources. These alternative fuels can be combusted themselves or be used to generate H_2 directly feeding a fuel cell.

Research will be conducted in this project to the implementation of two processes related to the LOHC technologies:

i) The selective low temperature decomposition of formic acid by heterogeneous catalysis to the on-demand production of carbon monoxide free hydrogen.

ii) The hydrogen production by reforming of alcohols (i.e. biomethanol) in heterogeneous photocatalytic processes.

Catalysis is playing the key role in the implementation of these lwo processes. Therefore the main objectives and activities in the project are the rational design and preparation of catalysts and supports to study composition-structure-performance relationships for the two above mentioned processes. The innovative approach is the application of plasma assisted techniques, like the magnetron sputtering for thin film growth, as well as plasma treatments of oxidation, reduction and etching for the development of nanostructured catalytic coatings and supported nanoparticles. Porous carbon foam supports and Pd based catalysts including Pd, Pd-C, Pd-B or Pd-Cu will be developed for the study of the formic acid decomposition reaction. TiO_2-TiO_x photocatalytic films with Pt (and/or gold) as co-catalysts will be investigated for the photo-reforming of methanol.

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/N2-O2 (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 nano-porous 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

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 realizado 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.

Modelado e implementación de la técnica Freeze-Casting: gradientes de porosidad con un equilibrio tribo-mecánico y comportamiento celular electro-estimulado
Modeling and implementation of the freeze casting technique: gradients of porosity with a tribo-mechanical equilibrium and electro-stimulated cellular behavior

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Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-12597711	01-02-2020 31-01-2022	Junta de Andalucía	90.000 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El titanio comercialmente puro (Ti c.p.) y la aleación Ti6Al4V, son los biomateriales metálicos con el mejor pronóstico para la reparación clínica del tejido óseo. Sin embargo, a pesar de sus ventajas, 5-10% de los implantes fallan durante los cinco años post-implantación. Éstos se asocian fundamentalmente al apantallamiento de tensiones (diferencias de rigidez entre el implante-hueso), el empleo de criterios de diseño (fractura y fatiga) no adecuados para biomateriales, a los fenómenos de tribo-corrosión en condiciones de servicio y a los problemas que ocurren en la intercara (micromovimientos y/o presencia de bacterias) que limitan la capacidad de oseointegración. En este proyecto se propone fabricar e implementar un dispositivo sencillo y económico para obtener cilindros con porosidad controlada (gradiente) y alargada mediante la técnica de congelación dirigida. Se desarrollarán modelos de elementos finitos para estimar el crecimiento geométrico de las dendritas de hielo y el comportamiento mecánico de los cilindros porosos (distribución de esfuerzos y deformaciones), usando radiografías en tiempo real del proceso de congelación dirigida, así como los parámetros que caracterizan la microestructura (proporción, tamaño, morfología de la porosidad) y el comportamiento a compresión (rigidez y límite de fluencia). Además, se plantea la generación de patrones de rugosidad superficial mediante el bombardeo de iones, encaminados a mejorar la unión intima entre el implante y el tejido óseo. Por otra parte, se plantean protocolos in-vitro adecuados para evaluar la citotoxicidad, la adhesión, diferenciación y proliferación celular. Finalmente, se desarrollará un sistema de medida de bio-impedancia que permita racionalizar la influencia de la porosidad, el acabado superficial y los estímulos eléctricos en el comportamiento in-situ de osteoblastos. En este contexto, el objetivo principal es fabricar cilindros con una porosidad controlada y su superficie modificada, que permita garantizar un mejor equilibrio biomecánico, tribo-corrosivo y biofuncional (in-growth y oseointegración del tejido óseo y el implante).

Commercial pure Titanium (c.p. Ti) and Ti6Al4V alloy are metal biomaterials with the best properties for clinical repair bone tissue. However, despite their advantages, 5-10 % of implants fail during the five years post-implantation. They are mainly associated with stress shielding (difference stiffness between bone and implant), the use of design criteria (fracture and fatigue) not suitable for biomaterials, the tribo-corrosion phenomena in service conditions and the interface problems (micro-movements and / or the presence of bacteria) that limit the capacity of osseointegration. This project proposes the manufacture and implementation of a simple and economical device to obtain cylinders with controlled (gradient) and elongated porosity by the freeze casting technique. Finite element models will be developed to estimate the geometric growth of the ice dendrites and the mechanical behaviour of the porous cylinders (distribution of stresses and deformations), using real-time radiographs of the directed freezing process, as well as the parameters that characterize the microstructure (amount, size and morphology of porosity) and compression behaviour (stiffness and yield strength). In addition, the generation of surface roughness patterns by ion sputtering is proposed, with the aim to improve the close bond between the implant and the bone tissue. Furthermore, suitable in-vitro protocols are proposed to evaluate cytotoxicity, adhesion, differentiation and proliferation cell. Finally, a bio-impedance measuring system will be developed in order to rationalize the influence of porosity, finished surface and electrical stimulus on the in-situ behaviour of osteoblasts. In this context, the main objective is to manufacture cylinders with a controlled porosity and modified surface, with enhanced biomechanical, tribo-corrosive and biofunctional balance (in-growth and osseointegration of the bone tissue and the implant).

Plasmas atmosféricos de arco deslizante para la producción sostenible de amoniaco e hidrógeno

Atmospheric Pressure Gliding-arc Plasmas for the Sustainable Production of Ammonia and Hydrogen | ARCPLAS

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-1380977	01-02-2021 31-12-2022	Junta de Andalucía	77.987 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

El proyecto "*Plasmas atmosféricos de arco deslizante para la producción sostenible de amoniaco e hidrógeno*", ARCPLAS en adelante, pretende el desarrollo de procesos de transformación química de gases mediante tecnologías de plasma atmosférico que usan la electricidad como vector energético directo. En concreto se persigue la puesta a **punto de un reactor de Plasmas Atmosféricos de Arco Deslizante (PAAD) para inducir dos procesos de gran impacto industrial y medioambiental, como son la síntesis de amoniaco (NH_3) y la producción de hidrógeno (H_2).** 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, de sobra es conocido que el camino hacia una economía basada en dicho combustible es uno de los retos del siglo XXI. ARCPLAS propone, en una primera etapa, desarrollar la tecnología PAAD mediante el diseño, construcción, modelización y puesta a punto de un reactor de arco deslizante. La complejidad de los procesos básicos implicados 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, características químicas de los gases implicados y otros parámetros básicos de operación. Tanto la caracterización experimental como 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 su rendimiento químico, así como el rendimiento energético del reactor. Finalmente, en una última etapa del proyecto, se explorarán posibles modificaciones sobre

el modelo de reactor PAAD desarrollado, 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.

The project "*Atmospheric Gliding-arc Plasmas for the Sustainable Production of Ammonia and Hydrogen*", hereinafter ARCPLAS, **aims to develop gas chemical transformation processes through atmospheric pressure plasma technologies that use electricity as a direct energy vector. Specifically, the objective is to fine-tune a Plasma Atmospheric Gliding Arc Reactor (PAAD) to induce two processes of great industrial and environmental impact, such as the synthesis of ammonia (NH_3) and the production of hydrogen (H_2).** Ammonia is the base substance of fertilizers used in agriculture, and its demand is increasing in line with world food needs. Regarding hydrogen, it is well known that the path towards an economy based on it is one of the challenges of the 21st century. ARCPLAS proposes, in a first stage, to develop PAAD technology through the design, construction, modelling and commissioning of a gliding arc reactor. The complexity of the basic processes involved in this type of reactors will require a fundamental study of their electrical response and mass and charge transport phenomena, as well as an exhaustive characterization and diagnosis of the plasma based on parameters such as gas flow, interaction between excited species, residence time, chemical characteristics of the gases involved and other basic operating parameters. Both the experimental and theoretical characterization of the reactor, the latter carried out using computational methods, will be essential for its correct operation and optimization of the processes. In a second stage, the study of the reactions to obtain H_2 and NH_3 will be addressed, with the aim of maximizing their chemical yield, as well as the energy yield of the reactor. Finally, possible modifications of the PAAD reactor will be explored, contemplating the effect of the incorporation of piezoelectric materials to induce secondary electron emission phenomena, the modification of the surface of the electrodes or the geometry of the system in order to promote an improvement in the performance of the processes studied.

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
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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).

Tecnología de plasma para el desarrollo de una nueva generación de conductores de huecos en celdas solares de perovskita

Plasma technology for the development of a new generation of hole transport layers in perovskite solar cells | PLASMACELLS

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-1263142	01-02-2020 31-12-2022	Junta de Andalucía	30.000 €

Investigador Principal Research Head	Componentes Research Group
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RESUMEN / ABSTRACT

Las celdas solares (CSs) de tercera generación son dispositivos nanotecnológicos que convierten directamente la luz solar en electricidad y suponen el paradigma de la investigación en energías renovables de cuyo aprovechamiento dependerá el futuro energético del planeta. Recientemente, un ejemplo particular de CSs que contienen una perovskita de haluro organometálico como absorbedor de luz han centrado la atención de la comunidad científica debido, ante todo, a su alta eficiencia y bajo coste. Estas características las convierten en una alternativa prometedora a las celdas actuales (de Si y calcogenuros). Sin embargo, para que la realización final y comercial de las celdas de perovskita sea posible es necesario que alcancen una mayor estabilidad, durabilidad y reproducibilidad. Los avances más importantes alcanzados se han debido a la intensa investigación sobre los elementos que integran esta CS: conductor de electrones, perovskita y conductor de huecos. En concreto, este último elemento ha tenido una importancia crucial en su evolución tras la implementación de los conductores de huecos en estado sólido.

PlasmaCells persigue abordar por primera vez la síntesis de una nueva familia de conductores de huecos por técnicas 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 PlasmaCells es la integración de estos nuevos conductores de huecos procesados por plasma en CSs de perovskita. La importancia del proyecto se basa en resultados recientes obtenidos por el Investigador Principal (IP) que demuestran que la aproximación propuesta

puede ser una de las vías más prometedoras para el aumento de la estabilidad, durabilidad y reproducibilidad de estas CSs, que actualmente suponen el cuello de botella que impide su industrialización. Cabe destacar que no existe en la bibliografía ningún ejemplo sobre esta aproximación sintética para el desarrollo de conductores de huecos. Se espera que esta oportunidad permita demostrar las ventajas y versatilidad de esta metodología innovadora en un campo de alto impacto, que se enmarca dentro de las áreas prioritarias RIS3 Andalucía y en el PAIDI 2020 de crecimiento sostenible, eficiencia energética y energías renovables.

Third generation solar cells (SCs) are nanotechnological devices that directly convert sunlight into electricity and represent the paradigm of research in renewable energies, the use of which will depend on the energy future of the planet. Recently, a particular example of SCs containing an organometallic halide perovskite as a light absorber have attracted the attention of the scientific community due, above all, to their high efficiency and low cost. These characteristics make them a promising alternative to current cells (Si and chalcogenides). However, for the commercial realization of perovskite cells, it is necessary to achieve greater stability, durability and reproducibility. The most important advances have been achieved due to the intense research on the elements that integrate a SC: electron transport layer, perovskite and hole transport layer. Specifically, this latter element has been crucial for its evolution after the implementation of solid state hole conductors.

PlasmaCells pursuits to address for the first time the synthesis of a new family of hole transporters by vacuum and plasma techniques. These methodologies are industrially scalable and have great advantages over solution methodologies (the most used), among which stand out: their high versatility, composition and microstructural control, low cost, are environmental friendly since they do not require solvents, do not produce polluting emissions and are compatible with current semiconductor technology.

The main objective of PlasmaCells is the integration of these new plasma-processed hole transport layers into perovskite SCs. The importance of the project is based on recent results obtained by the Principal Investigator (PI) that demonstrate that the proposed approach may be one of the most promising ways to increase the stability, durability and reproducibility of these SCs, which currently represent the bottleneck that prevents their industrialization. It should be noted that there is no example in the literature of this synthetic approach for the development of hole transporters. It is expected that this opportunity will allow to demonstrate the advantages and versatility of this innovative methodology in a high-impact field, which is framed within the priority areas RIS3 Andalucía and in the PAIDI 2020 of sustainable growth, energy efficiency and renewable energies.

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 31-12-2022	Junta de Andalucía	119.800 €

Investigador Principal Research Head	Componentes Research Group
Ángel Barranco Quero Alberto Palmero Acebedo	Ana María Gómez Ramírez Juan Ramón Sánchez Valencia Víctor J. Rico Gavira Rafael Álvarez Molina Francisco Yubero Valencia Juan Pedro Espinós Manzorro Ana Isabel Borrás Martos Agustín R. González-Elipe

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 31-12-2022	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".

Funcionalización superficial y modelos de difusión de factores de germinación en semillas tratadas con plasmas

Surface functionalization and diffusion models of germination factors in plasma-treated seeds | PLASMASEED

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
US-1381045	01-01-2021 31-12-2022	Junta de Andalucía	79.866 €

Investigador Principal Research Head	Componentes Research Group
María del Carmen López Santos Antonio Prados Montaño (US)	Agustín Rodríguez González-Elipe Francisco Yubero Valencia

RESUMEN / ABSTRACT

PLASMASEED aborda la inclusión de la tecnología de vacío y plasma para la funcionalización superficial de semillas como una estrategia eficaz y limpia para que los cultivos sean menos dependientes de los cambios del entorno. Se pretenden analizar los factores y mecanismos básicos que inciden en la mejora de la germinación tratando las semillas desde una aproximación multidisciplinar que combina conceptos básicos de biofísica, caracterización avanzada y procesado por vacío y plasma. El efecto de campos eléctricos asociados a los plasmas y las características físico-químicas de estos, la influencia de la difusión de otros factores de germinación además del agua (oxígeno, luz, etc.), la difusión de nutrientes como especies nitratos u otras de interés para la germinación, etc., son factores experimentales que se modelizan usando procedimientos de Monte Carlo y mecánica estadística para proponer modelos holísticos de difusión de factores de germinación a través de las membranas de semillas y de la influencia de los tratamientos superficiales con técnicas de plasma para modificar y / o controlar tales procesos.

PLASMASEED addresses the inclusion of vacuum and plasma technology for the surface functionalization of seeds as an effective and clean strategy to make crops less dependent on environmental changes. The aim is to analyze the basic factors and mechanisms that affect the improvement of germination by treating the seeds from a multidisciplinary approach that combines basic concepts of biophysics, advanced characterization and vacuum and plasma processing. The effect of electric fields associated with plasmas and their physical-chemical features, the influence of the diffusion of other germination factors besides water (oxygen, light, etc.), the diffusion of nutrients such as nitrates or other species of interest for germination, etc., are experimental factors that are simulated using Monte Carlo procedures and statistical mechanics to propose holistic models of diffusion of germination factors through seed membranes and the influence of surface treatments by plasma techniques to modify and/or control such processes.

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 |PlasmaDielec

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

Estudios preliminares para la aplicación de nanocomposites sólido-gas como blancos sólidos en estudios de reacciones nucleares y alta densidad de energía (PRE-TARGETS)

Periodo/Period:	1-07-2021 / 31-12-2022
Entidad Financiadora:	CSIC (Intramural)
Importe total/Total amount:	14.000 €
Investigador responsable/Research head:	Asunción Fernández Camacho

Ondas acústicas superficiales y su transferencia para aplicaciones de relevancia industrial

Periodo/Period:	1-02-2021 / 31-01-2024
Entidad Financiadora:	CSIC (Intramural)
Importe total/Total amount:	47.640 €
Investigador responsable/Research head:	Ana Isabel Borrás Martos

Nanostructures with atomic precision for next generation energy harvesting devices

Código/Code:	LINKA20346
Periodo/Period:	01-01-2021 / 31-12-2022
Organismo Financiador/Financial source:	CSIC
Importe total/Total amount:	16.093 €
Investigador responsable/Research head:	Mariona Coll Bau (ICMAB)
Participantes del ICMS:	Ángel Barranco Quero, Ana Isabel Borrás Martos, Xabier García Casas, Víctor J. Rico Gavira, Agustín R. González-Elipe

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

New ideas for the use of Commercial Off The Shelf (COTS) components

Código/Code:	ITT/AO/2-1785/20/NL/GLC
Periodo/Period:	01-01-2021 / 31-12-2022
Entidad Financiadora:	ESA; Coordinator ALTER Technikigt TÜV NORD SAU
Importe total/Total amount:	25.000 €
Investigador principal/Research head:	Angel Barranco Quero

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

AYUDAS PARA LA ADQUISICIÓN DE EQUIPOS

Goniómetro para medidas de ángulo de contacto de superficies en ambiente controlado (IE_19_142 USE)

Financia: Junta de Andalucía
Importe Concedido: 82.000,00 €
Periodo: 29-12-2020 / 28-12-2022

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Caracterización microestructural y química de materiales para avisadores sonoros

Periodo/Period:	19-01-2010 / 31-12-2022
Organismo Financiador/Financial source:	CLARTON HORN
Importe total/Total amount:	48.872 €
Investigador responsable/Research head:	Asunción Fernández Camacho

Nuevo sistema de propulsión espacial basado en el principio de Mach

Periodo/Period:	02-12-2019 / 30-12-2022
Organismo Financiador/Financial source:	ARQUIMEA INGENIERIA, S.L.
Importe total/Total amount:	100.000 €
Investigador responsable/Research head:	Agustín R. González-Elipe

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 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

Sistema de generación de hidrógeno a partir de gasoil

Periodo/Period:	09-04-2020 / 1-11-2022
Entidad Financiadora:	INYECCIONES PLÁSTICAS MECACONTROL, S.L.
Importe total/Total amount:	45.000 €
Investigador responsable/Research head:	Ana María Gómez Ramírez
Componentes/Research group:	Agustín R. González-Elipe, José Cotrino Bautista, Manuel Oliva Ramírez

Proyecto de consultoría "PULSAR"

Periodo/Period:	19-10-2021 / 18-04-2022
Organismo Financiador/Financial source:	ARQUIMEA CENTRO DE INVESTIGACIONES AVANZADAS, S.L.U.
Importe total/Total amount:	27.000 €
Investigador responsable/Research head:	Agustín R. González-Elipe

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

Patentes / Patents

Máquina universal de ensayo de materiales a temperatura y humedad controlada para determinar su mojado y la formación, acumulación, adhesión y fusión de hielo

Inventores: Víctor J. Rico, Ana I. Borrás, Agustín R. González-Elipe, Laura Montes, Jaime del Moral, Juan R. Sánchez Valencia, Jorge Gil-Rostra, Angel Barranco
Tipo de Patente: Secreto Industrial
Número de Solicitud: 112556Z
Fecha Solicitud: 9 agosto de 2022
Entidades Titulares: Consejo Superior de Investigaciones Científicas, Universidad de Sevilla

Dispositivo de eliminación y prevención de formación de hielo en superficies

Inventores: Ana Isabel Borrás Martos, Agustín R. González-Elipe, Víctor J. Rico Gavira, Aurelio García Valenzuela. Laura Montes Montañez, Carmen López Santos, Manuel Oliva Ramírez
Tipo de Patente: Internacional
Número de Solicitud: PCT/ES22/070383
Fecha Solicitud: 17 de junio de 2022
Entidades Titulares: Consejo Superior de Investigaciones Científicas, Universidad de Sevilla

Energy harvesting device and self-powered sensor using the same
Inventores: Xabier García Casas, Ángel Barranco Quero, Ali Ghaffarinejad, Juan Ramón Sánchez Valencia, Ana Isabel Borrás Martos
Tipo de Patente: Internacional
Número de Solicitud: PCT/EP22/073950
Fecha Solicitud: 29 de agosto de 2022
Entidades Titulares: Consejo Superior de Investigaciones Científicas, Universidad de Sevilla

Porous Ionomer free layered metal alloy electrocatalyst electrode
Inventores: Jorge Gil Rostra, Agustín R. González-Elipe, Francisco Yubero Valencia, Ester López Fernández, Juan Pedro Espinós Manzorro
Tipo de Patente: Nacional
Número de Solicitud: PCT/EP22/079454
Fecha Solicitud: 21 de octubre de 2022
Entidades Titulares: Consejo Superior de Investigaciones Científicas, Universidad de Castilla-La Mancha, Fundación Domíngo Martínez

INFORMES TÉCNICOS / TECHNICAL REPORTS

Infiltración de Alúmina
Autores: Gloria Montero, Ana Borrás, Ángel Barranco, Juan R. Sánchez-Valencia
Destinatario: CTECH Nano
Fecha: 4 de octubre de 2022

Artículos Publicados en Revistas SCI / Papers In SCI Journals

Highly Anisotropic Organometal Halide Perovskite Nanowalls Grown by Glancing-Angle Deposition

Castillo-Seoane, J; Contreras-Bernal, L; Obrero-Pérez, JM; García-Casas, X; Lorenzo-Lazaro, F; Aparicio, FJ; López-Santos, C; Rojas, TC; Anta, JA; Borrás, A; Barranco, A; Sánchez-Valencia, JR
Advanced Materials, **34** (2022) 2107739
Marzo, 2022 | **DOI:** 10.1002/adma.202107739

Polarizers are ubiquitous components in current optoelectronic devices as displays or photographic cameras. Yet, control over light polarization is an unsolved challenge, since the main drawback of the existing display technologies is the significant optical losses. In such a context, organometal halide perovskites (OMHP) can play a decisive role given their flexible synthesis with tunable optical properties such as bandgap and photoluminescence, and excellent light emission with a low non-radiative recombination rate. Therefore, along with their outstanding electrical properties have elevated hybrid perovskites as the material of choice in photovoltaics and optoelectronics. Among the different OMHP nanostructures, nanowires and nanorods have lately arisen as key players in the control of light polarization for lighting or detector applications. Herein, the fabrication of highly aligned and anisotropic methylammonium lead iodide perovskite nanowalls by glancing-angle deposition, which is compatible with most substrates, is presented. Their high alignment degree provides the samples with anisotropic optical properties such as light absorption and photoluminescence. Furthermore, their implementation in photovoltaic devices provides them with a polarization-sensitive response. This facile vacuum-based approach embodies a milestone in the development of last-generation polarization-sensitive perovskite-based optoelectronic devices such as lighting appliances or self-powered photodetectors.

Ultrathin Plasma Polymer Passivation of Perovskite Solar Cells for Improved Stability and Reproducibility

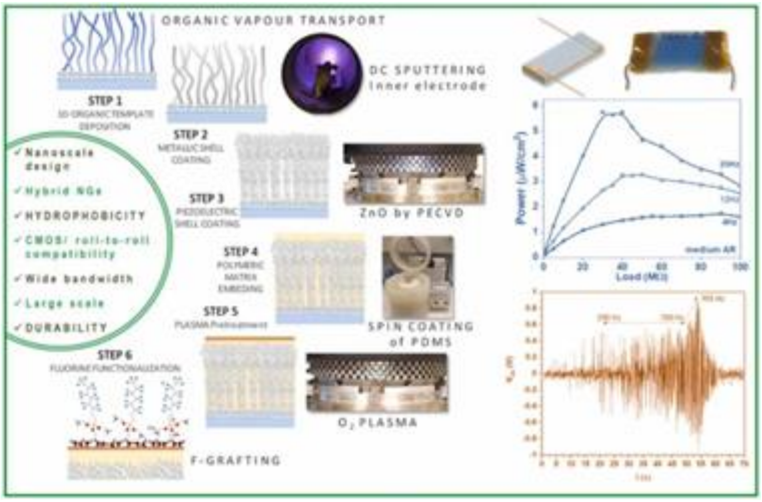
Obrero-Pérez, JM; Contreras-Bernal, L; Nuñez-Galvez, F; Castillo-Seoane, J; Valadez-Villalobos, K; Aparicio, FJ; Anta, JA; Borrás, A; Sánchez-Valencia, JR; Barranco, A
Advanced Energy Materials, 12 (2022) 2200812
Julio, 2022 | **DOI:** 10.1002/aenm.202200812

Despite the youthfulness of hybrid halide perovskite solar cells, their efficiencies are currently comparable to commercial silicon and have surpassed quantum-dots solar cells. Yet, the scalability of these devices is a challenge due to their low reproducibility and stability under environmental conditions. However, the techniques reported to date to tackle such issues recurrently involve the use of solvent methods that would further complicate their transfer to industry. Herein a reliable alternative relaying in the implementation of an ultrathin plasma polymer as a passivation interface between the electron transport layer and the hybrid perovskite layer is presented. Such a nanoengineered interface provides solar devices with increased long-term stability under ambient conditions. Thus, without involving any additional encapsulation step, the cells retain more than 80% of their efficiency after being exposed to the ambient atmosphere for more than 1000 h. Moreover, this plasma polymer passivation strategy significantly improves the coverage of the mesoporous scaffold by the perovskite layer, providing the solar cells with enhanced performance, with a champion efficiency of 19.2%, a remarkable value for Li-free standard mesoporous n-i-p architectures, as well as significantly improved reproducibility.

Plasma engineering of microstructured piezo-Triboelectric hybrid nanogenerators for wide bandwidth vibration energy harvesting

García-Casas, X; Ghaffarinehad, A; Aparicio, FJ; Castillo-Seoane, J; López-Santos, C; Espinos, JP; Cotrino, J; Sánchez-Valencia, JR; Barranco, A; Borrás, A

Nano Energy, **91** (2022) 106673
Enero, 2022 | **DOI:** 10.1016/j.nanoen.2021.106673

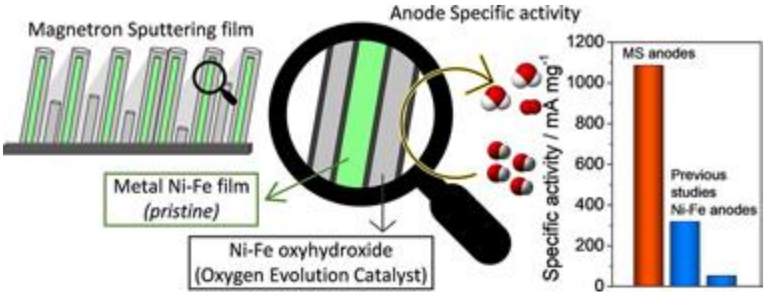


We introduce herein the advanced application of low-pressure plasma procedures for the development of piezo and triboelectric mode I hybrid nanogenerators. Thus, plasma assisted deposition and functionalization methods are presented as key enabling technologies for the nanoscale design of ZnO polycrystalline shells, the formation of conducting metallic cores in core@shell nanowires, and for the solventless surface modification of polymeric coatings and matrixes. We show how the perfluorinated chains grafting of polydimethylsiloxane (PDMS) provides a reliable approach to increase the hydrophobicity and surface charges at the same time that keeping the PDMS mechanical properties. In this way, we produce efficient Ag/ZnO convoluted piezoelectric nanogenerators supported on flexible substrates and embedded in PDMS compatible with a contact-separation triboelectric architecture. Factors like crystalline texture, ZnO thickness, nanowires aspect ratio, and surface chemical modification of the PDMS are explored to optimize the power output of the nanogenerators aimed for harvesting from low-frequency vibrations. Just by manual triggering, the hybrid device can charge a capacitor to switch on an array of color LEDs. Outstandingly, this simple three-layer architecture allows for harvesting vibration energy in a wide bandwidth, thus, we show the performance characteristics for frequencies between 1 Hz and 50 Hz and demonstrate the successful activation of the system up to ca. 800 Hz.

Ionomer-Free Nickel-Iron bimetallic electrodes for efficient anion exchange membrane water electrolysis

López-Fernandez, E; Gomez-Sacedon, C; Gil-Rostra, J; Espinos, JP; González-Elipe, AR; Yubero, F; De Lucas-Consuegra, A

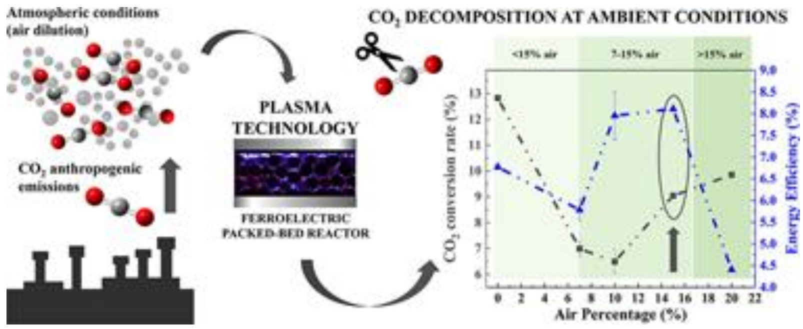
Chemical Engineering Journal, **433** (2022) 133774
Abril, 2022 | **DOI:** 10.1016/j.cej.2021.133774



A bottleneck for the deployment of the Anion Exchange Membrane Water Electrolysis (AEMWE) is the manufacturing of efficient and long lasting anodes and cathodes for the cells. Highly performant bimetallic Ni/Fe catalyst films with various atomic ratios have been prepared by magnetron sputtering in an oblique angle configuration (MS-OAD) and used as anodes for AEMWE. Electrocatalytic experiments in a small three-electrode cell and a thorough analysis of the electrode properties with various physico-chemical characterization tech-niques have been used to select the nanostructured anode catalyst which, depicting an optimized Ni/Fe ratio, presents the maximum activity for the oxygen evolution reaction. These anode layers are then scale-up for their integration in an AEMWE cell where the influence of assembly conditions and the effect of adding an ionomer to the anodes have been studied. The obtained results have demonstrated the outstanding properties of the fabri-cated bimetallic films in terms of activity, stability, and operation under ionomer-free conditions. Current density values around 400 and 600 mA cm^{-2} at 40ºC and 60ºC (2.0 V), respectively, much higher than those obtained with pure Ni, were obtained with an optimized membrane electrode assembly. The high yield obtained with these electrodes gains further relevance when considering that the current yield per unit mass of the anodic active phase catalyst (i.e., 1086 mA mg^{-1} at 2.0 V and 40 ºC) is the highest among equivalent values reported in literature. The possibilities and prospects of the use of bimetallic catalyst films prepared by MS-OAD for AEMWE are discussed.

Plasma assisted CO_2 dissociation in pure and gas mixture streams with a ferroelectric packed-bed reactor in ambient conditions

Navascues, P; Cotrino, J; González-Elipe, AR; Gomez-Ramírez, A
Chemical Engineering Journal, **430** (2022) 133066
Febrero, 2022 | **DOI:** 10.1016/j.cej.2021.133066



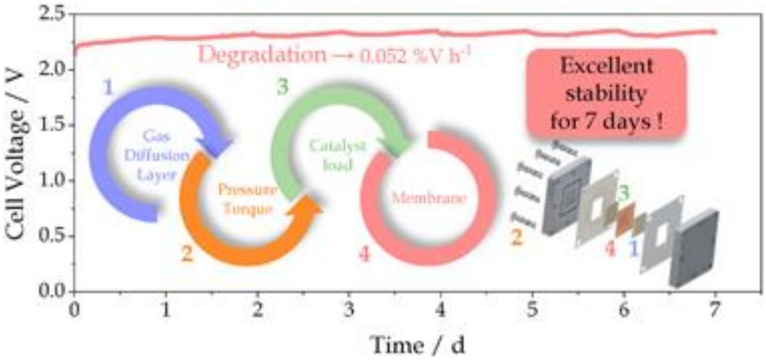
Carbon dioxide decomposition is a challenging target to combat climate change. Nonthermal plasmas are advantageous for this purpose because they operate at ambient conditions and can be easily scaled-up. In this study, we attempt the CO_2 splitting into CO and O_2 in a parallel plate packed-bed plasma reactor moderated with Lead Zirconate Titanate (PZT) as fermelectric component, achieving conversion rates and energy efficiencies higher than those obtained with $BaTiO_3$ in our experimental device. The analysis of the reaction mechanisms with optical emission spectroscopy under various operating conditions has shown a direct correlation between energy efficiency and intensity of CO* emission bands. These results and those obtained with a $LiNbO_3$ plate placed onto the active electrode suggest that high temperature electrons contribute to the splitting of CO_2 through an enhancement in the formation of CO_2^+ intermediate species. Results obtained for $CO_2 + O_2$ mixtures confirm this view and suggest that back recombination processes involving CO and O_2 may reduce the overall splitting efficiency. The study of mixtures of CO_2 and dry air has proved the capacity of fermelectric packed-bed reactors to efficiently decompose CO_2 with no formation of harmful N_xO_y subproducts in conditions close to those in real facilities. The found enhancement in energy efficiency with respect to that found for the pure gas decomposition supports that new reaction pathways involving nitrogen molecules are contributing to the dissociation reaction. We conclude that PZT moderated packed-bed plasma reactors is an optimum alternative for the decompositon of CO_2 in real gas flows and ambient conditions.

One-Dimensional Photonic Crystal for Surface Mode Polarization Control
Mogni, E; Pellegrini, G; Gil-Rostra, J; Yubero, F; Simone, G; Fossati, S; Dostalek, J; Vazquez, RM; Osellame, R; Celebrano, M; Finazzi, M; Biagioni, P
Advanced Optical Materials, **10** (2022) 2200759
Agosto, 2022 | **DOI:** 10.1002/adom.202200759

Bloch surface waves sustained by truncated 1D photonic crystals (1DPCs) are well known tools for surface-enhanced spectroscopy. They provide strongly confined fields with uniform distribution over a large surface area, a characteristic exploited in standard refractometric sensing. However, their application to polarization-sensitive investigations is not straightforward because the transverse electric (TE) and magnetic (TM) surface modes possess distinct dispersion relations, therefore their relative phase is not conserved along propagation and the polarization state of any wave obtained by combining these modes is ill-defined. In this work, a novel design of a 1DPC is realized in which the TE and TM modes exhibit the same phase velocity over a broadband spectral range and thus their dispersion relations overlap. The capability to simultaneously excite TE and TM modes with a well-defined phase relation allows the generation of surface waves with a controlled polarization state. This paves the way to polarization-resolved surface-enhanced analysis, including, for example, linear and circular dichroism spectroscopy of grafted molecular layers at the photonic crystal surface.

Optimization of anion exchange membrane water electrolyzers using ionomer-free electrodes
López-Fernandez, E; Gomez-Sacedon, C; Gil-Rostra, J; Espinos, JP; Brey, JJ; González-Elipe, AR; de Lucas-Consuegra, A.; Yubero, F
Renewable Energy, **197** (2022) 1183-1191
Septiembre, 2022 | **DOI:** 10.1016/j.renene.2022.08.013

This work is carried out in the context of the anion exchange membrane water electrolysis (AEMWE) and pursuits to determine the influence of different cell components on the global electrochemical performance. Ionomer-free electrodes consisting of anodic Ni-Fe and cathodic Ni electrocatalysts deposited by magnetron sputtering in an oblique angle deposition configuration were utilized for this study. In addition to the characteristics and equivalent thickness of the electrocatalysts, other factors affecting the efficiency that have been considered in this study encompass the type of gas diffusion layer (GDLs), including carbon paper and stainless-steel fiber paper supports, and several commercial anion exchange membranes. The electrocatalytic performances in both a threeelectrode and complete single cell AEMWE set-ups, together with the physico-chemical characterization of the electrodes before and after operation, have served to select the optimum



components for the utilized cell configuration. Thus, current densities of 670 mAcm^{-2}, at polarization voltage of 2.2 V, 1.0 M KOH electrolyte and 40 °C were obtained in a membrane electrode assembly. A seven days chronopotentiometry experiment at a fixed current of 400 mAcm^{-2} demonstrated a noticeable stability of this type of AEMWE cells incorporating ionomer-free electrodes.

Morphologically diverse $CaCO_3$ microparticles and their incorporation into recycled cellulose for circular economy

Guerra-Garces, J; García-Negrete, CA; Pastor-Sierra, K; Arteaga, GC; Barrera-Vargas, M; de Haro, MJ; Fernandez, A

Materials Today Sustainability, **19** (2022) 100166
Noviembre, 2022 | **DOI:** 10.1016/j.mtsust.2022.100166

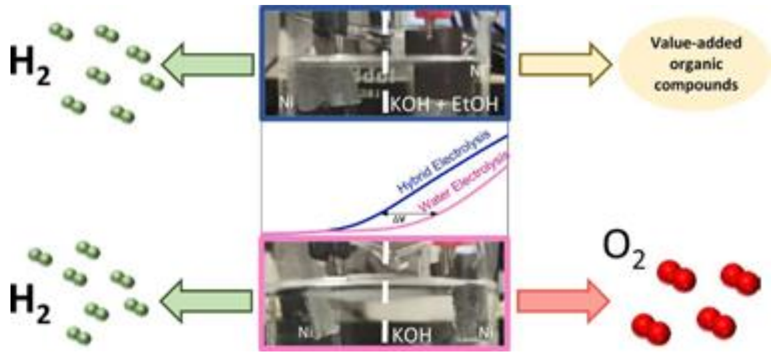
The main raw material for manufacture of paper is cellulose fibers that can be virgin or recycled. Globally, 70% of the Tetra Pak packages sold are not recycled and remain as unused wastes. Therefore, the development of alternatives to promote greater recycling and sustainable use of these packages is of great interest. In this study, the formation of precipitated calcium carbonates (PCC) in the presence of carboxymethyl cellulose (CMC) is studied at different temperatures, and the morphologically diverse particles obtained are explored as filler for composites based on cellulosic fibers recovered from Tetra Pak containers. It was found that the addition of filler does not lead to deterioration of either tensile strength or thermal and stability of the obtained composite samples. Results also suggest that the morphological diversity of the filler contributes to a more efficient filling of the interfibrillar spaces of cellulosic fibers and, in turn, to the fiber and filler compatibility.

Nanostructured nickel based electrocatalysts for hybrid ethanol-water anion exchange membrane electrolysis

López-Fernandez, E; Gomez-Sacedon, C; Gil-Rostra, J; Espinos, JP; González-Elipe, AR; Yubero, F

Journal of Environmental Chemical Engineering, **10** (2022) 107994
Junio, 2022 | **DOI:** 10.1016/j.jece.2022.107994

Ni and Ni-Fe nanostructured layers prepared by magnetron sputtering in an oblique angle deposition configuration (MS-OAD) have been used as anode and cathode catalysts for hybrid ethanol-water electrolysis in an anion exchange membrane (AEM) electrolyser. Physico-chemical and electrochemical characterization in a threeelectrode cell has been carried out to determine the optimal characteristics of the anodic films. Current densities up to 434 mAcm^{-2} at 2.0 V in a 1.5 M EtOH and 2.0 M KOH fuel solution were achieved with excellent operational stability for 3 days. These experiments show that the



oxygen evolution reaction taking place at the anode is completely replaced by the ethanol oxidation reaction under our explored reaction conditions. The obtained results evidence the interest of this kind of organic vs. pure water electrolysis to decrease the overall electrical energy consumption for the production of hydrogen.

Multiscale ultrafast laser texturing of marble for reduced surface wetting

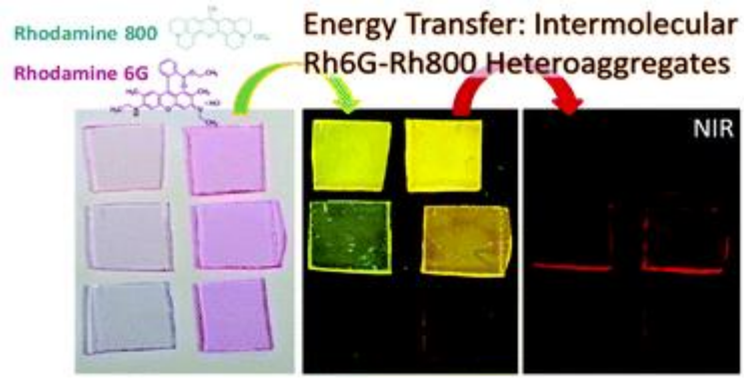
Ariza, R; Alvarez-Alegria, M; Costas, G; Tribaldo, L; González-Elipe, AR; Siegel, J; Solis, J
Applied Surface Science, **577** (2022) 152850
Marzo, 2022 | **DOI:** 10.1016/j.apsusc.2021.151850

The modification of the wetting properties of marble surfaces upon multi-scale texturing induced by ultrafast laser processing (340 fs pulse duration, 1030 nm wavelength) has been investigated with the aim of evaluating its potential for surface protection. The contact angle (CA) of a water drop placed on the surface was used to assess the wettability of the processed areas. Although the surfaces are initially hydrophilic upon laser treatment, after a few days they develop a strong hydrophobic behavior. Marble surfaces have been irradiated with different scan line separations to elucidate the relative roles of multi-scale roughness (nano-and micro-texture) and chemical changes at the surface. The time evolution of the contact angle has been then monitored up to 11 months after treatment. A short and a long-term evolution, associated to the combined effect of multi-scale roughness and the attachment of chemical species at the surface over the time, have been observed. XPS and ATR measurements are consistent with the progressive hydroxylation of the laser treated surfaces although the additional contribution of hydrocarbon adsorbates to the wettability evolution cannot be ruled-out. The robustness of the results has been tested by CA measurements after cleaning in different conditions with very positive results.

Rhodamine 6G and 800 intermolecular heteroaggregates embedded in PMMA for near-infrared wavelength shifting

Castillo-Seoane, J; González-García, L; Obrero-Pérez, JM; Aparicio, FJ; Borrás, A; González-Elipe, AR; Barranco, A; Sánchez-Valencia, JR
Journal of Materials Chemistry C, **10** (2022) 7119-7131
Marzo, 2022 | **DOI:** 10.1039/d1tc06167d

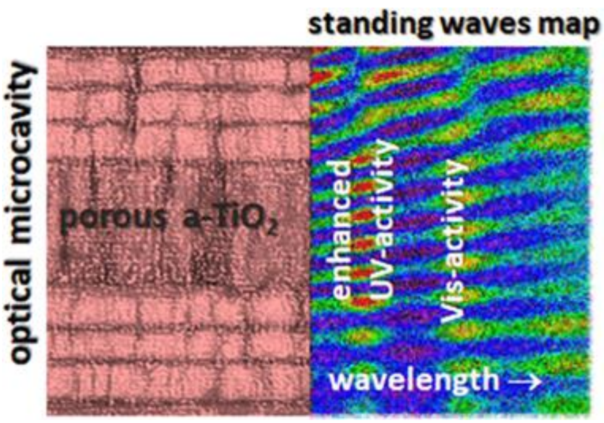
The opto-electronic properties of small-molecules and functional dyes usually differ when incorporated into solid matrices with respect to their isolated form due to an aggregation phenomenon that alters their optical and fluorescent properties. These spectroscopic modifications are studied in the framework of the exciton theory of aggregates, which has been extensively applied in the literature for the study of molecular aggregates of the same type of molecules (homoaggregation). Despite the demonstrated potential of the control of the heteroaggregation process (aggregation of different types of molecules), most of the reported works are devoted to intramolecular aggregates, complex molecules formed by several chromophores attached by organic linkers. The intramolecular aggregates are specifically designed to hold a certain molecular structure that, on the basis of the exciton theory,



modifies their optical and fluorescent properties with respect to the isolated chromophores that form the molecule. The present article describes in detail the incorporation of Rhodamine 6G (Rh6G) and 800 (Rh800) into polymeric matrices of poly-(methyl methacrylate), PMMA. The simultaneous incorporation of both dyes results in an enhanced fluorescent emission in the near-infrared (NIR), originating from the formation of ground-state Rh6G-Rh800 intermolecular heteroaggregates. The systematic control of the concentration of both rhodamines provides a model system for the elucidation of the heteroaggregate formation. The efficient energy transfer between Rh6G and Rh800 molecules can be used as wavelength shifters to convert effectively the light from visible to NIR, a very convenient wavelength range for many practical applications which make use of inexpensive commercial detectors and systems.

Titania Enhanced Photocatalysis and Dye Giant Absorption in Nanoporous 1D Bragg Microcavities

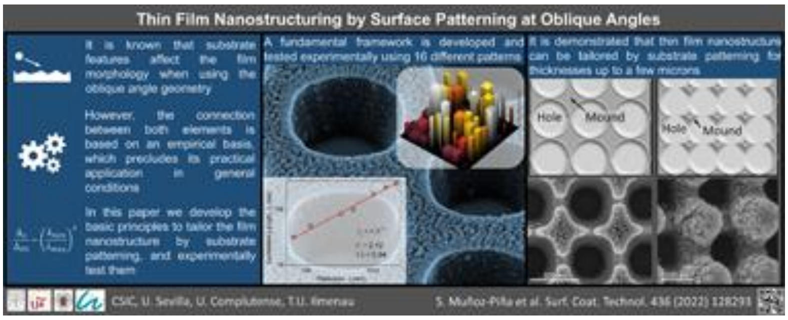
Rico, VJ; Turk, H; Yubero, F; González-Elipe, AR
ACS Applied Nano Materials, **5** (2022) 5487-5497
Junio, 2022 | **DOI:** 10.1021/acsanm.2c00477



Light trapping effects are known to boost the photocatalytic degradation of organic molecules in 3D photonic structures of anatase titania (a-TiO_2) with an inverse opal configuration. In the present work, we show that photocatalytic activity can also be enhanced in a-TiO_2 thin films if they are incorporated within a nanoporous 1D optical resonant microcavity. We have designed and manufactured multilayer systems that, presenting a high open porosity to enable a straightforward diffusion of photodegradable molecules, provide light confinement effects at wavelengths around the absorption edge of photoactive a-TiO_2. In brief, we have observed that a nanoporous 1D Bragg microcavity prepared by electron beam evaporation at oblique angles comprising a central defect layer of nanoporous a-TiO_2 boosts the photocatalytic degradation of nitrobenzene and methyl orange dye solutions. The multilayer structure of the microcavity was designed to ensure the appearance of optical resonances at the a-TiO_2 layer location and wavelengths around the absorption onset of this semiconductor. In this porous 1D Bragg microcavity, the diffusion constraints of molecules through the capping layers covering the a-TiO_2 are effectively compensated by an increase in the photocatalytic activity due to the light confinement phenomena. We also report that the absorption coefficient of methyl orange dye solution infiltrated within the pore structure of the microcavity is exalted at the wavelengths of the corresponding optical resonances. This effect gives rise to a small but non-negligible visible light photodegradation of dye molecules. The possibilities of tailoring the design of 1D photonic systems to boost the photocatalytic activity of a-TiO_2 are discussed.

Thin film nanostructuring at oblique angles by substrate patterning

Muñoz-Pina, S; Alcaide, AM; Limones-Ahijon, B; Oliva-Ramírez, M; Rico, V; Alcalá, G; González, MU; García-Martín, JM; Alvarez, R; Wang, D; Schaaf, P; González-Elipe, AR; Palmero, A
Surface & Coatings Technology, **436** (2022) 128293
Abril, 2022 | **DOI:** 10.1016/j.surfcoat.2022.128293



It is demonstrated that, besides classical nanocolumnar arrays, the oblique angle geometry induces the growth of singular structures in the nanoscale when using wisely designed patterned substrates. Well-ordered array of crosses, cylindrical nanorods or hole structures arranged in square or hexagonal regular geometries are reported as examples, among others. The fundamental framework connecting substrate topography and film growth at oblique angles is presented, allowing the use of substrate patterning as a feasible thin film nanostructuring technique. A systematic analysis of the growth of TiO2 thin films on 4 different lithographic patterned substrates in 4 different scale lengths is also presented. A first conclusion is the existence of a height-based selective growth in the initial stages of the deposition, by which the film preferentially develops on top of the tallest substrate features. This behavior is maintained until the film reaches a critical thickness, the so-called Oblivion Thickness, above which the film topography becomes gradually independent of the substrate features. A general formula relating the spatial features of the pattern, the coarsening exponent and the Oblivion Thickness has been deduced.

High-Quality SiO_2/O-Terminated Diamond Interface: Band-Gap, Band-Offset and Interfacial Chemistry

Canas, J; Reyes, DF; Zakhtser, A; Dussarrat, C; Teramoto, T; Gutierrez, M; Gheeraert, E
Nanomaterials, **12** (2022) 4125
Diciembre, 2022 | **DOI:** 10.3390/nano12234125

Silicon oxide atomic layer deposition synthesis development over the last few years has open the route to its use as a dielectric within diamond electronics. Its great band-gap makes it a promising material for the fabrication of diamond-metal-oxide field effects transistor gates. Having a sufficiently high barrier both for holes and electrons is mandatory to work in accumulation and inversion regimes without leakage currents, and no other oxide can fulfil this requisite due to the wide diamond band-gap. In this work, the heterojunction of atomic-layer-deposited silicon oxide and (100)-oriented p-type oxygen-terminated diamond is studied using scanning transmission electron microscopy in its energy loss spectroscopy mode and X-ray photoelectron spectroscopy. The amorphous phase of silicon oxide was successfully synthesized with a homogeneous band-gap of 9.4 eV. The interface between the oxide and diamond consisted mainly of single- and double-carbon-oxygen bonds with a low density of interface states and a straddling band setting with a 2.0 eV valence band-offset and 1.9 eV conduction band-offset.

Multiscale Kinetic Monte Carlo Simulation of Self-Organized Growth of GaN/AlN Quantum Dots

Budagosky, JA; García-Cristobal, A
Nanomaterials, **12** (2022) 3052
Septiembre, 2022 | **DOI:** 10.3390/nano12173052

A three-dimensional kinetic Monte Carlo methodology is developed to study the strained epitaxial growth of wurtzite GaN/AlN quantum dots. It describes the kinetics of effective GaN adatoms on an hexagonal lattice. The elastic strain energy is evaluated by a purposely devised procedure: first, we take advantage of the fact that the deformation in a lattice-mismatched heterostructure is equivalent to that obtained by assuming that one of the regions of the system is subjected to a properly chosen uniform stress (Eshelby inclusion concept), and then the strain is obtained by applying the Green's function method. The standard Monte Carlo method has been modified to implement a multiscale algorithm that allows the isolated adatoms to perform long diffusion jumps. With these state-of-the art modifications, it is possible to perform efficiently simulations over large areas and long elapsed times. We have taylored the model to the conditions of molecular beam epitaxy under N-rich conditions. The corresponding simulations reproduce the different stages of the Stranski-Krastanov transition, showing quantitative agreement with the experimental findings concerning the critical deposition, and island size and density. The influence of growth parameters, such as the relative fluxes of Ga and N and the substrate temperature, is also studied and found to be consistent with the experimental observations. In addition, the growth of stacked layers of quantum dots is also simulated and the conditions for their vertical alignment and homogenization are illustrated. In summary, the developed methodology allows one to reproduce the main features of the self-organized quantum dot growth and to understand the microscopic mechanisms at play.

Analysis of the effect of cationic ratio Bi^{3+}/Fe^{3+} on the magnetic and multiferroic properties of $BiFeO_3$ nanoparticles synthesized using a sonochemical-assisted method

Palomino-Resendiz, RL; Bolarin-Miro, AM; Pedro-García, F; Sánchez-De Jesus, F; Espinos-Manzorro, JP; Cortes-Escobes-Escobedo, CA
Ceramics International, **48** (2022) 14746-14753
Mayo, 2022 | **DOI:** 10.1016/j.ceramint.2022.02.011

This study examined the effects of the cationic ratio of Bi^{3+}/Fe^{3+} via X-ray photoelectron spectroscopy (XPS) on the magnetic and multiferroic properties of $BiFeO_3$ nanoparticles synthesized using a sonochemical-assisted method. X-ray diffraction revealed the successful synthesis of single-phase $BiFeO_3$ powder after annealing the sonicated material at 723 K. The powder was composed of agglomerates of rounded particles with a mean particle size of 35 nm. XPS was performed to determine the Bi^{3+}/Fe^{3+} ratio as a function of the heat treatment process and its relationship with secondary phases, which can modulate the magnetic properties of the nano powders. The cationic ratio obtained by XPS confirmed that the powders obtained at 623 and 923 K have excess Bi^{3+} and Fe^{3+}, respectively, which induces the formation of $Bi_{24}Fe_2O_{39}$ and $Bi_2Fe_4O_9$ as the majority phases. Powder annealing at 723 K revealed a ferromagnetic order with specific magnetization of 1.8 Am^2/kg. This ferromagnetic behavior

was preserved after applying spark plasma sintering (SPS) at 923 K. By contrast, conventional sintering at 1023 K promotes antiferromagnetic order. In addition, the dielectric properties of the ceramic material of the sintered powders showed a behavior related to a typical ferroelectric material.

Pd supported on defective TiO_2 polymorphic mixtures: Effect of metal-support interactions upon glycerol selective oxidation

Rinaudo, MG; Beltran, AM; Fernandez, A; Cadus, LE; Morales, MR
Results in Engineering, **16** (2022) 100737
Diciembre, 2022 | **DOI:** 10.1016/j.rineng.2022.100737

Palladium catalysts supported on defective mixes of anatase, TiO_2 (II) and rutile crystalline phases, previously obtained by high-energy ball milling, were synthesized and tested for glycerol selective oxidation. A deep characterization of these unusual materials was carried out to elucidate catalytic and physicochemical features. Electron density transfer from support to metal or vice versa, depending on the polymorphs present, could not only alter palladium particle sizes and its surface oxidation state but also reducibility and oxygen mobility of catalysts. Furthermore, acid-base properties achieved also influenced catalytic activity under mild conditions of liquid-phase glycerol oxidation. A conversion of 94% and a selectivity to glyceric and lactic acids of 48% and 22% respectively were obtained for the Pd catalyst supported on mechanochemically activated anatase. The presence of several polymorphs in a metal oxide support could therefore benefit or handicap catalytic cycle for a particular reaction. Metal-support interactions play a key role in heterogenous catalysts and thus the rational design of supports comes on the scene.

Design and Characterization of ITO-Covered Resonant Nanopillars for Dual Optical and Electrochemical Sensing

Tramarin, L; Casquel, R; Gil-Rostra, J; González-Martínez, MA; Herrero-Labrador, R; Murillo, AMM; Laguna, MF; Banuls, MJ; González-Elipe, AR; Holgado, M
Chemosensors, **10** (2022) 393
Octubre, 2022 | **DOI:** 10.3390/chemosensors10100393

In this work we present a dual optical and electrochemical sensor based on SiO_2/Si_3N_4 resonant nanopillars covered with an indium tin oxide (ITO) thin film. A 25-30 nm thick ITO layer deposited by magnetron sputtering acts as an electrode when incorporated onto the nanostructured array, without compromising the optical sensing capability of the nanopillars. Bulk sensing performances before and after ITO deposition have been measured and compared in accordance with theoretical calculations. The electrochemical activity has been determined by the ferri/ferrocyanide redox reaction, showing a remarkably higher activity than that of flat thin films of similar ITO nominal thickness, and proving that the nanopillar system covered by ITO presents electrical continuity. A label-free optical biological detection has been performed, where the presence of amyloid-beta has been detected through an immunoassay enhanced with gold nanoparticles. Again, the experimental results have been corroborated by theoretical simulations. We have demonstrated that ITO can be a beneficial component for resonant nanopillars sensors by adding potential electrochemical sensing capabilities, without significantly altering their optical properties. We foresee that resonant nanopillars coated with a continuous ITO film could be used for simultaneous optical and electrochemical biosensing, improving the robustness of biomolecular identification.

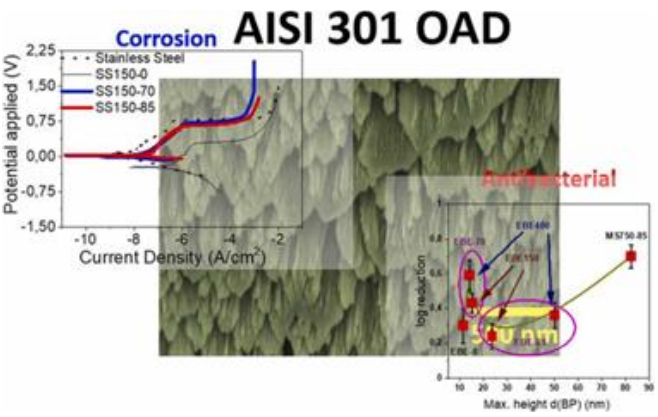
Mesoporous Silica-Based Nanoparticles as Non-Viral Gene Delivery Platform for Treating Retinitis Pigmentosa

Valdes-Sánchez, L; Borrego-González, S; Montero-Sánchez, A; Massalini, S; De la Cerda, B; Díaz-Cuenca, A; Díaz-Corrales, FJ
Journal of Clinical Medicine, **11** (2022) 2170
Abril, 2022 | **DOI:** 10.3390/jcm11082170

Background: Gene therapy is a therapeutic possibility for retinitis pigmentosa (RP), in which therapeutic transgenes are currently delivered to the retina by adeno-associated viral vectors (AAVs). Although their safety and efficacy have been demonstrated in both clinical and preclinical settings, AAVs present some technical handicaps, such as limited cargo capacity and possible immunogenicity in repetitive doses. The development of alternative, non-viral delivery platforms like nanoparticles is of great interest to extend the application of gene therapy for RP. Methods: Amino-functionalized mesoporous silica-based nanoparticles (N-MSiNPs) were synthesized, physico-chemically characterized, and evaluated as gene delivery systems for human cells in vitro and for retinal cells in vivo. Transgene expression was evaluated by WB and immunofluorescence. The safety evaluation of mice subjected to subretinal injection was assessed by ophthalmological tests (electroretinogram, funduscopy, tomography, and optokinetic test). Results: N-MSiNPs delivered transgenes to human cells in vitro and to retinal cells in vivo. No adverse effects were detected for the integrity of the retinal tissue or the visual function of treated eyes. N-MSiNPs were able to deliver a therapeutic transgene candidate for RP, PRPF31, both in vitro and in vivo. Conclusions: N-MSiNPs are safe for retinal delivery and thus a potential alternative to viral vectors.

Electron beam evaporated vs. magnetron sputtered nanocolumnar porous stainless steel: Corrosion resistance, wetting behavior and anti-bacterial activity

Bobaru, S; Rico-Gavira, V; García-Valenzuela, A; López-Santos, C; González-Elipe, AR
Materials Today Communications, **31** (2022) 103266
Junio, 2022 | **DOI:** 10.1016/j.mtcomm.2022.103266



Stainless steel (SS), widely used because of its outstanding corrosion protection properties, does not possess any particular anti-stain or anti-bacterial activity as required for household and sanitary applications. This work reports the fabrication of SS thin films that, keeping a similar corrosion resistance than the bulk material, presents hydrophobicity and anti-bacterial activity. These thin films are prepared at ambient temperature by physical vapor deposition (PVD), either electron beam evaporation (EBE) or magnetron sputtering (MS), at oblique angles (OAD). According to their scanning electron microcopy and atomic force microscopy analysis, the microstructure of the OAD-SS thin films consisted of tilted and separated nanocolumns defining a surface topology that, characterized by a high percentage of void space, varied with the deposition conditions and procedure, either EBE or MS. It has been shown that particularly the nanocolumnar MS-OAD thin films preserved and even improved the high corrosion resistance of compact SS, as determined by electrochemical analysis. Besides, all OAD-SS thin films depict hydrophobicity and a high antibacterial activity. These features, particularly remarkable for the

MS-OAD thin films, have been related with their tip-like termination at the surface and the existence of large void spaces separating the nanocolumns. This topology appears to affect negatively the bacteria's deployment onto the surface and therefore the survival rate. Differences in the corrosion and antibacterial performance between EBE and MS-OAD thin films have been related with the specificities of these two PVD methods of thin film preparation. A relatively high abrasion resistance, as determined by abrasion tests, supports the use of MS-OAD thin films for the protection of commodity materials.

Influence of the carbon incorporation on the mechanical properties of TiB_2 thin films prepared by HiPIMS

Sala, N; Abad, MD; Sánchez-López, JC; Crugeira, F; Ramos-Masana, A; Colominas, C
International Journal of Refractory Metals & Hard Materials, **107** (2022) 105884
Septiembre, 2022 | **DOI:** 10.1016/j.ijrmhm.2022.105884

Nanostructured TiB_2 and TiBC thin films with carbon contents up to 11 at. % were prepared by physical vapor deposition using high power impulse magnetron sputtering (HiPIMS) technology. The influence of carbon incorporation during the deposition of TiB_2 coatings was investigated on the chemical composition, microstructure and mechanical properties by means of scanning electron microscopy, atomic force microscopy, x-ray photoelectron spectroscopy (XPS), x-ray diffraction (XRD), nanoindentation, scratch test, calotest and adhesion Daimler-Benz test. The results indicated that small additions of carbon up to 3 at. % improved the mechanical behavior and increased the adhesion of the TiB_2 thin films. Hardnesses up to 37 GPa were reached and the adhesion of the coating to AISI D2 steel substrates increased from 11 to 18 N. XRD and XPS results showed that the carbon atoms are either occupying interstitial sites within the hexagonal structure of the TiB_2 or forming bonds with titanium and boron atoms. The preferred orientation of the films determined by XRD also changed with the increasing carbon content in the (001) crystalline plane.

Coarse-grained approach to amorphous and anisotropic materials in kinetic Monte Carlo thin-film growth simulations: A case study of TiO_2 and ZnO by plasma-enhanced chemical vapor deposition

Budagosky, J; García-Casas, X; Sánchez-Valencia, JR; Barranco, A; Borrás, A
Plasma Processes and Polymers, **19** (2022) e2100179
Enero, 2022 | **DOI:** 10.1002/ppap.202100179

The growth of TiO_2 and ZnO thin films is studied by means of coarse-grained kinetic Monte Carlo simulations under conditions typically encountered in plasma-enhanced chemical vapor deposition experiments. The basis of our approach is known to work well to simulate the growth of amorphous materials using cubic grids and is extended here to reproduce not only the morphological characteristics and scaling properties of amorphous TiO_2 but also the growth of polycrystalline ZnO with a good approximation, including the evolution of the film texture during growth and its dependence on experimental conditions. The results of the simulations have been compared with available experimental data obtained by X-ray diffraction, analysis of the texture coefficients, atomic force microscopy, and scanning electron microscopy.

Comparative analysis of the germination of barley seeds subjected to drying, hydrogen peroxide, or oxidative air plasma treatments

Perea-Brenes, A; Gomez-Ramírez, A; López-Santos, C; Oliva-Ramírez, M; Molina, R; Cotrino, J; García, JL; Cantos, M; González-Elipe, ARA

Plasma Processes and Polymers, **19** (2022) e2200035
Junio, 2022 | **DOI:** 10.1002/ppap.202200035

Acceleration in germination time by 12-24 h for barley seeds treated with atmospheric air plasmas may have a significant economic impact on malting processes. In this study, the increase in germination rate and decrease in contamination level upon plasma treatment could not be directly correlated with any significant increase in the water uptake capacity, except for seeds exposed to mild drying treatment. A variety of germination essays have been carried out with seeds impregnated with an abscisic acid solution, a retarding factor of germination, treated with a peroxide solution, and/or subjected to the plasma and drying treatments. Results suggest that plasma and hydrogen peroxide treatments induce the formation of reactive oxygen and nitrogen species that affects the abscisic acid factor and accelerate the germination rate.

Compositional gradients at the nanoscale in substoichiometric thin films deposited by magnetron sputtering at oblique angles: A case study on SiOx thin films

García-Valenzuela, A; Alcaide, AM; Rico, V; Ferrer, FJ; Alcalá, G; Rojas, TC; Alvarez, R; González-Elipe, AR; Palmero, A

Plasma Processes and Polymers, **19** (2022) e2100116
Enero, 2022 | **DOI:** 10.1002/ppap.202100116

We demonstrate the existence of stoichiometric variations at the nanoscale when growing nanocolumnar SiOx thin films by reactive magnetron sputtering deposition at oblique angles. Results show stoichiometric variations in the range $0.3 < x < 1.3$ when growing a $SiO_{0.5}$ thin film. This agrees with results from a numerical growth model that obtains a shift of the stoichiometry in all nanocolumns from lower values at the side facing the Si target to higher values at the opposite side. The different momentum distribution of the gaseous reactive and sputtered species results in preferential incorporation of the latter at a particular side of the nanocolumns. The general occurrence of this mechanism during the reactive magnetron sputtering deposition of substoichiometric thin films at oblique angles is discussed.

Influence of Femtosecond Laser Modification on Biomechanical and Biofunctional Behavior of Porous Titanium Substrates

Beltran, AM; Giner, M; Rodríguez, A; Trueba, P; Rodríguez-Albelo, LM; Vázquez-Gámez, MA; Godinho, V; Alcudia, A; Amado, JM; López-Santos, C; Yadir, T

Materials, **15** (2022) 2969
Mayo, 2022 | **DOI:** 10.3390/ma15092969

Bone resorption and inadequate osseointegration are considered the main problems of titanium implants. In this investigation, the texture and surface roughness of porous titanium samples obtained by the space holder technique were modified with a femtosecond Yb-doped fiber laser. Different percentages of porosity (30, 40, 50, and 60 vol.%) and particle range size (100-200 and 355-500 μm) were compared with fully-dense samples obtained by conventional powder metallurgy. After

femtosecond laser treatment the formation of a rough surface with micro-columns and micro-holes occurred for all the studied substrates. The surface was covered by ripples over the micro-metric structures. This work evaluates both the influence of the macro-pores inherent to the spacer particles, as well as the micro-columns and the texture generated with the laser, on the wettability of the surface, the cell behavior (adhesion and proliferation of osteoblasts), micro-hardness (instrumented micro-indentation test, P-h curves) and scratch resistance. The titanium sample with 30 vol.% and a pore range size of 100-200 μm was the best candidate for the replacement of small damaged cortical bone tissues, based on its better biomechanical (stiffness and yield strength) and biofunctional balance (bone in-growth and in vitro osseointegration).

Role of Surface Topography in the Superhydrophobic Effect-Experimental and Numerical Studies

Ibrahim, SH; Wejrzanowski, T; Przybyszewski, B; Kozera, R; García-Casas, X; Barranco, A
Materials, **15** (2022) 3112
Mayo, 2022 | **DOI:** 10.3390/ma15093112

Within these studies, the effect of surface topography for hydrophobic coatings was studied both numerically and experimentally. Chemically modified polyurethane coating was patterned by application of a laser beam. A set of patterns with variously distant linear peaks and grooves was obtained. The cross section of the pattern showed that the edges of the peaks and grooves were not sharp, instead forming a rounded, rectangle-like shape. For such surfaces, experimental studies were performed, and in particular the static contact angle (SCA), contact angle hysteresis (CAH), and roll-off angle (ROA) were measured. Profilometry was used to create a numerical representation of the surface. Finite volume method was then applied to simulate the behavior of the water droplets. The model developed herewith enabled us to reproduce the experimental results with good accuracy. Based on the verified model, the calculation was extended to study the behavior of the water droplet on the simulated patterns, both spiked and rectangular. These two cases, despite a similar SCA of the water droplet, have shown extremely different ROA. Thus, more detailed studies were dedicated to other geometrical features of such topography, such as the size and distance of the surface elements. Based on the results obtained herewith, the future design of superhydrophobic and/or icephobic topography is discussed.

Sol-Gel Synthesis of Endodontic Cements: Post-Synthesis Treatment to Improve Setting Performance and Bioactivity

Song, X; Diaz-Cuenca, A
Materials, **15** (2022) 6051
Septiembre, 2022 | **DOI:** 10.3390/ma15176051

The sol-gel process is a wet chemical technique that allows very fine control of the composition, microstructure, and final textural properties of materials, and has great potential for the synthesis of endodontic cements with improved properties. In this work, the influence of different sol-gel synthesis variables on the preparation of endodontic cement based on calcium silicate with Ca/Si stoichiometry equal to 3 was studied. Starting from the most optimal hydraulic composition selected, a novel second post-synthesis treatment using ethanol was essayed. The effects of the tested variables were analyzed by X-ray diffraction, infrared spectroscopy, scanning electron microscopy, nitrogen physisorption, and Gillmore needles to determine the setting time and simulated body fluid (SBF) immersion to measure the bioactive response in vitro. The results indicated that the sol-gel technique is effective in obtaining bioactive endodontic cements (BECs) with high content of the hydraulic compound tricalcium silicate (C3S) in its triclinic polymorph. The implementation of a novel post-synthesis treatment at room temperature using ethanol allows obtaining a final BEC product with a finer particle size and a higher $CaCO_3$ content, which results in an improved material in terms of setting time and bioactive response.

QUEELS: Software to calculate the energy loss processes in TEELS, REELS, XPS and AES including effects of the core hole
Tougaard, S; Pauly, N; Yubero, F
Surface and Interface Analysis, **54** (2022) 820-833
Abril, 2022 | **DOI:** 10.1002/sia.7095

We present the user-friendly and freely available software package QUEELS (QUantitative analysis of Electron Energy Losses at Surfaces) that allows to calculate effective inelastic scattering cross sections within the dielectric response description, for swift electrons travelling nearby surfaces in several environments. We briefly describe the underlying theoretical models and illustrate its use to evaluate the distribution of energy losses taking place in electron spectroscopies like transmission electron energy loss spectroscopy (TEELS), X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES) and reflection electron energy loss spectroscopy (REELS), which are widely used for material analysis. This includes the intrinsic excitations due to the core hole in XPS and AES.

LIBROS Y OTRAS PUBLICACIONES / BOOKS AND OTHER PUBLICATIONS

Funcionalización superficial mediante recubrimientos PVD (deposición física en fase vapor) de materiales fabricados aditivamente
R. Escobar-Galindo, J. Hernández-Saz, B. Palacios-I, T.C. Rojas, J.C. Sánchez-López, S.I. Molina
Libros de Actas del Congreso Nacional de Materiales (CNMAT2022), pag. 19
ISBN: 978-84-09-38118-0

Diseño y comportamiento de recubrimientos solares selectivos basados en Cr(Al)N
J.C. Sánchez-López, T.C. Rojas, A. Caro, R. Escobar-Galindo
Libros de Actas del Congreso Nacional de Materiales (CNMAT2022), pag. 34
ISBN: 978-84-09-38118-0

Diseño de recubrimientos solares selectivos para alta temperatura basados en Cr(Al)N: Microestructura y propiedades ópticas de capas de CrN_y and $Cr_{1-x}Al_xN_y$
T.C. Rojas, A. Caro, G. Lozano, J.C. Sánchez-López
Libros de Actas del Congreso Nacional de Materiales (CNMAT2022), pag. 45
ISBN: 978-84-09-38118-0

Crecimiento de aleaciones de TiAlV y TiNbZrTa sobre probetas de titanio poroso magnetron sputtering
J.C. Sánchez-López, M. Rodríguez-Albelo; M. Sánchez-Pérez; V. Godinho; C. López-Santos; Y. Torres
Libros de Actas del Congreso Nacional de Materiales (CNMAT2022), pag. 51
ISBN: 978-84-09-38118-0

Desarrollo de sistemas tándem basados en multicapas CrAlN/Al2O3 usando HiPIMS como absorbedores solares selectivos
M. Sánchez-Pérez, T.C. Rojas, F.J. Ferrer, G. Lozano, A. Morales, S. Mato, R. Escobar-Galindo, J.C. Sánchez-López
Libros de Actas del Congreso Nacional de Materiales (CNMAT2022), pag. 638
ISBN: 978-84-09-38118-0

Low friction/wear properties of snake skins: a case study for mimicking nature tribological behavior
J.C. Sánchez-López, C.F. Clemens, S.N. Gord
Book of Abstracts Ibertrib2022, pag. 61-62
ISBN: 978-989-53890-4-9

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

11th International Conference on Plasma Nanoscience | IPlasmaNano XI
12 septiembre [Sevilla, España]

Ana Isabel Borrás (Chair)

European Materials Research Society | EMRS Fall Meeting 2022
19 – 22 septiembre [Varsovia, Polonia]

Ana Isabel Borrás (Participación en la organización del simposium “Materials, components and characterization of energy harvesters for self-powered electronics”

COMUNICACIONES / COMMUNICATIONS

16th Annual Meeting RSC Biomaterials Chemistry Group
10 – 12 enero [Online, Reino Unido]

Comunicación Oral: **Metallic phytate derivatives for biomedical applications. Structural characterization and biological activity.** G. Asensio; A.M. Hernández-Arriaga; A.M. Prieto; A.R. González-Elipe; L. Rojo; B. Vázquez-Lasa

The 3rd International Conference on Nanomaterials Applied to Life Sciences | NALS 2022
27 – 29 abril [Santander, España]

Comunicación Oral: **Nanocolumnar films: sustainable manufacturing and applications in biomedicine.** M.U. González; R. Álvarez; D. Medina-Cruz; P. Díaz-Núñez; S. Mobini; I. Izquierdo-Barba; D. Arcos; I. Fernández-Martínez; O. Peña-Rodríguez; A. Palmero; J. M. García-Martín

Surfaces, Interfaces and Coatings Technologies International conference | SICT2022
27 – 29 abril [Barcelona, España]

Conferencia Invitada: **Optical design, microstructural characterization and high-temperature in-air stability study of solar selective coatings based on aluminium-(titanium, chromium) oxynitride multilayers.** R. Escobar Galindo; I. Heras; E. Guillén; F. Munnik; I. Azkona; A. Caro; T.C. Rojas; J.C. Sánchez-López; M. Krause

14Th International Conference on Hybrid and Organic Photovoltaics HOPV22
23 – 25 mayo [Valencia, España]

Comunicación Oral: **Two Step Glancing Angle Deposition of Supported Vertically Aligned Organometallic Halide Perovskite Nanostructures.** J. Castillo-Seoane; L. Contreras-Bernal; J.M. Obrero-Pérez; X. García-Casas; F.J. Aparicio; M.C: López-Santos; T. C. Rojas; J. A. Anta; A. Borrás; A. Barranco; J.R. Sánchez-Valencia

Comunicación Oral: **Organic plasma polymer for improving the stability of perovskite solar cells.** J. Obrero-Pérez; L. Contreras-Bernal; F. Nuñez-Galvez; J. Castillo-Seoane; K. Valadez-Villobos; F.J. Aparicio; J.A. Anta; A. Borrás; J. Sánchez-Valencia; A. Barranco

European Conference on Applications of Surface and Interface Analysis | ECASIA22
29 mayo – 3 junio [Limerick, Irlanda]

Comunicación Oral: **Enhanced photocatalysis and dye giant absorption in Bragg microcavities.** F. Yubero; A.R. González-Elipe; V.J. Rico

European Materials Research Society | EMRS Spring Meeting 2022
30 mayo – 3 junio [Virtual Conferencia]

Conferencia Invitada: **3D Nanoarchitectures as building blocks for single and hybrid energy harvesters,** X. García-Casas; J. Castillo-Seoane; F.J. Aparicio; A. Ghaffarinejad; L. Contreras-Bernal; J. Budagoski; M.C: López-Santos; A. Barranco; J.R. Sánchez-Valencia; A. Borrás

Conferencia Invitada: **Coarse-grained approach in growth simulations of metal oxides and polymers on planar and nanostructured substrates.** J. Budagosky, X. García-Casas, J.R. Sánchez-Valencia, A. Barranco, A. Borrás

Women in Renewable Energy | WiRE 2022
3 junio [Online, Estrasburgo, Francia]

Conferencia Invitada: **3D Nanoarchitectures as building blocks for single and hybrid energy harvesters .** A. Borrás

16th International Conference on Nanostructured Materials | NANO2022
6 – 10 junio [Sevilla, España]

Comunicación Oral: **Enhanced photocatalysis and dye giant absorption in Bragg Microcavities.** F. Yubero; A.R. González-Elipe; V.J. Rico

Comunicación Oral: **Magnetron sputtering as an efficient method for electrodes development in AEMWE cell.** A. De Lucas Cansuegra; E. López Fernández; C. Gómez-Sacedón; J. Gil-Rostra; J.P. Espinós; A.R. González-Elipe; F. Yubero

Comunicación Oral: **Towards superchiral surface waves in a microfluidic chip sensor.** R. Martínez-Vázquez; E. Mogni; G. Pellegrini; S. Fossati; J. Dostalek; J. Gil-Rostra; F. Yubero; G. Simone; M. Celebrano; M. Finazzi; R. Osellame; P. Biagioni

Comunicación Oral: **Organometal halide perovskite nanowalls with high anisotropy grown by Glancing Angle Deposition.** J. Castillo-Seoane; L. Contreras-Bernal; J.M. Obrero-Pérez; X. García-Casas; F.J. Aparicio; M.C. López-Santos; T.C.Rojas; J.A. Borrás; A. Barranco; J.R. Sánchez Valencia

Comunicación Oral: **Plasma processing of metal phthalocyanines and porphyrins for the development of supported porous nanostructures.** J.M. Obrero; A.N. Filippin; M. Alcaire;J.R. Sánchez Valencia; Matei; F.J. Aparicio; M. Macias Montero; T.C. Rojas; Saghi; A. Barranco; A. Borrás

Comunicación Oral: **Paper-based sensor and piezoelectric nanogenerators developed by plasma assisted deposition.** X. García-Casas; F.J. Aparicio; A. Ghaffarinejad; L. Contreras-Bernal; J.R. Sánchez-Valencia; A. Barranco; A. Borrás, A.

Comunicación Oral: **Ultrathin plasma polymer passivation of perovskite solar cells for improved stability and reproducibility.** L. Contreras-Bernal; J. Obrero-Pérez; F. Nuñez-Galvez; J. Castillo-Seoane; K. Valez-Villalobos; F.J. Aparicio; J.A. Anta; A. Borrás; J.R. Sánchez-Valencia; A. Barranco

Comunicación Oral: **From tunable wetting and liquid filtration to self cleaning and anti icing properties of TiO_2 3D nanomembranes fabricated by plasma assisted technology.** L. Montes, J. Román, X. García Casas, J. Castillo Seoane, J. Mora, P. García, F. Carreño, V.J. Rico, J. Sánchez Valencia, A. Barranco, C. López Santos

Comunicación Oral: **Effect of charged and functionalized surfaces in enhancing the output power of drop energy harvesters.** A. Ghaffarinejad, X. García Casas, F. Núñez, C.L. Santos, J.R.S. Valencia, A. Barranco, A. Borrás

Comunicación Oral: **Coarse-grained approach in kinetic Monte Carlo growth simulations of metal oxides and polymers on planar and nanostructured substrates.** J. Budagosky, X. García-Casas, J.R. Sánchez-Valencia, A. Barranco, A. Borrás

Comunicación Oral: **Implementation of nanostructured electrodes in dye – sensitized solars cells working at indoor illumination.** J. Castillo-Seoane, L. Contreras-Bernal, J. Gil-Rostra, J.A. Antab, A. Barranco, J.R. Sánchez-Valencia, A. Borrás

Comunicación Oral: **Photoelectrochemical water splitting by ITO/WO_3/$BiVO_4$ hollow multichell nanotubes fabricated by a soft-template approach.** J. Gil, J. Castillo-Seoane, Qian Luo, A. Jorge Sobrido, A. Borrás, A. R. González-Elipe

Póster: **Droplet-based energy harvesters developed by laser micro-texturing and plasma assisted deposition.** X. García-Casas; A. Salmoral-Reina; J. Castillo-Seoane; M.C. López-Santos; A. Ghaffarinejad; F.J. Aparicio; L. Contreras-Bernal; J. Gil-Rostra; J.R. Sánchez-Valencia; A. Barranco; A. Borrás

6th International Conference on Nanogenerators and Piezotronics | NGPT2022
20 – 23 junio [Online]

Comunicación Oral: **Porous ZnO thin films on paper substrates for the development of piezoelectric nanogenerators and self-powered sensors.** X. García-Casas; F.J. Aparicio; J. Budagosky; A. Ghafarinejad; J.R. Sánchez-Valencia; A. Barranco; A. Borrás

Comunicación Oral: **Plasma engineering of microstructured piezo – triboelectric hybrid nanogenerators for wide bandwidth vibration energy harvesting.** X. García-Casas; A. Ghafarinejad; F.J. Aparicio; J. Castillo-Seoane; M.C. López-Santos; J.P. Espinos; J. Cotrino; J.R. Sánchez-Valencia; A. Barranco; A: Borrás

Symposium of Nanoscience and Nanomaterials 2022
31 agosto – 2 septiembre [Ensenada B.C., México]

Conferencia Invitada: **Applied thin film growth technology @ NoSP.** F. Yubero

11th International Conference on Plasma Nanoscience | IPlasmaNano XI
12 septiembre [Sevilla, España]

Conferencia Invitada: **Plasma Polymers in Perovskite Solar Cells.** A. Barranco; A. Borrás; F.J. Aparicio; J.R. Sánchez-Valencia; L. Contreras; J. Castillo; J.M. Obrero

Conferencia Invitada: **Metal and metal oxide porous thin films and nanostructures from metalorganic solid precursors.** J.R. Sánchez Valencia; J.M. Obrero; F.J. Aparicio; A. Borrás; A. Barranco

Conferencia Invitada: **Plasma nanofabrication of hybrid piezo/triboelectric nanogenerators.** X. García-Casas; F.J. Aparicio; A. Ghaffarinejad; J. Castillo-Seoane; M.C. López-Santos; J.P. Espinós, J.Cotrino; J.R. Sánchez-Valencia; A. Barranco; A. Borrás

Conferencia Invitada: **Plasmas and Acoustic Waves Come Together for the 2D Patterning of Thin Films.** V. Rico, A. García-Valenzuela, H. Reichel, M. Oliva-Ramírez, G. Regodon-Harkness, A. M. Alcaide, A. Espino, T.C. Rojas, J. Palomares, A. Fakhfouri, A. Borrás, A. Winkler, R. Alvarez, A. Palmero, A. R. González-Elipe

Conferencia Invitada: **Plasma polymers in perovskite solar cells.** L. Contreras-Bernal, J. Obrero-Pérez, F.J. Aparicio, F. Nuñez-Galvez, J. Castillo-Seoane, K. Valez-Villalobos, J.A. Anta, A. Borrás, J.R. Sánchez-Valencia, A. Barranco

Conferencia Invitada: **Latest advances in wetting tunable and anti-icing surfaces by plasma deposition and laser patterning.** L. Montes, V. Rico, J. Mora, M. González del Val, G. de la Fuente, L. Angurel, A.R. González-Elipe, A. Borrás, C. López-Santos

Comunicación Oral: **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: **Novel perfluorinated polymeric thin films for the development of controlled wetting surfaces with multirepellency applications.** T. Czermak-Alvarez; M.C. López-Santos; A. Borrás; F.J. Aparicio; A. Barranco

Póster: **PDMS based triboelectric nanogenerators optimization by surface treatment with plasmas at different pressures.** X. García-Casas; A. Ghaffarinejad; F.J. Aparicio; J.P. Espinós; J. Cotrino; A.R. González-Elipe; A. Gómez-Ramírez; M.C. López-Santos; A. Borrás

Póster: **First step toward the development of nanogenerators based in barium titanate nanostructures by magnetron sputtering.** D. Jumilla-Núñez, X. García-Casas, J. Gil-Rostra, J.R. Sánchez Valencia, V. Godinho, A. Borrás

Póster: **From thin film to hierarchical nanostructures of indium tin oxide by vacuum and plasma soft-template methodology.** A. Perea-Brenes, A. Gómez-Ramírez, R. Molina, J.L. García, M. Cantos, A.R. González-Elipe, C. López-Santos

Póster: **Effects of high-pressure plasma treatments on the germination of barley seeds under stressful environments.** J. Castillo-Seoane, J. Gil-Rostra, G. Lozano, K. (Ken) Ostrikov, A.R. González-Elipe, A. Barranco, J.R. Sánchez-Valencia, A. Borrás

Póster: **Hydrophobic fluorinated (CFx) coatings by plasma assisted deposition to protect perovskite solar cells from environmental degradation.** F. Núñez-Gálvez, A. Descalzo, X. García-Casas, J.M. Obrero-Pérez, J.R. Sánchez-Valencia, C. López-Santos

Póster: **Droplet-based energy harvesters developed by laser micro-texturing and plasma assisted deposition.** X. García-Casas, A. Salmoral-Reina, J. Castillo-Seoane, C. López-Santos, A. Ghaffarinejad, F.J. Aparicio, L. Contreras-Bernal, J. Gil-Rostra, J,R. Sánchez-Valencia, A. Barranco, A.Borrás

Póster: **1D nanoelectrodes synthesized by soft-template vacuum and plasma techniques for dye-sensitized solar cells.** L. Contreras-Bernal, J. Castillo-Seoane, J. Gil-Rostra, J. Antonio-Anta, A. Barranco, J.R. Sánchez-Valencia, A. Borrás

Póster: **Plasma assisted fabrication of photocatalytic TiO2 surfaces with 1D to 3D nanoarchitectures.** L. Montes-Montañez, V.J. Rico, J. Castillo-Seoane, J.R. Sánchez-Valencia, A. González-Elipe, C. López-Santos, A. Borrás

Póster: **Development of conformal highly porous oxide thin films by plasma deposition of metal phthalocyanines and porphyrins.** J.M. Obrero, G.P. Moreno, J.R. Sánchez-Valencia, F.J. Aparicio, T.C. Rojas, A. Borrás, A, Barranco

Póster: **Novel perfluorinated polymeric thin films for the development of controlled wetting surfaces with multirepellency applications.** T. Czermak Álvarez, M. C. López Santos, A. Borrás, F. J. Aparicio, A. Barranco

Póster: **PECVD of ZnO and CFX thin films for multifunctional anti-icing and de-icing acoustic wave devices.** J. del Moral, L. Montes, V.J. Rico, C. López-Santos, S. Jacob, M. Oliva, J. Gil, A. Fakhfouri, S. Pandey, M. González, J. Mora, P. García-Gallego Mora, P.F. Ibáñez-Ibáñez, M.A. Rodríguez-Valverde, A. Winkler, A. Borrás, A.R. González-Elipe

18th International Conference on Plasma Surface Engineering | PSE2022
12 – 15 septiembre [Erfurt, Alemania]

Comunicación Oral: **Design and performance of high-temperature solar-selective coatings based on Cr(Al)N.** J.C. Sánchez-López; T.C. Rojas; A. Caro; R. Escobar-Galindo

Comunicación Oral: **Oxidation resistance, adhesion improvement and tribo-mechanical properties of CrAlN coatings deposited by HiPIMS.** S. Domínguez-Meister; A. Dianova; I. Ibáñez; I. Braceras; M. Brizuela; I. Tabares; J.C. Sánchez-López; T.C. Rojas

Póster: **Design of high-temperature solar selective coatings based on Cr(Al)N: Microstructure and optical properties of CrNy and Cr1-xAlxNy films.** T.C. Rojas; A. Caro; G. Lozano; J.C. Sánchez-López

Póster: **Development of multi-layered CrAlN/Al_2O_3 tandem coating using HiPIMS for solar selective applications.** M. Sánchez-Pérez; T.C. Rojas; F. J. Ferrer; G. Lozano; A. Morales; S. Mato; R. Escobar-Galindo; J.C. Sánchez-López

Póster: **Functionalization of additively manufactured materials using physical vapour deposition coatings.** R. Escobar Galindo; J. Hernández-Saz; B. Palacios-I; T.C. Rojas; J.C. Sánchez-López; S.I. Molina

Póster: **Implementation of Ti6Al4V coatings on porous titanium samples.** J.C. Sánchez-López; M. Rodríguez-Albelo; M. Sánchez Pérez; V. Godinho; Y. Torres

The European Optical Society Annual Meeting | EOSAM22
12 – 16 septiembre [Oporto, Portugal]

Comunicación Oral: **One-dimensional photonic crystal for polarization-sensitive surface-enhanced spectroscopy.** E. Mogni; G Pellegrini; J. Gil-Rostra; F. Yubero; G. Simone; S. Fossati; J. Dostálek; R. Martínez-Vazquez; R. Osellame; M. Celebrano; M. Finazzi; P. Biagioni

European Materials Research Society | EMRS Fall Meeting 2022
19 – 22 septiembre [Varsovia, Polonia]

Comunicación Oral: **Interface engineering of ZnO thin films by remote plasma assisted vacuum deposition for the solvent-less fabrication of piezoelectric nanogenerators and UV piezo-phototronic detectors.** X. García-Casas; F.J. Aparicio; Q. He; A. Ghaffarinejad; J. Briscoe; A. Barranco; A. Borrás

Comunicación Oral: **1D nanostructured electrodes in dye-sensitized solar cells for indoor light harvesting.** L. Contreras Bernal; J. Castillo Seoane; J. Gil Rostra; J. Antonio Anta; A. Barranco; J.R. Sánchez Valencia; A. Borrás

Comunicación Oral: **Plasma engineering of microstructured piezo-Triboelectric hybrid nanogenerators for wide bandwidth vibration energy harvesting.** X. García-Casas; A. Ghaffarinejad; F.J. Aparicio; J. Castillo Seoane; C. López-Santos; J. Budagosky; J. Gil-Rostra; J.R. Sánchez-Valencia; A. Barranco; A. Borrás

Comunicación Oral: **PECVD of ZnO and CFX thin films for multifunctional anti-icing and de-icing acoustic wave devices.** J. del Moral, L. Montes, V.J. Rico, C. López-Santos, S. Jacob, M. Oliva, J. Gil, A. Fakhfouri, S. Pandey, M. González, J. Mora, P. García-Gallego Mora, P.F. Ibáñez-Ibáñez, M.A. Rodríguez-Valverde, A. Winkler, A. Borrás, A.R. González-Elipe

Comunicación Oral: **Triboelectric Pixels for large area integration of drop energy harvesters.** A. Ghaffarinejad, X. García-Casas, F. Núñez Gálvez, C. López Santos, J. Ramón Sánchez-Valencia, A. Barranco, A. Borrás

IX Jornadas de I+D+i & 1st International Workshop on STEM
3 – 4 octubre [Sevilla, España]

Comunicación Oral: **Effect of Ti6Al4V coatings on PM titanium samples using high-power impulse magnetron sputtering.** J.C. Sánchez-López, M. Rodríguez-Albelo, M. Sánchez-Pérez, V. Godinho, C. López-Santos, Y.Torres

11th Iberian Conference on Tribology | IBERTRIB 2022
6 – 7 octubre [Setúbal, Portugal]

Comunicación Oral: **Low friction/wear properties of snake skins: a case study for mimicking nature tribological behaviour.** J.C. Sánchez-López; C.F. Schaber; S.N. Gorb

Acoustofluidics 2022
19 – 21 octubre [Glasgow, Reino Unido]

Comunicación Oral: **Acoustic wave activation of the growth of dielectric and metal thin films by plasma deposition techniques.** M. Oliva-Ramírez; A. García-Valenzuela; V. Rico; J.P. Espino; TC Rojas; G. Regodon-Harkness; J. Gil-Rostra; A. Gómez-Ramírez; R. Alvarez; A. Borrás; A. Palmero; A. Winkler; A.R. González-Elipe

Póster: **A holistic solution to icing by acoustic waves on piezoelectric plates.** J.del Moral; L. Montes; V.J. Rico; C. López-Santos; S. Jacob; M. Oliva; J. Gil-Rostra; A. Fakhfouri; S. Pandey; M. González del Val; J. Mora; P. García-Gallego; P.F. Ibáñez-Ibáñez; M.A. Rodríguez-Valverde; A. Winkler; A. Borrás; A.R. González-Elipe

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESSES AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

Conferencia Plenaria: **Synthesis and applications of multifunctional 3D Nanoarchitectures.** A. Borrás

LVIII Congreso de la Sociedad Española de Cerámica y Vidrio
3 – 6 mayo [Madrid, España]

Conferencia Invitada: **Synthesis and applications of multifunctional 3D nanoarchitectures.** X. García-Casas; J. Castillo-Seoane; L. Montes-Montañez; A.N. Filippin; F.J. Aparicio; A. Ghaffarinejad; L. Contreras-Bernal; J. Gil-Rostra; J. Budagoski; V. López-Flores; M.C. López-Santos; J.R. Sánchez-Valencia; A. Barranco; A. Borrás

Conferencia Invitada: **Functional applications of nanostructured surfaces: from energy harvesting to wetting.** X. García Casas; J. Castillo Seoane; L. Montes Montañez; A.N. Filippin; F.J. Aparicio; A. Ghaffarinejad; L. Contreras Bernal; J. Gil Rostra; J. Budagosky; V. López Flores; M.C. López Santos; J.R. Sánchez Valencia; A. Barranco; A. Borrás

Comunicación Oral: **Plasma processing of metal phthalocyanines and porphyrins for the development of supported porous nanostructures for energy applications.** J.M. Obrero; A.N. Filippin; F.J. Aparicio; Saghi; J.R. Sánchez Valencia; A. Barranco; A. Borrás

XVI Congreso Nacional de Materiales | CNMAT2022
28 junio – 1 julio [Ciudad Real, España]

Comunicación Oral: **Diseño y comportamiento de recubrimientos solares selectivos basados en Cr(Al)N.** J.C. Sánchez-López; T.C. Rojas; A. Caro; R. Escobar-Galindo

Comunicación Oral: **Funcionalización superficial mediante recubrimientos PVD (deposición física en fase vapor) de materiales procesados por fabricación aditiva.** R. Escobar-Galindo; J. Hernández-Saz; B. Palacios-I; M. Sánchez-Pérez; T.C. Rojas; J.C. Sánchez-López; S.I. Molina

Comunicación Oral: **Diseño de recubrimientos solares selectivos para alta temperatura basados en Cr(Al)N: Microestructura y propiedades ópticas de capas de CrNy and Cr1-xAlxNy.** T.C.Rojas; A. Caro; G. Lozano; J.C. Sánchez-López

Comunicación Oral: **Crecimiento de aleaciones de TiAlV y TiNbZrTa sobre probetas de titanio poroso mediante magnetrón sputtering.** J.C. Sánchez-López; M. Rodríguez-Albelo; M. Sánchez-Pérez; V. Godinho; C. López-Santos; Y. Torres

Comunicación Oral: **Nanoestructuración a la Carta de Películas Delgadas en Geometría de Ángulo Oblicuo Mediante el Control Topográfico del Sustrato.** S. Muñoz-Piña; A.M. Alcaide; B. Limones-Ahijón; M. Oliva-Ramírez; V. Rico; G. Alcalá; M.U. González; J.M. García-Martín; R. Alvarez; D. Wang; P. Schaaf; A.R. González-Elipe; A. Palmero

Comunicación Oral: **Recubrimientos antibacterianos de Ti nanoestructurado mediante pulverización catódica: del laboratorio a escala semiindustrial.** R. Alvarez; S. Muñoz-Piña; M.U. González; I. Fernández-Martínez; V. Rico; A.M. Alcaide; G.F. Regodón; J.M. arcía-Martín; A.R. González-Elipe; A. Palmero

Comunicación Oral: **Fabricación de nanomateriales funcionales 1D y 3D para sistemas de captación de energía mecánica local.** X. García-Casas; A. Ghaffarinejad; F.J. Aparicio; M.C. López-Santos; J.R: Sánchez-Valencia; A. Barranco; A: Borrás

Comunicación Oral: **Fabricación de nanoestructuras de perovskita altamente anisotrópicas mediante depósito por evaporación térmica en ángulo rasante.** J. Castillo-Seoane; L. Contreras-Bernal; J. M. Obrero; X. García-Casas; F.J. Aparicio; M.C: López-Santos; T.C: Rojas; J.A. Anta; A. Borrás; A.Barranco; J.R. Sánchez-Valencia

Comunicación Oral: **Sculptural fabrication of perovskite nanostructures by thermal evaporation deposition at glancing angles.** J. Castillo-Seoane, L. Contreras-Bernal, J.M. Obrero, X. García-Casas, F.J. Aparicio, C. López-Santos, T. Cristina Rojas, J.A. Anta, A. Borrás, A. Barranco, J.R. Sánchez-Valencia

Comunicación Oral: **Influencia de la modificación con láser de femtosegundo en el comportamiento biomecánico y biofuncional de sustratos de titanio porosos.** J.M. Amado, A.M. Beltrán, M.Giner, A.Rodríguez, P.Trueba, L.M. Rodríguez-Albelo, M.A.Vázquez-Gámez, V.Godinho, A.Alcudia, C. López-Santos,Y.Torres

Comunicación Oral: **Composites antibacterianos para aplicación en profilaxis de implantes dentales porosos.** B. Begines, A. Alcudia, P. Rodríguez-Lejarraga, V. Greyer, V. Godinho, E. Pajuelo, E. Delgado, A. El Hadad, Y. Torres

Comunicación Oral: **Recubrimientos de espumas de titanio con nanocomposites poliméricos para mejorar la biocompatibilidad y la resistencia a la corrosión.** C. García Cabezón, V. Godinho, C. García Hernandez, F. J. García-García, J. de la Rosa, Y. Torres, F. Martín-Pedrosa

Póster: **Desarrollo de sistemas tándem basados en multicapas CrAlN/Al_2O_3 usando HiPIMS como absorbedores solares selectivos.** M. Sánchez-Pérez;T. C. Rojas;F. J. Ferrer;G. Lozano;Á. Morales;S. Mato;R. Escobar-Galindo;J.C. Sánchez-López

XLIV Congreso de la Sociedad Ibérica de Biomecánica y Biomateriales
25 – 26 Noviembre [Cáceres, España]

Comunicación Oral: **Bioactive coatings for titanium dental implants containing Sr/Zn phytates: osteogenic and antibacterial properties.** G. Asensio; A.M. Hernández-Arriaga; A.M. Prieto; A.R. González-Elipe; L. Rojo; B. Vázquez-Lasa

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título: **Porous ionomer free layered metal alloy electrocatalyst electrode**
Autor: Ester López Fernández
Directores: Antonio de Lucas Consuegra, Francisco Yubero Valencia
Centro: Universidad Castilla-la Mancha
Fecha Defensa: 21 de enero de 2022

Título: **Atmospheric pressure plasmas for more sustainable chemical processes and environmental applications**
Autor: Paula de Navascués Garvín
Directores: Agustín R. González-Elipe, Ana María Gómez Ramírez
Centro: Universidad de Sevilla
Fecha Defensa: 1 de junio de 2022

Título: **Recubrimientos nanocolumnares estructurados sobre sustratos rugosos y litografiados en condiciones industriales**
Autor: Sandra Muñoz Piña
Directores: Germán Alcalá Penadés, Rafael Álvarez Molina, Alberto Palmero Acebedo
Centro: Universidad Complutense de Madrid
Fecha Defensa: 15 de julio de 2022

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título: **Fenómenos de Histéresis en reactores de plasma de pulverización catódica reactiva**
Autor: Teresa Víctoria López Carmona
Tutores: José Cotrino Bautista, Alberto Palmero Acebedo
Grado: Trabajo Fin de Grado
Centro: Universidad de Sevilla
Fecha Defensa: 19 de septiembre de 2022

Título: **Desarrollo de láminas delgadas y nanoestructuras de NiOx por magnetrón sputtering como contacto selectivo en celdas solares de perovskita**
Autor: Mikel Martínez Olaizola
Tutores: Jorge Gil Rostra, Lidia Contreras Bernal
Grado: Trabajo Fin de Máster
Centro: Universidad de Sevilla
Fecha Defensa: 29 de noviembre de 2022

Título:	**Nanogeneradores piezo- y piroeléctricos para componentes microelectrónicos**
Autor:	Juan Delgado Álvarez
Tutores:	Francisco Javier Aparicio Rebollo, Víctor López Flores
Grado:	Trabajo Fin de Máster
Centro:	Universidad de Sevilla
Fecha Defensa:	8 de diciembre de 2022

PREMIOS Y RECONOCIMIENTOS / PRIZES AND ACKNOWLEDGEMENTS

Medalla de Sevilla
Dra. Asunción Fernández Camacho

XII Premios cicCartuja EBRO FOODS
Xavier García Casas
Primer Premio al mejor artículo para Jóvenes Investigadores del cicCartuja

Premio SOCIEMAT al Joven Investigador
Javier Castillo Seoane por su trabajo "Sculptural fabrication of perovskite nanostructures by thermal evaporation deposition at glancing angles"

IX Edición Premios Losada Villasante
Dra. Ana Isabel Borrás Martos
Premio a la Investigación en Innovación por el trabajo "Materiales avanzados para la captación de energía ambiental: luz, movimiento y temperatura"

Miguel Angel Castro Arroyo (Rector de la Universidad de Sevilla), Ana Isabel Borrás, Rogelio Velasco (Consejero de Economía, Conocimiento, Empresas y Universidad de la Junta de Andalucia) (Fotografía: Fundación Cajasol)

ESTANCIAS Y VISITAS DE PERSONAL DEL ICMS EN OTROS CENTROS
PERSONNEL OF THE ICMS IN OTHER LABORATORIES

University Queen Mary of London
Londres, Reino Unido — **José Obrero Pérez** — 04/04/22 - 04/07/22

ESIEE Paris, l'école de l'innovation technologique
París, Francia — **Ali Ghaffarinajad** — 05/10/22 - 14/10/22

Tampere University
Tempere, Finlandia — **Ana Isabel Borrás Martos** — 22/08/22 - 27/08/22
Laura Montes Montañez — 22/08/22 - 27/08/22
Jaime del Moral Jalón — 22/08/22 - 27/08/22

Instituto de Nanociencia y Materiales de Aragón (INMA)
Zaragoza, España — **Laura Montes Montañez** — 04/07/22 - 15/07/22

Institut de recherche interdisciplinaire de Grenoble – French Alternative Energies and Atomic Energy Commission (IRIG-CEA)
Grenoble, Francia — **Lidia Bernal Contreras** — 01/11/22 - 30/11/22

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

Universidad Rey Juan Carlos
Madrid, España — **María del Carmen López González** — 01/07/22 – 31/07/22

University Queen Mary of London
Londres, Reino Unido — **Chloe Forrester** — 03/07/22 – 17/07/22
Joseph Briscoe — 03/07/22 – 06/07/22

Universidad Federal de Pernambuco
Brasil — **Kamilla Veronika Rodrigues de Andrade Silva** — 24/11/22 – 31/05/23

Instituto Nacional de Técnica Aeroespacial (INTA)
Madrid, España — **Pilar García Parejo** — 15/06/22 – 17/06/22

Universidad Autónoma de Yucatán
Mérida, México — **Mahmoud Nabil Hassan Mahmoud** — 01/12/22 – 31/05/23

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 °C (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 °C) –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 °C (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

PERSONAL / PERSONNEL

Profesores de Investigación	Dr. Hernán R. Míguez García
	Dr. Manuel Ocaña Jurado
Científicos Titulares	Dra. Ana Isabel Becerro Nieto
	Dr. Mauricio E. Calvo Roggiani
	Dr. Gabriel Lozano Barbero
	Dra. Nuria Ofelia Núñez Álvarez
Investigadores Distinguidos	Dr. Juan Francisco Galisteo López
Doctores Contratados	Dr. Víctor Castaing
	Dra. Laura Caliò
	Dr. Daniel González Mancebo
	Dr. Ngo Thi Tuyen
Investigadores en Formación	Gda. Encarnación Arroyo Porriño
	Gda. Clara Bujalance Aguilera
	Gda. Elena Cabello Olmo
	Gda. Beatriz De Sola Báez
	Gda. Elisabet Gómez González
	Gda. María Morán Pedroso
	Gdo. Manuel Romero Aguilar
	Gdo. Carlos Romero Pérez
	Gdo. David Otto Tiede
	Gdo. José María Viaña Jorge
Técnicos Contratados	Lda. Lucía T. Castillo Flores
	Lda. M. Carmen Gutiérrez Lázaro

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
Gabriel S. Lozano Barbero

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.

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
Hernán R. Míguez García

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.

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
Hernán R. Míguez García Juan Francisco Galisteo López	Gabriel S. Lozano Barbero Mauricio Calvo Roggiani

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 absoprtion 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 perovksite 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

MINISTERIO DE CIENCIA E INNOVACIÓN

AGENCIA ESTATAL DE INVESTIGACIÓN

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
Hernán R. Míguez García Mauricio E. Calvo Roggiani	Gabriel S. Lozano Barbero Juan Francisco Galisteo López

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.

Biosondas basadas en lantánidos para la obtención de bioimagen mediante resonancia magnética y luminiscencia persistente
Lanthanide-based bioprobes for MRI and persistent luminescence imaging

MINISTERIO DE CIENCIA E INNOVACIÓN
UNIÓN EUROPEA
FONDO EUROPEO DE DESARROLLO REGIONAL
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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
Manuel Ocaña Jurado Ana Isabel Becerro Nieto	Nuria O. Núñez Álvarez

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.

Nanopartículas multifuncionales para la obtención de bioimágenes mediante luminiscencia, resonancia magnética y tomografía computerizada de Rayos X
Multifunctional nanoparticles for luminescent, magnetic resonance and X-ray computed tomography bioimaging

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Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
RTI2018-094426-B-100	01-01-2019 30-09-2022	Ministerio de Ciencia e Innovación	193.600 €

Investigador Principal Research Head	Componentes Research Group
Manuel Ocaña Jurado Ana Isabel Becerro Nieto	Nuria O. Núñez Álvarez

RESUMEN / ABSTRACT

El proyecto persigue la preparación de nanopartículas (NPs) multifuncionales con propiedades mejoradas y características (tamaño, estabilidad coloidal y toxicidad) adecuadas que puedan emplearse en más de una modalidad de obtención de imágenes de órganos, tejidos y células, cuyo principal interés radica en que mediante un único tipo de sonda se podría obtener información complementaria esencial para un diagnóstico clínico más riguroso. En concreto, se estudiarán sondas bifuncionales para la obtención de imágenes mediante luminiscencia y resonancia magnética (MRI) o tomografía computarizada de rayos X (CT), y sondas trifuncionales con utilidad para las tres modalidades mencionadas. Se abordarán dos tipos de biosondas luminiscentes. Por una parte, se diseñarán NPs luminiscentes constituidas por matrices singulares dopadas con cationes lantánidos (Nd^{3+} o Er^{3+}:Yb^{3+} o Tm^{3+}:Yb^{3+}), cuya excitación y emisión tiene lugar 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. Por otra parte, se persigue la obtención de NPs cuya luminiscencia persiste después de eliminar la excitación, evitándose así los posibles efectos no deseados de ésta (autofluorescencia de los tejidos, radiaciones dañinas). En el primer caso, se pretende conseguir una mayor estabilidad química y térmica de las sondas mediante la selección de matrices tipo oxifluoruro más estables que las de tipo fluoruro propuestas hasta ahora, En el segundo caso, se abordarán sistemas con luminiscencia persistente en el NIR con composición $ZnGa_2O_4$:Cr^{3+} y $Y_3Al_2Ga_3O_{12}$:Ce^{3+},Cr^{3+},Nd^{3+}, para los que es prioritario desarrollar nuevos métodos de síntesis que permitan la obtención de NPs uniformes, necesarias para este tipo de aplicaciones. Respecto a la modalidad MRI y en respuesta a la necesidad de desarrollar agentes de contraste para las más modernas técnicas que operan a campos magnéticos altos para aumentar la resolución de las imágenes y así obtener un diagnóstico más preciso, se planea desarrollar NPs constituidas por compuestos (oxifluoruros, vanadatos, fosfatos) de Dy y Ho. Por último, debido al alto número atómico de los elementos constituyentes de las sondas anteriores, es de esperar que éstas también tengan una alta capacidad de atenuación de rayos X, siendo por tanto también potencialmente útiles como agentes de contraste para CT. En este caso, el empleo de las NPs objeto de estudio aportará importantes ventajas respecto a los agentes comerciales utilizados en la actualidad que se traducen en un mayor control del tiempo de residencia en el organismo y de su biodistribución y, por tanto, en la posibilidad de disminuir las dosis utilizadas reportando así un beneficio para el paciente. El proyecto contempla tanto la fabricación de las sondas optimizadas como la exploración de su aplicabilidad al campo del diagnóstico clínico mediante la obtención de imágenes in vivo en ratones. El equipo investigador posee gran experiencia en la síntesis de NPs inorgánicas basadas en tierras raras y dispone de la mayoría de los medios necesarios para su caracterización. Además, dicho equipo cuenta con el apoyo de investigadores de otras instituciones, expertos en diversos aspectos del proyecto, que colaborarán en el desarrollo de algunas tareas del mismo como vienen haciendo desde hace varios años, lo que garantiza el correcto desarrollo de la propuesta.

The project pursues the preparation of multifunctional nanoparticles (NPs) with improved properties and suitable characteristics (size, colloidal stability and toxicity) that can be used to get images of cells, tissues and organs by means of more than one bioimaging technique, thus providing complementary information essential for a more reliable medical diagnosis. Specifically, we shall study bifunctional probes for both, luminescence and magnetic resonance (MRI) or luminescence and X-ray computed tomography (CT), and trifunctional probes that are useful for the three imaging techniques. Two types of luminescent probes will be addressed. On the one hand, luminescent NPs will be designed consisting of single matrices doped with lanthanide cations (Nd^{3+} o Er^{3+}:Yb^{3+} o Tm^{3+}:Yb^{3+}), whose excitation and emission takes place in the near-infrared (NIR) region known as the biological window (650-1800 nm), in which radiation is not harmful to tissues and has a high penetration power. On the

other hand, nanoprobes whose luminescence persists after ceasing the excitation will be also developed, thus avoiding the possible undesirable effects of the excitation radiation on the tissues. In the first case, our aim is to achieve greater chemical and thermal stability of the probes by selecting oxifluoride-type matrices, more stable than the fluoride-type matrices proposed so far. In the second case, the aim of the project resides in the exploration of new synthetic routes to obtain nanoparticulated $ZnGa_2O_4:Cr^{3+}$ and $Y_3Al_2Ga_3O_{12}:Ce^{3+}$, Cr^{3+}, Nd^{3+}, with uniform size and shape, which are essential for bioapplications. Regarding MRI technique, this project aims at developing NPs made up of Dy- and Ho-based oxifluorides, vanadates and phosphates in response to the need of new contrast agents that work at high magnetic fields, which are increasingly being used in clinics to improve image resolution. Finally, due to the high atomic number of the constituent elements of the selected probes, it is expected that they show a high X-ray attenuation capacity, being therefore also useful as CT contrast agents. The advantage of the NPs proposed in this research with respect to the CT CAs currently used in clinics is the longer circulation time of the former, which will allow decreasing considerably the dosage to be given to the patient. The project contemplates both the manufacture of optimised probes and the exploration of their applicability to the field of medical diagnosis by obtaining "in vivo" images in mice. The research team has long experience in the synthesis of rare earths-based inorganic NPs and has most of the necessary equipment for their characterisation. The participation in the work plan of researchers from other institutions, with long expertise on various aspects of the project, who have successfully collaborated with the research team, gives further support to the viability of the proposal.

Nuevos agentes de contraste multimodales para el diagnóstico médico por imagen
New multimodal contrast agents for medical diagnostic imaging

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_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 volframatos 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.

Desarrollo de Dispositivos Emisores de Luz basados en Perovskita Nanoestructurada

Development of light emitting devices based on nanostructured perovskite | Nano-ABX LED

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
P18-RT-2291	01-02-2020 31-12-2022	Junta de Andalucía	122.968 €

Investigador Principal Research Head	Componentes Research Group
Hernán R. Míguez García	Juan Francisco Galisteo López Mauricio E. Calvo Roggiani Gabriel S. Lozano Barbero

RESUMEN / ABSTRACT

El proyecto Nano-ABX LED se centra en encontrar vías de solución a los principales retos que enfrenta el campo de la emisión de luz basada en perovskitas. Estos son la inestabilidad química y térmica de las perovskitas, así como la dificultad de mantener una eficiencia cuántica elevada independientemente del color de emisión, lo que dificulta la obtención tanto de una gama de colores variada como de distintos tonos de blanco (i.e., distintas temperaturas de color).

El proyecto Nano-ABX LED surge con la motivación de encontrar soluciones a estos problemas. Partiendo de resultados preliminares recientes del grupo de Materiales Ópticos Multifuncionales, se intentará demostrar que la integración de nanocristales de perovskita híbrida en el interior de matrices con porosidad controlada mejora extraordinariamente la estabilidad ambiental de estos materiales, un aspecto que el grupo solicitante de esta propuesta ha estudiado en profundidad, así como permite aumentar el rendimiento cuántico luminiscente a longitudes de onda de emisión controladas. En otra vertiente del proyecto, se explorará el aumento de eficiencia y prestaciones (direccionalidad, control espectral) de los dispositivos a través de la integración de distintas estructuras fotónicas, tomando como punto de partida.

The Nano-ABX LED project focuses on finding ways to solve the main challenges facing the field of perovskite-based light emission. These are the chemical and thermal instability of perovskites, as well as the difficulty of maintaining a high quantum efficiency regardless of the emission color, which makes it difficult to obtain both a varied color range and different shades of white (i.e., different temperatures color).

The Nano-ABX LED project arises with the motivation to find solutions to these problems. Based on recent preliminary results of the Multifunctional Optical Materials Group, an attempt will be

made to demonstrate that the integration of hybrid perovskite nanocrystals inside matrices with controlled porosity dramatically improves the environmental stability of these materials, an aspect that the group requesting this proposal has studied in depth, as well as it allows to increase the luminescent quantum efficiency at controlled emission wavelengths. In another aspect of the project, the increase in efficiency and performance (directionality, spectral control) of the devices will be explored through the integration of different photonic structures, taking as a starting point.

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

Ayudas extraordinarias para la preparación de proyectos 2021. Proyecto: RTI2018-094426-B-100

Código/Code: 2021AEP088
Periodo/Period: 01-01-2022 / 31-08-2022
Organismo Financiador/Financial source: CSIC
Importe total/Total amount: 10.000 €
Investigador responsable/Research head: Manuel Ocaña Jurado

CONVENIOS Y CONTRATOS / CONTRACTS AND AGREEMENTS

Diseño y preparación de filtros dicroicos para su integración en módulos fotovoltaicos

Periodo/Period: 01-01-2021 / 31-12-2022
Organismo Financiador/Financial source: BLUESOLAR FILTERS, S.L.
Importe total/Total amount: 181.500 €
Investigador responsable/Research head: Hernán Míguez García

PATENTES / PATENTS

Dysprosium nanoparticles, process for obtaining said nanoparticles and use of said nanoparticles as a contrast agent
Inventores: Ana Isabel Becerro Nieto, Elisabet Gómez González, Carlos Alberto Caro Salazar (CIN2), Nuria O. Núñez Álvarez, María Luisa García Martín (IIBM), Manuel Ocaña Jurado
Tipo de Patente: Nacional
Número de Solicitud: 22382507
Fecha Solicitud: 26 de mayo de 2022
Entidad Titular: Servicio Andaluz de Salud, Consejo Superior de Investigaciones Científicas

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Optoelectronic Devices Based on Scaffold Stabilized Black-Phase CsPbI3 Nanocrystals
Romero-Pérez, C; Rubino, A; Calio, L; Calvo, ME; Miguez, H
Advanced Optical Materials, **10** (2022) 2102112
Enero, 2022 | **DOI:** 10.1002/adom.202102112

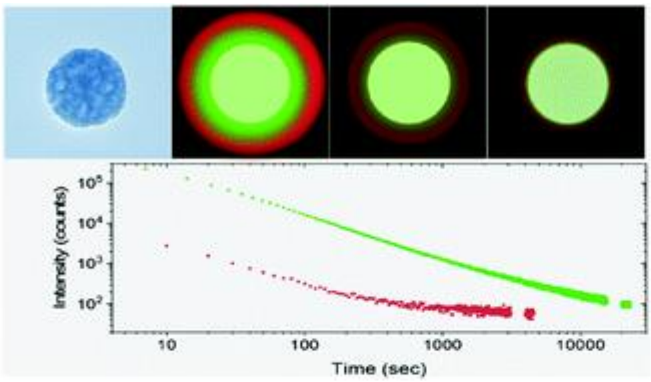
The optoelectronic properties of lead halide perovskites are intimately related to their crystalline phase. For the case of cesium lead iodide ($CsPbI_3$) several polymorphs meet the Goldschmidt tolerance factor, which determines their stability, and form broad band absorber and luminescent phases. However, at room temperature none of them are stable, which prevents their use in optoelectronics. In this work, bare $CsPbI_3$ nanocrystals are synthesized in the sub-10 nm range in the "black", light emitting, crystalline phase, using a pore controlled SiO_2 matrix that limits crystal size and confers a certain degree of strain that favors their stability. Quantum confinement effects allow the tuning of the optical properties of the $CsPbI_3$ nanocrystals by means of the crystal size. Their suitability as optoelectronic materials is demonstrated by building scaffold supported $CsPbI_3$ quantum dot based photovoltaic and light emitting devices.

Molecular Interface Engineering via Triazatruxene-Based Moieties/NiOx as Hole-Selective Bilayers in Perovskite Solar Cells for Reliability
Hemasiri, NH; Calio, L; Pegu, M; Kazim, S; Ahmad, S
Solar RRL. **6** (2022) 2100793
Enero, 2022 | **DOI:** 10.1002/solr.202100793

Interface engineering is an effective approach to decrease nonradiative recombination and the energy barrier at the perovskite/hole transporting layer (HTL) interfaces. To overcome such limitations, an organic semiconductor (DTT-EHDI2) is proposed, which is, composed of dithienothiophene (DTT) as the core and a planar triazatruxene incorporating an alkyl chain as the side group. This is noted to be an effective interfacial layer for inverted planar perovskite solar cells (PSCs). The altered interface effectively minimizes the detrimental charge recombination and tailors the photoinduced charge transfer dynamics at the interface of the inorganic HTL/perovskite. The pi-conjugation in DTT-EHDI2 induces high hole mobility and electrical conductivity via electron-donating properties and strong pi-pi intermolecular interaction. The synergetic approach leads to a substantial performance enhancement in dopant-free DTT-EHDI2-based inverted planar PSCs, achieving 18.15% power conversion efficiency with negligible hysteresis effect. The present approach provides an effective direction of the cost-effective thiophene derivative as an interfacial agent to escalate the optoelectronic performances in photovoltaics.

Highly uniform $Y_3Al_2Ga_3O_{12}$-based nanophosphors for persistent luminescence bioimaging in the visible and NIR regions

Arroyo, E; Herrero, BT; De la Fuente, JM; Ocaña, M; Becerro, AI
Inorganic Chemistry Frontiers, **9** (2022) 2454-2461
Abril, 2022 | **DOI:** 10.1039/d2qi00480a

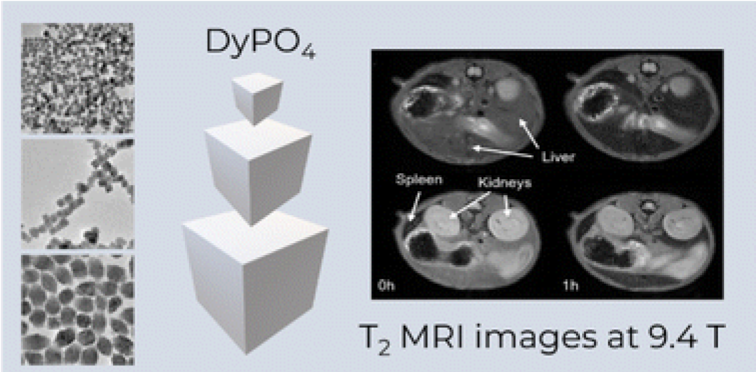


In the last few years, persistent phosphors with a garnet crystal structure have attracted a great deal of interest for a plethora of applications ranging from bioimaging to anti-counterfeiting technologies. However, the development of synthesis methods to fabricate uniform garnet-based micro and nanoparticles, that are needed for such applications, is not mature at all. This study reports the synthesis of highly uniform yttrium aluminum gallium garnet nanospheres. The method is based on homogeneous precipitation in a polyol medium followed by silica coating and calcination. The nanoparticles resulting after silica removal were also uniform and were easily functionalized with polyacrylic acid. The colloidal stability of the latter in physiological media and their biocompatibility were analyzed. The luminescence of the particles, doped with Ce^{3+}, Cr^{3+}, and Nd^{3+}, was studied by recording emission and excitation spectra and persistent luminescence decay curves. Due to their uniform morphology, high colloidal stability, absence of toxicity, and persistent emission in the visible and near-infrared regions, the reported nanospheres show great potential as persistent luminescent bioimaging probes. In addition, the synthesis method paves the way for future use of this persistent material in other applications that require the phosphor to be in the form of highly uniform nanoparticles.

Outstanding MRI contrast with dysprosium phosphate nanoparticles of tuneable size

Gómez-González, E.; Caro, C.; García-Martín, ML; Becerro, AI; Ocaña, M.
Nanoscale, **14** (2022) 11461-11470
Agosto, 2022 | **DOI:** 10.1039/d2nr02630a

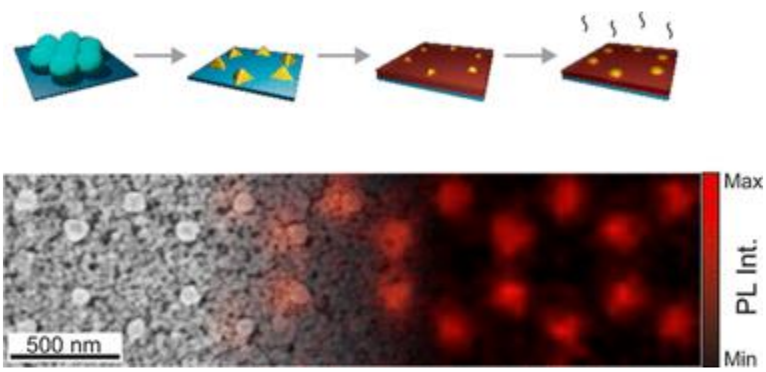
The use of high-field magnets for magnetic resonance imaging (MRI) is expected to experience the fastest growth rate during the present decade. Although several CAs for MRI scanners using high magnetic fields have been reported, they are mostly based on fluoride matrices, which are known for their low chemical stability in aqueous suspensions. Chemically stable MRI CAs for high-field magnets



are therefore needed to enable the advances in MRI technique. Herein, we synthesized uniform $DyPO_4$ nanoparticles (NPs) with tuneable sizes between 23 and 57 nm using homogeneous precipitation in butanol. The NPs were successfully functionalized with polyacrylic acid (PAA) and showed good colloidal stability in aqueous suspensions. Chemical stability was also assessed in PBS, showing negligible solubility. The effect of particle size on the transversal relaxivity value (r_2) was further explored at 9.4 T, finding a clear increase in r_2 with particle size. The r_2 value found for the largest NPs was 516 $mM^{-1}s^{-1}$, which is, to the best of our knowledge, the highest r_2 value ever reported at 9.4 T for any Dy-based nanometric particles in the literature. Finally, the latter NPs were submitted to biosafety studies after polyethylene glycol (PEG) functionalization. Cell morphology, induction of necrotic/late apoptotic cells, and mitochondrial activity were thoroughly analyzed. The results clearly indicated negligible toxicity effects under the assayed conditions. Short- and long-term in vivo pharmacokinetics of the intravenously injected NPs were assessed by dynamic T_2-weighted MRI and quantitative T_2 mapping, revealing faster liver than spleen uptake, while no accumulation was observed in the kidneys. Finally, no histopathological changes were observed in any of the studied organs, including the liver, kidney, spleen, and lung, which provide further evidence of the biocompatibility of $DyPO_4$ NPs and, therefore, their suitability as bioimaging probes.

Nanoantennas Patterned by Colloidal Lithography for Enhanced Nanophosphor Light Emission

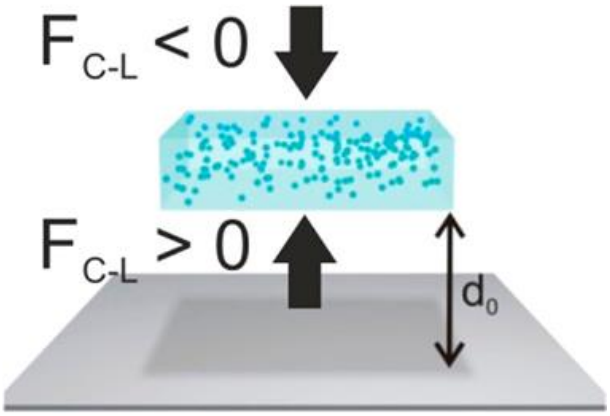
Viana, JM; Romero, M; Lozano, G; Míguez, H
ACS Applied Nano Materials, **5**(11) (2022) 16242-16249
Noviembre, 2022 | **DOI:** 10.1021/acsanm.2c03258



Transparent coatings made of rare-earth doped nanocrystals, also known as nanophosphors, feature efficient photoluminescence and excellent thermal and optical stability. Herein, we demonstrate that the optical antennas prepared by colloidal lithography render thin nanophosphor films with a brighter emission. In particular, we fabricate gold nanostructures in the proximity of $GdVO_4:Eu^{3+}$ nanophosphors by metal evaporation using a mask made of a monolayer of polymer beads arranged in a triangular lattice. Optical modes supported by the antennas can be controlled by tuning the diameter of the polymer spheres in the colloidal mask, which determines the shape of the gold nanostructure, as confirmed by numerical simulations. Confocal microscopy reveals that metallic antennas induce brighter photoluminescence at specific spatial regions of the nanophosphor film at targeted frequencies as a result of the coupling between gold nanostructures and nanophosphors. Patterning of nanophosphor thin layers with arrays of metallic antennas offers an inexpensive nanophotonic solution to develop bright emitting coatings of interest for color conversion, labeling, or anti-counterfeiting.

Effect of Spatial Inhomogeneity on Quantum Trapping

Esteso, V; Carretero-Palacios, S; Miguez, H
Journal of Physical Chemistry Letters, **13** (2022) 4513-4519
Junio, 2022 | **DOI:** 10.1021/acs.jpclett.2c00807

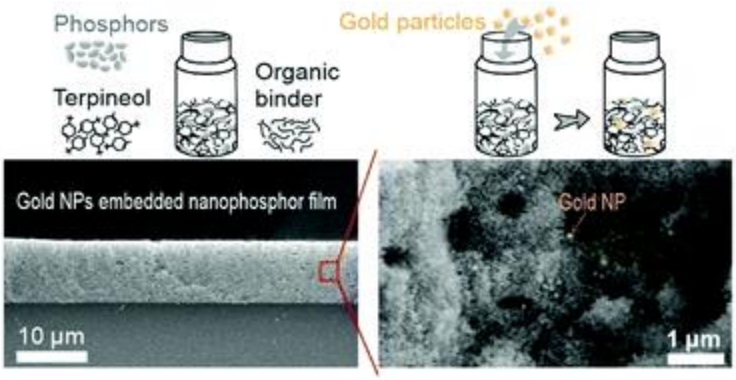


An object that is immersed in a fluid and approaching a substrate may find a potential energy minimum at a certain distance due to the balance between attractive and repulsive Casimir–Lifshitz forces, a phenomenon referred to as quantum trapping. This equilibrium depends on the relative values of the dielectric functions of the materials involved. Herein, we study quantum trapping effects in planar nanocomposite materials and demonstrate that they are strongly dependent on the characteristics of the spatial inhomogeneity. As a model case, we consider spherical particles embedded in an otherwise homogeneous material. We propose an effective medium approximation that accounts for the effect of inclusions and find that an unprecedented and counterintuitive intense repulsive Casimir–Lifshitz force arises as a result of the strong optical scattering and absorption size-dependent resonances caused by their presence. Our results imply that the proper analysis of quantum trapping effects requires comprehensive knowledge and a detailed description of the potential inhomogeneity (caused by imperfections, pores, inclusions, and density variations) present in the materials involved.

Enhanced up-conversion photoluminescence in fluoride-oxyfluoride nanophosphor films by embedding gold nanoparticles

Ngo, TT; Lozano, G; Miguez, H
Materials Advances, **3** (2022) 4235-4242
Abril, 2022 | **DOI:** 10.1039/D2MA00068G

Owing to their unique non-linear optical character, lanthanide-based up-converting materials are potentially interesting for a wide variety of fields ranging from biomedicine to light harvesting. However, their poor luminescent efficiency challenges the development of technological applications. In this context, localized surface plasmon resonances (LSPRs) have been demonstrated as a valuable strategy to improve light conversion. Herein, we utilize LSPR induced by gold nanoparticles (NPs) to enhance up-conversion photoluminescence (UCPL) in transparent, i.e. scattering-free, films made of



nanophosphors formed by fluoride–oxyfluoride host matrix that feature high thermal stability. Transparency allows excitation by an external source without extinction losses caused by unwanted diffuse reflection. We provide a simple method to embed gold NPs in films made of YF/YOF:Yb^{3+},Er^{3+} UC nanophosphors, via preparation of a viscous paste composed of both UC nanophosphors and colloidal gold NPs, reducing complexity in sample fabrication. The dimensions of gold NPs are such that their associated LSPR matches spectrally with the green emission band of the Er^{3+} doped nanophosphors. In order to demonstrate the benefits of plasmonic nanoparticles for UCPL in nanophosphor films, we provide a careful analysis of the structural properties of the composite thin films along with precise characterization of the impact of the gold NPs on the photophysical properties of UC nanophosphors.

Transparent Phosphor Thin Films Based on Rare-Earth-Doped Garnets: Building Blocks for Versatile Persistent Luminescence Materials

Castaing, V; Lozano, G; Míguez, H

Advanced Photonics Research, **3** (2022) 2100367
Abril, 2022 | **DOI:** 10.1002/adpr.202100367

Afterglow properties of persistent phosphors are attracting a great deal of attention in the fields of bioimaging, sensing, labeling, safety, or security. Complex garnet oxides, especially those doped with Ce^{3+} and Cr^{3+}, are particularly relevant to this end since their persistent luminescence can be tuned through matrix composition and activated by visible light, in contrast to the vast majority of persistent phosphors that require UV excitation. Most extended preparation routes yield micrometer-sized phosphors that display strong light scattering, which limits their versatility and applicability. Herein, nanostructured garnet oxide-based thin films that are transparent and feature persistent luminescence properties are demonstrated. Following a sol–gel route and after high temperature annealing, few hundred nanometre-thick $Y_3Al_2Ga_3O_{12}$:Ce^{3+},Cr^{3+} transparent films showing efficient green emission and afterglow are attained. $Gd_3Al_2Ga_3O_{12}$:Ce^{3+},Cr^3 transparent thin films displaying yellow afterglow with distinct persistent kinetics are demonstrated, to prove the generality of the approach herein proposed. Its versatility is further demonstrated by developing layered phosphors with time-dependent chromaticity due to the unique persistent emission color – upon blue light excitation – and kinetics of each layer forming the stack. The results pave an avenue toward nanodevices and multifunctional coatings in which afterglow offers hitherto unexplored properties.

Neodymium doped lanthanide fluoride nanoparticles as contrast agents for luminescent bioimaging and X-ray computed tomography

González-Mancebo, D; Becerro, AI; Calderon-Olvera, RM; Cantelar, E; Corral, A; Balcerzyk, M; De la Fuente, JM; Ocaña, M

Boletin de la Sociedad Española de Ceramica y Vidrio, **61** (2022) 540-549
Mayo, 2022 | **DOI:** 10.1016/j.bsecv.2021.07.004

The synthesis of uniform neodymium-doped lanthanum trifluoride nanoparticles with lenticular shape and a mean diameter around 45 nm by using a homogeneous precipitation method is reported. The luminescent properties of the synthesized samples in terms of their emission spectra and emission lifetime are analyzed as a function of the Nd content to find the optimum phosphor and its suitability for luminescent imaging in the second biological window. The X-ray attenuation properties of the optimum phosphor are evaluated to investigate their additional ability as contrast agent for X-ray computed tomography. Finally, the colloidal stability of the obtained nanoparticles in physiological medium and their cytotoxicity are also analyzed to assess their aptness for in vivo bioimaging applications.

Enhanced red-UC luminescence through Ce^{3+} co-doping in $NaBiF_4$:Yb^{3+}/Ho^{3+}(Er^{3+})/Ce^{3+} phosphors prepared by ultrafast coprecipitation approach

Giordano, L; Du, H; Castaing, V; Luan, F; Guo, D; Viana, B

Optical Materials X, **16** (2022) 100199
Octubre, 2022 | **DOI:** 10.1016/j.omx.2022.100199

Series of Yb^{3+}/Ho^{3+}(Er^{3+})/Ce^{3+} co-doped $NaBiF_4$ phosphors were synthesized through an ultrafast co-precipitation reaction technique at room temperature. The effect of the Ce^{3+} ions on the crystal structure and upconversion (UC) luminescence properties of the studied samples were investigated in detail. FTIR and XPS demonstrated the pre-formation of $NaBiF_4$ and the introduction of Yb^{3+}, Ho^{3+}, Er^{3+} and Ce^{3+} all as dopants in the host materials. Under 980 nm excitation, $NaBiF_4$:Yb^{3+},Ho^{3+}(Er^{3+}),Ce^{3+}performed the characteristic emission of the activator ion, and the introduction of Ce^{3+} did not change the emission wavelengths, only the relative intensities. Due to partial good energy overlap when $^2F_{7/2}$ Ce^{3+} manifold is populated, raising Ce^{3+} ions concentration enhanced the red UC emission versus green UC emission but also lead to significant decrease in the average lifetimes of all monitored emissions for Ho^{3+} and Er^{3+}. These lifetime decreases are explained by the energy loss in non-radiative pathways after the introduction of Ce^{3+}. In addition, the green to yellow color emission change through addition of Ce^{3+} was explored in $NaBiF_4$: Yb^{3+},Ho^{3+},Ce^{3+} to propose a novel application in two-level anti-counterfeiting.

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

COMUNICACIONES / COMMUNICATIONS

SPIE OPTO
22 – 27 enero [San Francisco, California, Estados Unidos de América]

Conferencia Invitada: **Tailoring the optical properties of broad-band molecular solar absorbers embedded into a Fabry-Pérot cavity.** L.Caliò; V. Esteso; C. Bujalance; H. Espinós; G. Lavarda; T. Torres; J. Feist; F.J. García-Vidal; G. Bottari; H. Míguez

Nanolight
6 – 12 marzo [Benasque, Huesca, España]

Conferencia Invitada: **Strong exciton-photon coupling in optoelectronic materials.** L.Caliò; H. Míguez

Póster: **Determination of the optical constants of transparent nanophosphor thin films.** M. Romero; E. Cabello-Olmo; G. Lozano; H. Míguez

Póster: **Plasmon-enhanced up-conversion photoluminescence in fluoride-oxyfluoride nanophosphor films.** T.T. Ngo; G. Lozano; H. Míguez

Póster: **Emission Properties of Lead-Halide Perovskite Nanocrystals and its Environmental Interaction.** M. Morán-Pedroso; A. Rubino; M.E. Calvo; J.P. Espinós; J.F. Galisteo-López; H. Míguez

Póster: **Optoelectronic devices based on scaffold stabilized black-phase $CsPbI_3$ quantum dots.** C. Romero-Pérez; A. Rubino; L. Caliò; M.E. Calvo; H. Míguez

Póster: **Optical antennas prepared by colloidal lithography enhance nanophosphor light emission.** J.M. Viaña; M. Romero; G. Lozano; H. Míguez

SPIE Photonics Europe 2022
3 – 7 abril [Estrasburgo, Francia]

Comunicación Oral: **Imprinted periodic surface textures enhace the directionality of the emission of thin phosphor films.** E. Cabello-Olmo; P. Molet; A. Mihi; G. Lozano Barbero; H. Míguez

Comunicación Oral: **Nanophosphor-based photonic architectures for efficient light conversion.** E. Cabello-Olmo; J.M. Viaña; T.T. Ngo; V. Castaing; G. Lozano; H. Míguez

PERSEPHONe Training Event (TE2)
5 abril [Sevilla, España]

Conferencia Invitada: **Optical modelling of planar perovskite structures and devices.** G. Lozano

2nd meeting Excelence Network of the Red MODE-Fotovoltaica
27 – 28 abril [Madrid, España]

Conferencia Invitada: **The Role of the Atmosphere on the Photophysics of Ligand-Free Lead-Halide Perovskite Nanocrystals.** M. Morán-Pedroso; A. Rubino; M.E. Calvo; J.P. Espinós; J.F. Galisteo-López; H. Míguez

14Th International Conference on Hybrid and Organic Photovoltaics HOPV22
23 – 25 mayo [Valencia, España]

Conferencia Invitada: **Ligand-free perovskite quantum dots embedded in porous matrices: synthesis, properties and optoelectronic devices.** H. Míguez

Comunicación Oral: **Template-assisted synthesis of optically active $CsPbI_3$ quantum dots.** C. Romero Pérez; A. Rubino, L. Caliò, M. Calvo Roggiani, H. Míguez García

Comunicación Oral: **Iodide Nanodomain Formation as Local Rearrangement Process during Phase Segregation in Mixed Halide Perovskites.** D.O. Tiede; J.F. Galisteo-López; M.E. Calvo; H. Míguez

Póster: **Optoelectronic devices base don scaffold stabilized black-phase $CsPbI_3$ quantum dots.** C. Romero Pérez; A. Rubino, L. Caliò, M. Calvo Roggiani, H. Míguez García

European Materials Research Society | EMRS Spring Meeting 2022
30 mayo – 3 junio [Virtual Conferencia]

Conferencia Invitada: **Transparent persistent luminescence films: from design to shimmering perspectives.** H. Miguez; G. Lozano; M. Ocaña; A.I. Becerro; E. Arroyo; V. Castaing

Comunicación Oral: **Highly versatile up-converting oxyfluoride-based nanophosphor films.** T. Tuyen Ngo; E. Cabello-Olmo; E. Arroyo; A.I. Becerro; M. Ocaña; G. Lozano; H. Míguez

3rd International Conference on Interface Properties In organic and Hybrid Electronic: Perspectives & Key Challenges | IPOE-2022
13 – 16 junio [Málaga, España]

Comunicación Oral: **Exciton-Photon Coupling of Subphthalocyanine-based Solar Absorbers Embedded into a Fabry-Pérot Cavity.** L. Caliò; V. Esteso; C. Bujalance; H. Espinós; G. Lavarda; T. Torres; J. Feist; F.J. García-Vidal; G. Bottari; H. Míguez

12th International Conference on Metamaterials, Photonic Crystals and Plasmonics
19 – 22 julio [Torremolinos, España]

Conferencia Invitada: **Localized Surface plasmon resonance in perovskite thin film embedding metallic nanoparticles.** L. Caliò; A. Bayles; S. Carretero-Palacios; A. Jiménez-Solano; G. Lozano; M.E. Calvo; H. Míguez

Applied Photonics
19 agosto [Vietnam]

Conferencia Invitada: **Upconverting nanophosphor-based photonics for different applications.** T. Tuyen Ngo; E. Cabello-Olmo; E. Arroyo; A.I. Becerro; M. Ocaña; G. Lozano; H. Míguez

Complex Nanophotonics Science Camp
2 - 5 agosto [Exeter, Reino Unido]

Comunicación Oral: **Ultra-Strong coupling phenomena in broadband light-harvesting molecules.** L. Caliò; V. Esteso; H. Míguez; C. Bujalance

The 6th International Conference on the Physics of Optical Materials and Devices And The 5th International Workshop of Persistent and Photostimulable Phosphors IWPPP-5
29 agosto – 2 septiembre [Belgrado, Serbia]

Conferencia Invitada: **Nanophosphor-based Photonic Materials provide fine control over the emission properties of rare-earth nanocrystals.** G. Lozano

Conferencia Invitada: **Transparent persistent luminescence films: from design to glowing perspectives.** V. Castaing; E. Arroyo; M. Ocaña; A.I. Becerro; G. Lozano; H. Míguez

Materials Science and Engineering | MSE 2022
27 - 29 septiembre [Online & Darmstadt, Alemania]

Conferencia Invitada: **Imprinted periodic surface textures enhance the directionality of the emission of thin phosphor films.** G. Lozano; E. Cabello-Olmo; H. Míguez

Comunicación Oral: **Improvement of up-conversion photoluminescence in fluoride-oxyfluoride nanophosphor films by implanting gold nanoparticles.** T.T. Ngo; G. Lozano; H. Míguez

Comunicación Oral: **Transparent coatings based on rare-earth doped garnets: from design to unique chameleon-like time-dependent chromaticity.** V. Castaing; G. Lozano; H. Míguez

Emerging Light Emitting Materials | EMLEM22
3 – 5 octubre [Limassol, Chipre]

Conferencia Invitada: **Photophysics of perovskite quantum dots coupled to optical cavities.** H. Míguez

The Foremost Photonics 2022
10 – 14 octubre [Erice, Italia]

Conferencia Invitada: **Hybrid light-matter states of optoelectronic materials coupled to optical cavities.** L. Caliò; C. Bujalance; V. Esteso; G. Lavarda; J. Feist; F.J. García-Vidal; G. Bottari; T. Torres; H. Míguez

Póster: **Photonics structures to control the spectral and directional properties of outcoupled light from nanostructured emitters.** E. Cabello-Olmo; G. Lozano; H. Míguez

Póster: **Ultra-Strong coupling of broadband light-harvesting dyes to an optical cavity.** C. Bujalance; V. Esteso; L. Caliò; H. Míguez

Seventh International Conference on Multifunctional, Hybrid and Nanomaterials
19 – 22 octubre [Genova, Italia]

Comunicación Oral: **Mesoporous Matrices as Hosts for Ligand -Free ABX3 Perovskite Quantum Dots.** M.E. Calvo

Sustainable Metal-halide Perovskites for Photovoltaics, Optoelectronics and Photonics
12 – 13 diciembre [Valencia, España]

Conferencia Invitada: **Optoelectronic devices based on ligand-free lead halide quantum dots embedded in porous matrices.** H. Míguez

CONGRESOS Y REUNIONES NACIONALES / NATIONAL CONGRESS AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

M. Ocaña (Comité Organizador)
A.I. Becerro (Comité Organizador)
E. Arroyo (Comité Organizador)
E. Gómez González (Comité Organizador)

COMUNICACIONES / COMMUNICATIONS

XIX Reunión del Grupo Especializado de Química Inorgánica y XIII Reunión del Grupo Especializado de Química del Estado Sólido | QIES 22
30 enero – 2 febrero [Sevilla, España]

Comunicación Oral: **$ZnGa_2O_4$:Cr^{3+}nanospheres with persistent luminescence: suitable candidates for biomedicine and optoelectronics.** E. Arroyo; V. Castaing; G. Lozano; M. Ocaña; A.I. Becerro

Póster: **Nanopartículas basadas en $NaY(MoO_4)_2$ con propiedades luminiscentes y fotocatalíticas.** N.O. Núñez; E. Gómez-González; R.M. Calderón-Olvera; A.I. Becerro; G. Colón; M. Ocaña

XVIII Escuela Nacional de Materiales Moleculares | EMMM2022
20 – 24 marzo [Santiago de Compostela, España]

Conferencia Invitada: **Hybrid light-matter states in molecular materials coupled to optical cavities.** H. Míguez

Comunicación Oral: **Eficient Charge Transport in Ligand-free $MAPbI_3$ Quantum Dot Solar Cell based on Nanoporous SiO2 Matrices.** L. Caliò; A. Rubino; M. Calvo; H. Míguez

NanoSpain 2022
17 – 20 mayo [Madrid, España]

Conferencia Invitada: **$HoPO_4$ bioprobes to increase contrast in ultra-high field MRI scanners.** E. Gómez-González; M. Ocaña; A.I. Becerro

SEMINARIOS DEL GRUPO MATERIALES ÓPTICOS MULTIFUNCIONALES / MOM SEMINARS

12 enero | **Incorporation of large organic A-site cations in 3D and 2D hybrid perovskites**
Dr. Gustavo de Miguel
Universidad de Córdoba

2 marzo | **Halide perovskites for sustainable optoelectronic devices: from energy to healthcare**
Dr. Miguel Anaya
University of Cambridge

9 junio | **Cavity optomechanics with exciton-polaritons condensates**
Dr. Andrés Reynoso
Universidad de Sevilla and Centro Atómico Bariloche

FORMACION / TRAINING

FORMACIÓN DE GRADUADOS / MASTER DEGREE THESIS

Título:	**Sintesis y caracterización de nanopartículas basadas en Eu^{3+}:$NaBi(MoO_4)_2$ con posibles aplicaciones en biomedicina**
Autor:	Sara Ruiz Herrera
Tutores:	Nuria O. Nuñez Álvarez, José Antonio Navío Santos
Grado:	Trabajo Fin de Máster
Centro:	Universidad de Sevilla
Fecha Defensa:	12 de julio de 2022

Título:	**Materiales particulados con luminiscencia persistente**
Autor:	Mª Hiedra Acosta Rivera
Tutores:	Ana Isabel Becerro Nieto, Manuel Ocaña Jurado
Grado:	Trabajo Fin de Máster
Centro:	Universidad de Sevilla
Fecha Defensa:	20 de septiembre de 2022

DOCENCIA / TEACHING

Investigadores de esta unidad participan en el Máster Interuniversitario "Láser, Plasma y Tecnología de Superficies" (ver ACTIVIDADES DIVULGATIVAS Y FORMATIVAS)

ESTANCIAS Y VISITAS DE PERSONAL DEL ICMS EN OTROS CENTROS
PERSONNEL OF THE ICMS IN OTHER LABORATORIES

Universidad de Oxford
Oxford, Inglaterra **Carlos Romero** 15/09/22 - 16/12/22

Department of Chemical Engineering and Biotechnology. Universidad de Cambridge
Cambridge, Inglaterra **Elena Cabello** 01/07/22 - 31/08/22

Departamento de Física de la Universidad Wake Forest
Salem, Estados Unidos de América **David Otto Tiede** 27/07/22 - 06/12/22

Grupo de Biofuncionalización de Nanopartículas y Superficies del Instituto de Nanociencia y Materiales de Aragón (CSIC-UNIZAR)
Zaragoza, España **Encarnación Arroyo Porriño** 06/06/22 - 30/07/22

Grupo "Pharmaceutical Chemistry of Nanocarrier Drug Delivery Systems" de la "School of Pharmacy and Pharmaceutical Sciences" en el "Trinity College Dublin"
Dublin, Irlanda **Elisabet Gómez González** 19/08/22 - 14/12/22

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 360° 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	Dr. Alberto Criado Vega
	Dr. Luis Esquivias Fedriani
	Dr. Víctorino Franco García
	Dra. Ángela María Gallardo López
	Dr. Antonio Muñoz Bernabé
	Dr. Javier S. Blázquez Gámez
Profesores Titulares	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
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	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

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
Víctorino Franco García	Josefa María Borrego Moro Jhon Jairo Ipus Bados

Procesado y Caracterización de Composites Cerámicos con Nanomateriales Laminados Bidimensionales

Código Code	Periodo Period	Organismo Financiador Financial Source	Importe Total Total Amount
PGC2018-101377-B-I00	01-01-2019 31-12-2022	Ministerio de Ciencia e Innovación	121.000 €

Investigador Principal Research Head	Componentes Research Group
Ángela Gallardo López Rosalía Poyato Galán	Antonio Muñoz Bernabé Ana Morales Rodríguez Felipe Gutiérrez Mora

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

Influencia de excitaciones múltiples sobre transiciones de fase termomagnéticas para aplicaciones energéticas

Código Code	Periodo Period	Organismo Financiador Financial Source
US-1260179	01-02-2020 30-04-2022	Junta de Andalucía

Investigador Principal Research Head	Componentes Research Group
Víctorino Franco García	Javier Sebastián Blázquez Gámez Josefa María Borrego Moro Alejandro Conde Amiano Clara Francisca Conde Amiano Jhon Jairo Ipus Bados

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	01-02-2020 31-12-2022	Junta de Andalucía

Investigador Principal Research Head	Componentes Research Group
Víctorino Franco García	Javier Sebastián Blázquez Gámez Josefa María Borrego Moro Alejandro Conde Amiano Clara Francisca Conde Amiano Jhon Jairo Ipus Bados

Fabricación y caracterización microestructural y mecánica de cerámicas de carburo de boro con estequiometría controlada (BORONCARB)

Código Code	Periodo Period	Organismo Financiador Financial Source
P18-RTJ-1972	01-11-2021 31-12-2022	Junta de Andalucía

Investigador Principal Research Head	Componentes Research Group
Francisco Javier Martínez Vázquez Bibi Malmal Moshtaghion	Francisco Luis Cumbreras Hernández

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 31-12-2022	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

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:	Víctorino Franco García
Componentes/Research group:	Jia Yan Law, Luis Miguel Moreno Ramírez

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.
- Colaboración con grupo de Frank Kern – Andrea Gommeringer, Universitat Stuttgart, IFKB (Institut für Fertigungstechnologie keramischer Bauteile)
- Colaboración con Katalin Balazsi, Head of Thin Film Physics Department, Hungarian Academy of Sciences, Centre for Energy Research, Budapest, Hungría

ARTÍCULOS PUBLICADOS EN REVISTAS SCI / PAPERS IN SCI JOURNALS

Mechanical properties of ceramics reinforced with allotropic forms of carbon

Morales-Florez, V; Domínguez-Rodríguez, A

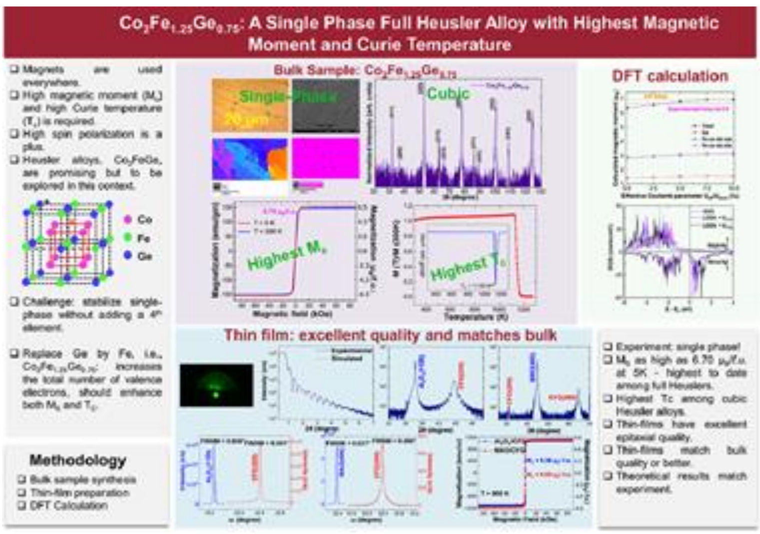
Progress in Materials Science, **128** (2022) 100966
Julio, 2022 | **DOI:** 10.1016/j.pmatsci.2022.100966

For decades, enormous investigation effort has been devoted to the fabrication of new ceramic matrix composites with enhanced mechanical properties. One of the most explored strategies is the addition of carbon allotropic phases such as carbon nanotubes, graphene, and carbon nanofibers due to their outstanding properties. In this review, the main fabrication protocols considered for the synthesis of the ceramic composites based on alumina and zirconia are shown, and their mechanical properties and the changes achieved by the addition of carbon allotropes are presented and discussed. Under particular circumstances, significant improvements in properties such as fracture toughness and wear at low temperature, or creep behavior and superplasticity at high temperature have been accomplished. Nevertheless, some critical aspects such as the homogenization of the carbon allotropes within the matrix are still lacking consolidated responses, which suggest that the potentialities of this reinforcing strategy have not yet been completely exploited. In summary, this work collects the fabrication strategies, major results, and main controversies of two decades of scientific research on the improvement of the fabrication methods and mechanical properties of ceramic matrix composites.

$Co_2Fe_{1.25}Ge_{0.75}$: A single-phase full Heusler alloy with highest magnetic moment and Curie temperature

Shambhu, KC; Mahat, R; Regmi, S; Law, JY; Franco, V; Mankey, G; Butler, WH; Gupta, A; LeClair, P

Acta Materialia, **236** (2022) 118112
Septiembre, 2022 | **DOI:** 10.1016/j.actamat.2022.118112



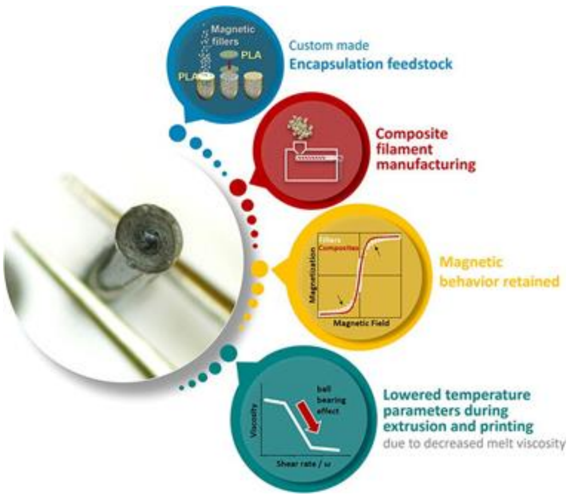
Elemental substitution by a different element is a well utilized technique of stabilizing a single-phase compound, in case the parent alloy is multi-phase, and this has been demonstrated specifically in a number of Heusler systems. This can, however, give an increased propensity for chemical disorder as well as adding complexity to synthesis and characterization.
In this paper, we present the successful synthesis of a single-phase compound, $Co_2Fe_{1.25}Ge_{0.75}$, by tuning the parent Co_2FeGe stoichiometry (which exhibits multi-phase structure) rather than introducing a fourth element. The compound is found to

crystallize in $L2_1$ structure (space group # 225). Magnetization measurements reveal $Co_2Fe_{1.25}Ge_{0.75}$ has a saturation magnetization as high as $6.7 \pm 0.1\ \mu_\beta$/f.u. at 5 K and a Curie temperature of 1135 ± 5 K – both being the highest reported to date for cubic full Heusler alloys to our knowledge. Thin films of $Co_2Fe_{1.25}Ge_{0.75}$ deposited on $Al_2O_3(110)$ and $MgAl_2O_4(100)$ substrates show excellent expitaxial quality, among the reported for Heusler films to date, and exhibit magnetic properties comparable to bulk samples. First principle calculations suggest the system exhibits total energy minimum at the experimentally-observed lattice parameter. Furthermore, the calculations corroborate the observed enhancement in magnetization and point to the importance of on-site Coulomb interactions. While our novel approach of substitution led to the discovery of stable $Co_2Fe_{1.25}Ge_{0.75}$ alloy with very high moment and Curie temperature that can be readily grown as a high-quality epitaxial thin film, making it a candidate for device applications, this approach can be taken as a new paradigm for the discovery of novel single-phase Heusler compounds with enhanced magnetic properties.

Functional, thermal and rheological properties of polymer-based magnetic composite filaments for additive manufacturing

Díaz-García, A; Law, JY; Felix, M; Guerrero, A; Franco, V

Materials & Design, **219** (2022) 110806
Julio, 2022 | **DOI:** 10.1016/j.matdes.2022.1108061

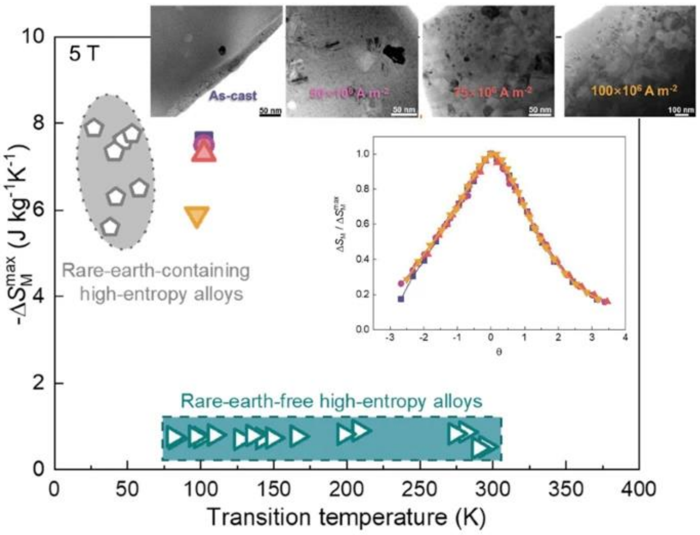


The design of functional composite filaments for fused filament fabrication requires a suitable polymer composition, functionality of particles, uniform distribution of fillers throughout the filament, and adequate printability. Uniform distribution at predictable concentrations is achieved by designing polymeric capsules containing the fillers and using them as feedstock for extrusion. Functionality can be inferred from that of the particles and target concentration. However, suitable conditions for printing strongly depend on polymer type and characteristics/concentration of fillers. Soft magnetic composite filaments were produced from polylactic acid (PLA) capsules filled with 30-52 wt. % maraging steel particles. Composite filaments preserve the soft magnetic character of the fillers. Fillers reduce the transition temperatures of the polymer by ti 5 K and have a profound impact on printability. Rheological characterization shows that the "ball bearing effect" of gas-atomized particles reduces the viscosity of the composites by more than one order of magnitude, decreasing printing temperature from 215 °C to 170 °C, associated with the lack of agglomeration of particles achieved by the proposed production method. Rheological experiments allow to detect the required changes in printing conditions without requiring an extensive and costly trial and error process of printing with a large set of printing parameters.

Enhancing the magnetocaloric response of high-entropy metallic-glass by microstructural control

Yin, HBC; Law, JY; Huang, YJ; Shen, HX; Jiang, SD; Guo, S; Franco, V; Sun, JF
Science China-Materials, **65** (2022) 1134-1142
Abril, 2022 | **DOI:** 10.1007/s40843-021-1825-1

Non-equiatomic high-entropy alloys (HEAs), the second-generation multi-phase HEAs, have been recently reported with outstanding properties that surpass the typical limits of conventional alloys and/or the first-generation equiatomic single-phase HEAs. For magnetocaloric HEAs, non-equiatomic $(Gd_{36}Tb_{20}Co_{20}Al_{24})_{100-x}Fe_x$ microwires, with Curie temperatures up to 108 K, overcome the typical low temperature limit of rare-earth-containing HEAs (which typically concentrate lower than around 60 K). For alloys with x = 2 and 3, they possess some nanocrystals, though very minor, which offers a widening in the Curie temperature distribution. In this work, we further optimize the magnetocaloric responses of x = 3 microwires by microstructural control using the current annealing technique. With this processing method, the precipitation of nanocrystals within the amorphous matrix leads to a phase compositional difference in the microwires. The multi-phase character leads to challenges in rescaling the magnetocaloric curves, which is overcome by using two reference temperatures during the scaling procedure. The phase composition difference increases with increasing current density, whereby within a certain range, the working temperature span broadens and simultaneously offers relative cooling power values that are at least 2-fold larger than many reported conventional magnetocaloric alloys, both single amorphous phase or multi-phase character (amorphous and nanocrystalline). Among the amorphous rare-earth-containing HEAs, our work increases the working temperature beyond the typical <60 K limit while maintaining a comparable magnetocaloric effect. This demonstrates that microstructural control is a feasible way, in addition to appropriate compositional design selection, to optimize the magnetocaloric effect of HEAs.



Additive manufacturing of magnetocaloric (La,Ce)(Fe,Mn,Si)$_{13}$–H particles via polymer-based composite filaments

Díaz-García, A; Revuelta, J; Moreno-Ramírez, LM; Law, JY; Mayer, C; Franco, V
Composites Communications, **35** (2022) 101352
Noviembre, 2022 | **DOI:** 10.1016/j.coco.2022.101352

Additive manufacturing could be an excellent way of shaping magnetocaloric heat exchangers in magnetic re-frigerators. However, the metal additive manufacturing techniques present the serious limitation that the melting of a magnetocaloric material can cause its transformation and the loss of functionality. Fused deposition modeling using polymer-based composite filaments is presented as a promising alternative as temperatures are low enough to preserve the magnetocaloric material. To prove this claim, a polymer-based composite filament containing 55 wt% of (La,Ce)(Fe,Mn,Si)$_{13}$-H magnetocaloric fillers has been manufactured using custom-made polymer capsules as the feedstock for the extrusion. Both adiabatic temperature change and isothermal en-tropy change have been characterized for the fillers, as-prepared filaments and as-printed parts, indicating that the magnetocaloric material functionality is not altered along the whole process. Printing resolution is comparable to the raw PLA filament.

Microstructure, magnetism and critical behavior of hot pressed Ni-Mn-Ga/Al magnetocaloric composites with enhanced thermal conductivity and mechanical properties

Zhang, YC; Franco, V; Wang, YF; Peng, HX; Qin, FX
Journal of Alloys and Compounds, **918** (2022) 165664
Junio, 2022 | **DOI:** 10.1016/j.jallcom.2022.165664

In the application of magnetic refrigeration technology, magnetocaloric materials are required to possess large magnetocaloric effect and broad working temperature range with good thermal conductivity and mechanical properties. To address this elusive combination of properties, we prepared Ni-Mn-Ga/Al magnetocaloric composites via hot pressing method. Phase composition and element distribution revealed the influence of sintering temperature on composites' microstructure. The magnetic properties and magnetocaloric effect of hot pressed Ni-Mn-Ga alloy and Ni-Mn-Ga/Al composites were studied, indicating their largely broadened working temperature range of 71 K and maximum magnetic entropy change of 2.2–3.0 J/(kg K). Based on thermomagnetic measurements, critical behavior was investigated via modified Arrott plots and Kouvel-Fisher method, and mean-field theory model could best explain the samples' critical behavior. The Ni-Mn-Ga/Al composite also possessed enhanced fracture stress of 306 MPa, much higher than that of bulk Ni-Mn-Ga alloy by arc melting. The good magnetocaloric response of the composites, which is comparable or even better than that of many other Ni-Mn-Ga particle and microwire counterparts, is accompanied by improved thermal conductivity and mechanical properties, extending the applicability of magnetocaloric materials with large specific surface area. The novel findings of this systematic study offer new insights into magnetocaloric composites and provide an approach to reach a significant balance when fulfilling multiple requirements of magnetic refrigeration technology.

Ageing-resistant zirconia/graphene-based nanostructures composites for use as biomaterials

Morales-Rodríguez, A; González-Orellana, C; Pérez-García, AA; López-Pernia, C; Muñoz-Ferreiro, C; Poyato, R; Gallardo-López, A
Journal of the European Ceramic Society, **42** (2022) 1784-1795
Abril, 2022 | **DOI:** 10.1016/j.jeurceramsoc.2021.11.060

This work explores the incorporation of graphene-based two-dimensional nanostructures as moisture barriers to delay hydrothermal ageing of yttria-stabilized zirconia and strengthen its use in biomedical applications. Two sets of highly dense zirconia composites incorporating multilayered graphene with very different lateral dimensions, few layer graphene and exfoliated graphene nanoplatelets, were prepared. The effect of the addition of graphene nanostructures on zirconia ageing was investigated by conducting accelerated hydrothermal degradation experiments in an autoclave. An improved resistance to low-temperature degradation and a high tolerance to damage were achieved in the composites compared to those of monolithic zirconia. The incorporation of 1 vol% multilayered graphene was very effective in restricting the hydrothermal degradation. In particular, the composite incorporating exfoliated graphene nanosheets exhibited outstanding resistance to ageing because of their fine dispersion throughout the matrix, which effectively seemed to restrict grain growth and slow the propagation of the transformation front to the ceramic bulk.

Rietveld analysis and mechanical properties of in situ formed La-β-Al_2O_3/Al_2O_3 composites prepared by sol-gel method

Rivero-Antunez, P; Morales-Florez, V; Cumbrera, FL; Esquivias, L
Ceramics International, **48** (2022) 24462-24470
Julio, 2022 | **DOI:** 10.1016/j.ceramint.2022.05.058

In this work, the crystal evolution of α-Al_2O_3 composites reinforced with LBA platelets were monitored by XRD Rietveld. In addition, the mechanical properties of totally densified specimens were researched by Vickers and Knoop indentations. These composite materials were prepared by a sol-gel process from alumina seeded boehmite sol and lanthanum nitrate. X-ray diffraction data have been studied by Rietveld refinements and line profile analyses, paying attention to the LBA formation, the evolution of vol%, and crystallite size of the different phases. It has been observed that the appearance of the LBA phase happens at a lower temperature than in samples prepared by a conventional solid state reaction. Indentation tests revealed that the presence of LBA microplatelets in the sol-gel samples leads to a significant increase of their indentation fracture resistance, in comparison to the conventional samples.

Fabrication of Porous Alumina Structures by SPS and Carbon Sacrificial Template for Bone Regeneration

González-Sánchez, M; Rivero-Antunez, P; Cano-Crespo, R; Morales-Florez, V
Materials, **15** (2022) 1754
Marzo, 2022 | **DOI:** 10.3390/ma15051754

In this work, a procedure for fabricating porous alumina with the use of a carbon sacrificial template has been tested in order to optimize the fabrication of porous structures mimicking the porosity and mechanical properties of the human cortical bone. Two different sources of sacrificial carbon were used and compared, and different sintering and calcination routes were considered. The porosity of the alumina structures studied by Hg porosimetry revealed that the amount of porosity and the size and shape of the pores are still below the required values, although some acicular pores were clearly observed by SEM. Moreover, measured mechanical properties (Young's modulus) remained below that of the bone, suggesting the need for further consolidation treatments. In summary, these encouraging results drive the optimization of future fabrication routes.

Effect of mixing the low-valence transition metal atoms *Y* = Co, Fe, Mn, Cr, V, Ti, or Sc on the properties of quaternary Hensler compounds $Co_{2-x}Y_xFeSi$ ($0 \leq x \leq 1$)

Mahat, R; Karki, U; Shambhu, KC; Law, JY; Franco, V; Galanakis, I; Gupta, A; LeClair, P
Physical Review Materials, **6** (2022) 064413
Junio, 2022 | **DOI:** 10.1103/PhysRevMaterials.6.064413

In this paper we report an experimental study of structural, magnetic, and mechanical properties of quaternary Heusler alloys $Co_{2-x}Y_xFeSi$ (Y = Co, Fe, Mn, Cr, V, Ti, or Sc, $0 \le x \le 1$) and the experimental findings are supported by ab initio electronic structure calculations. The alloys were synthesized using an arc-melting technique. Single phase microstructures are observed for all alloys substituted with low-valence transition metals *Y* except Sc. X-ray powder diffraction patterns at room temperature show the presence of Heusler-like face-centered cubic crystal structure in all single phase specimens. The low-temperature saturation magnetic moments, as determined from magnetization measurements, agree fairly well with our theoretical results and also follow the Slater-Pauling rule of thumb for half-metals, a prerequisite for half-metallicity. The alloys are predicted to exhibit half-metallic ferromagnetism by ab initio electronic structure calculations using the GGA+U approach. All stable compounds are observed to have high Curie temperatures with linear dependence with the valence electrons concentration in the alloys. Relatively high hardness values are also measured, approaching 15.7 GPa for Ti-substituted material, highest among the values reported for Heuslers so far. All these properties strongly suggest the alloys are promising for the spintronic applications at room temperature and above.

Enhanced Magnetocaloric Properties of Annealed Melt-Extracted $Mn_{1.3}Fe_{0.6}P_{0.5}Si_{0.5}$ Microwires

Luo, L; Law, JY; Shen, HX; Moreno-Ramírez, LM; Franco, V; Guo, S; Duc, NTM; Sun, JF; Phan, MH
Metals, **12** (2022) 1536
Septiembre, 2022 | **DOI:** 10.3390/met12091536

The highly regarded Fe_2P-based magnetocaloric materials are usually fabricated by ball milling, and require an additional extended annealing treatment at high temperatures (at temperatures up to 1423 K for several hours to days). In this work, we show that fabricating $Mn_{1.3}Fe_{0.6}P_{0.5}Si_{0.5}$ into the form of microwires attained 82.1 wt.% of the desired Fe_2P phase in the as-cast state. The microwires show a variable solidification structure along the radial direction; close to the copper wheel contact, Fe_2P phase is in fine grains, followed by dendritic Fe_2P grains and finally secondary $(Mn,Fe)_5Si_3$ phase in addition to the dendritic Fe_2P grains. The as-cast microwires undergo a ferro- to para-magnetic transition with a Curie temperature of 138 K, showing a maximum isothermal magnetic entropy change of 4.6 J kg^{-1} K^{-1} for a magnetic field change of 5 T. With further annealing, a two-fold increase in the maximum isothermal magnetic entropy change is found in the annealed microwires, which reveal 88.1 wt.% of Fe_2P phase.

Structural, Electronic, Magnetic, and Mechanical Properties of $Co_{2-x}V_xFeSi$ Heusler Alloys

Mahat, R; Shambhu, KC; Karki, U; Regmi, S; Law, JY; Franco, V; Galanakis, I; Gupta, A; LeClair, P
IEEE Transictions on Magnetics, **58** (2022) 2600105
Febrero, 2022 | **DOI:** 10.1109/TMAG.2021.3081466

The influence of V substitution for Co on the structural, electronic, magnetic, and mechanical properties of quaternary Heusler alloys $Co_{2-x}V_xFeSi$ (x = 0, 0.25, 0.50, 0.75, and 1) has been systematically investigated. The microstructural and the scanning profile using energy-dispersive X-ray analysis suggests the single-phase behavior in all alloys except for x = 1. The X-ray diffraction analysis at room temperature reveals the $L2_1$ crystal structure promoting lattice expansion after V substitution. The low-temperature saturation magnetic moments, as determined from magnetization measurements, agree fairly well with our theoretical results and also obey the Slater-Pauling rule. Very high Curie temperature is also observed. The alloys are mechanically robust. First-principles calculation with the implementation of a Hubbard correction term (U) is observed to predict half-metallic behavior.

CONGRESOS Y REUNIONES INTERNACIONALES / INTERNATIONAL CONGRESS AND MEETINGS

PARTICIPACIÓN EN LA ORGANIZACIÓN DE CONGRESOS Y REUNIONES / PARTICIPATION IN ORGANISING CONGRESSES AND MEETINGS

2022 Joint MMM-INTERMAG
10 enero – 15 enero [Nueva Orleans, Estados Unidos de América]

Víctorino Franco (General Chair)
Entidades Organizadoras: IEEE Magnetics Society y AIPP
Número de Participantes: 1509 participantes registrados

FORMACION / TRAINING

TESIS DOCTORALES/ DOCTOR DEGREE THESIS

Título:	**Effect of Microstructure on Magnetocaloric properties of High Entropy Alloys**
Autor:	Hangboce Yin
Directores:	Víctorino Franco García
Centro:	Universidad de Sevilla
Fecha Defensa:	2 de junio de 2022

Título:	**Métodos para la caracterización de materiales magnetocalóricos multifásicos**
Autor:	Álvaro Díaz García
Directores:	Víctorino Franco García
Centro:	Universidad de Sevilla
Fecha Defensa:	4 de julio de 2022

DOCENCIA / TEACHING

Investigadores de esta unidad participan en el Máster en Ciencia y Tecnología de Nuevos Materiales y en titulaciones de Grado y doble Grado de la Universidad de Sevilla (ver ACTIVIDADES DIVULGATIVAS Y FORMATIVAS)

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/cm^2 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 ESPECTROSCOPIAS / SPECTROSCOPY SERVICE

El Servicio de Espectroscopias incluye las Unidades de Espectroscopía Raman, Espectroscopía Infrarroja y Espectroscopía Ultravioleta-Visible. Este servicio está dedicado a la determinación de la estructura molecular de los compuestos químicos y la caracterización de materiales.

This Service consists of four different spectroscopies: Raman Spectroscopy, Infrared Spectroscopy and Ultraviolet-Visible 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. Juan Carlos Sánchez López, Dr. Hernán Míguez García y Dr. Miguel Ángel Centeno Gallego
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. Juan Carlos Sánchez López, Dr. Hernán Míguez García y Dr. Miguel Ángel Centeno Gallego
Personal Técnico/ Technical Assistant: Dr. Miguel Ángel Avilés Escaño

ESPECTROSCOPÍA ÓPTICA EN EL RANGO 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. Juan Carlos Sánchez López, Dr. Hernán Míguez García y Dr. Miguel Ángel Centeno Gallego
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 phyisisorption 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 Philips CM20 (200kV) con una resolución estructural de 0.14 nm entre líneas y 0.23 nm entre puntos, portamuestras de uno y dos giros y de calentamiento. 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.
  Philips CM200 microscope (200kV) with a structural resolution of 0.14 nm between lines and 0.23 nm between points. Sample holders with one and two angles and heating. It is equipped with a X-ray Energy Dispersive Analyzer (EDX X-Max 80T, Oxford Instruments) and a CCD GATAN camera for image acquisitions.

- 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: Dª Olga Montes Amorín (cicCartuja), 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)

Responsable Científico/ Scientific Responsible: Dra. Asunción Fernández Camacho, Dra. T. Cristina Rojas Ruiz

Personal Técnico/ Technical Assistant: Dª Olga Montes Amorín (cicCartuja) , 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, Dª Olga Montes Amorín (cicCartuja) y Dra. M. Carmen Jiménez de Haro

SERVICIO DE PREPARACIÓN Y CARACTERIZACIÓN DE SISTEMAS CATALÍTICOS HETEROGÉNEOS / SERVICE FOR THE 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

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).

Espectroscopía de Fotoemisión de Electrones / X-RAY Photoelectron Spectroscopy

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

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

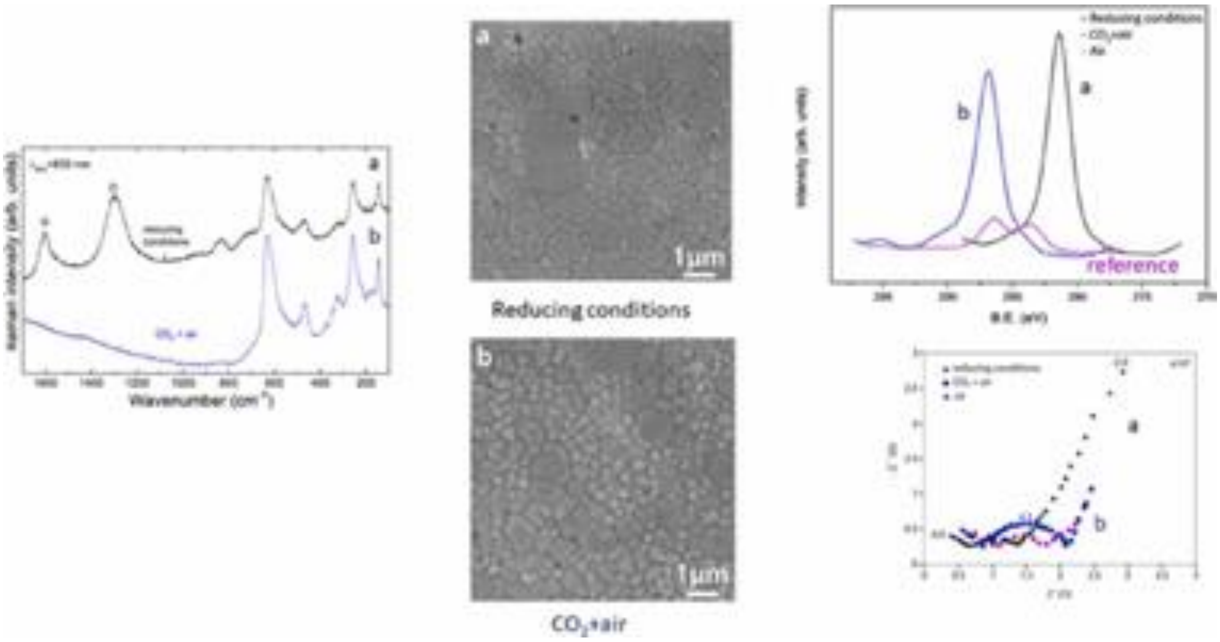
Personal Técnico/Technical Assistant: D. Juan Carlos Sánchez Martín, D. Adrián Gómez Castaño

Artículos Publicados en Revistas SCI / Papers In SCI Journals

Effect of sintering under $CO+N_2/H_2$ and CO_2+air atmospheres on the physicochemical features of a commercial nano-YSZ

MT Colomer, M. Simenas, J. Banys, F. Vattier, A. Gagor, M. Maczka

Journal of Alloys and Compounds, **904** (2022) 163976
Mayo, 2022 | **DOI:** 10.1016/j.jallcom.2022.163976



Given the need to process anodes and composites based on nano-YSZ in reducing or in air containing additional CO_2 atmospheres for the fabrication of solid oxide fuel cells (SOFCs), and solid oxide electrolysis cells (SOECs), we have studied the effect of the exposure to $CO+N_2/H_2$ or CO_2+air mixtures during sintering of YSZ green pellets, prepared from commercial nanopowders, on their structure, microstructure, chemical composition and their electrical properties. The reduced sample shows Raman bands at 1298 and 1605 cm−1 that are assigned to the D and G bands of carbon, respectively. The bands intensity ratio ID/IG indicates a larger content of disordered carbon. X-ray photoelectron spectroscopy (XPS) shows that C is present in the reduced samples as reduced carbon. However, the samples sintered in CO_2+air present C as carbonate-type. Impedance spectroscopy reveals that the highest total conductivity is for the reduced samples in the whole range of studied temperatures. In addition, sintering in CO_2+air causes a detrimental effect on the grain boundary conductivity and therefore, on the total electrical conductivity of YSZ. It can be due to the presence of impurities such as carbonates and oxidised or even, polymerised carbonaceous species located at those areas.

Monitoring the Simultaneous Implantation of Ti and Tb Cations to a Sacrificial Template and the Sol-Gel Synthesis of Tb-Doped TiO_2 (Anatase) Hollow Spheres and Their Transition to Rutile Phase

MT Colomer, F. Vattier
International Journal of Molecular Sciences, **23** (2022) 13162
Noviembre, 2022 | **DOI:** 10.3390/ijms232113162

Given Tb-doped TiO_2 (anatase) micro-hollow spheres (HSs) with nano-shells, in the range 0.00-3.00 at.% Tb, were successfully synthesized by a simultaneous chemical implantation route of both Ti and Tb cations from chlorides to a poly-styrene (PST)-co-poly-divinyl benzene (PDVB) sacrificial template, followed by controlled hydrolysis and polycondensation reactions. After water addition to the mixture of the precursors with the template, a decrease in the intensity and a shift to lower wavenumbers of the C=O absorption band in the IR spectra can indicate not only the anchoring of Ti and Tb ions to the carbonyl group of the template but also the hydrolysis of the implanted precursors. This latter process can involve a proton attack on the Ti-Cl, Tb-Cl and C=O bonds, the occupation of a vacant site by a water molecule, and then the dissociation of the dangling Ti-Cl, Tb-Cl ligands and C=O bonds. It gives rise to $Ti_{1-x}Tb_x[(OH)_{4-u}Cl_v]$@PST-PDVB and $Ti_{1-x}Tb_x[(OH)_{4-y}]$@PST-PDVB complexes (x = 0.00, 0.0012, 0.0170 and 0.030). Finally, polycondensation of these species leads to $Ti_{1-x}Tb_xO_2$-w'@PST-PDVB compounds. After subsequent thermal removal at 550 °C of the template, the IR bands of the core (template) totally vanished and new bands were observed in the 400-900 cm^{-1} region which can be attributed to the metalloxane bondings (M-O, M'-O, M-O-M, M-O-M' and/or M'-O-M', being M and M' = Ti and Tb, respectively, i.e., mainly vibration modes of anatase). Then, micron-sized HSs of TiO_2 and Tb-doped-TiO_2 (anatase) were obtained with nano-shells according to field emission gun scanning electron microscopy (FEG-SEM) and transmission electron microscopy (TEM) observations. Furthermore, X-ray photoelectron spectroscopy (XPS) measurements confirmed the presence of Tb^{4+} (38.5 and 41.2% for 1.70 and 3.00 at.% Tb, respectively) in addition to Tb^{3+} in the resulting HSs, with increasing Tb^{4+} content with both Tb doping and higher calcination temperatures. Then, these HSs can be considered as rare earth (RE) co-doped systems, at least for 1.70 and 3.00 at.% Tb contents being the transition to rutile phase favored by Tb doping for those compositions. Finally, diffusion of Tb from the inner parts to the surface of the HSs with the calcination treatments was also observed by XPS.

Reduction of N_2O with hydrosilanes catalysed by RuSNS nanoparticles

Molinillo, P; Lacroix, B; Vattier, F; Rendon, N; Suarez, A; Lara, P
Chemical Communication, **58** (2022) 7176-7179
Junio, 2022 | **DOI:** 10.1039/d2cc01470j

A series of RuSNS nanoparticles, prepared by decomposition of Ru(COD)(COT) with H_2 in the presence of an SNS ligand, have been found to catalyse the reduction of the greenhouse gas N_2O to N_2 employing different hydrosilanes.

Actividades Divulgativas y Formativas

Outreach and Teaching Activities

DOCENCIA / TEACHING

CURSOS DE POSTGRADO / POSTGRADUATE COURSES

MÉTODOS FÍSICOS DE ANÁLISIS DE CAPAS FINAS Y SUPERFICIES DE SÓLIDOS

Organizado por el Instituto de Ciencia de Materiales de Sevilla
Directores: Dr. Juan Pedro Espinós
Fecha de Celebración: 20 al 24 de junio de 2022
Horas lectivas: 25 de teoría + 15 de prácticas
Dirigido a: Grado de Doctor, Estudiante de Doctorado o Especialista de Empresa

Este curso de postgrado pretende familiarizar a los asistentes con algunos de los métodos físicos de análisis más utilizados en la actualidad para la caracterización, de materiales en general, y de capas finas y superficies en particular. El curso, de carácter intensivo y una semana de duración, consta de clases teóricas y sesiones prácticas. Estas últimas, desarrolladas con grupos de reducidos de alumnos, se realizarán con el equipamiento científico disponible en el Instituto de Ciencia de Materiales de Sevilla, el Centro Nacional de Aceleradores y el Servicio de Espectroscopía de Fotoelectrones de la Universidad de Sevilla.
El contenido y enfoque de los temas y otras actividades del curso son eminentemente prácticos, estando dirigido a científicos e ingenieros especializados en temas de análisis, diagnóstico, investigación en superficies, etc. También se considera especialmente adecuado para alumnos de tercer ciclo relacionados con la temática tratada.

Teoría**:**
Interacción de Fotones, Electrones e Iones con la Materia Condensada. Métodos Físicos de Análisis de Capas Finas y Superficies de Sólidos | Dr. Asunción Fernández Camacho
Espectroscopía de Fotoemisión de Rayos X: Composición Superficial | Dr. Juan Pedro Espinós
Espectroscopía de Fotoemisión de Rayos X: Estado Químico en la Superficie de Sólidos | Dr. Agustín R. González-Elipe
Pérdida de Energía de Electrones en Superficies: Perfiles de Composición y Caracterización Óptica en el EUV | Dr. Francisco Yubero Valencia
Plasmas en la Tecnología de Películas Delgadas | Dr. José Cotrino Bautista
Microscopía Electrónica de Efecto Túnel | Dr. Juan Ramón Sánchez Valencia
Microscopías de Fuerzas Atómicas | Dra. Carmen López Santos
Microscopía Electrónica de Transmisión: Fundamentos y Aplicaciones Generales | Dra. Asunción Fernández Camacho
Microscopía Electrónica de Barrido| Dra. María del Carmen Jiménez de Haro
Espectroscopías Electrónicas: X-EDS y EELS Imágenes Filtradas en Energía (EFTEM) | Dra. T. Cristina Rojas Ruiz

Nanomanipulación, Procesado y Análisis de Propiedades en el Microscopio Electrónico | Dra. Ana Borrás Martos
Análisis Tribológico y Mecánico de Capas Delgadas | Dr. Juan Carlos Sánchez López
La difracción y Reflectometría de Rayos X de Películas Delgadas | Dr. José María Martínez Blanes
Caracterización Óptica y Vibracional: UV-visible, Elipsometría y Color | Dr. Francisco Yubero Valencia
Caracterización Óptica y Vibracional: Fluorescencia, Infrarrojo y Raman | Dr. Ángel Barranco Quero
La absorción de Rayos X de Películas Delgadas | Dr. Juan Pedro Holgado Vázquez
Retrodispersión Rutherford: Perfiles de Composición | Dr. Francisco Javier Ferrer (CNA)

Prácticas:
a. Microscopías Electrónicas de Transmisión y Barrido | Dra. T. Cristina Rojas Ruiz | Dra. María del Carmen Jiménez de Haro | Lda. Olga Montes Amorín
b. Espectroscopía de Fotoemisión, XPS | Dr. Juan Pedro Holgado | Dra. Florencia Vattier
c. Difracción de Rayos X | Dr. José M. Martínez Blanes
d. Retrodispersión Rutherford | Dr. Javier Ferrer
e. Microscopía de Fuerzas Atómicas | Dr. Carmen López Santos | Dr. Juan Ramón Sánchez Valencia
f. Absorción de Rayos X, EXAFS y XANES | Dr. Juan Pedro Holgado

MÁSTER / MASTER

MÁSTER EN CIENCIA Y TECNOLOGÍA DE NUEVOS MATERIALES

Organizado por la Universidad de Sevilla
Coordinador: Dra. Regla Ayala Espinar
Fecha de Celebración: Curso Académico 2021-22
Créditos necesarios: 60
Dirigido a: Graduados en Física, Química, Ingeniería de Materiales, Ingeniería Química, Ingeniería de Sistemas de Defensa o Ingeniería Industrial.
Especialidades: Materiales para la Energía y el Medio Ambiente. Ingeniería de Superficies, Materiales Estructurales y Funcionales.
Mención de Calidad

Aplicaciones Tecnológicas de Materiales Funcionales (Créditos: 5) Dr. Víctorino Franco
Catalizadores para la Energía y el Medio Ambiente (Créditos: 5) Dra. Francisca Romero Sarria | Dr. José Manuel Córdoba Gallego
Corrosión y Recubrimientos Protectores (Créditos: 5) Dr. Leidy Marcela Martínez Tejada | Antonio Paul Escolano (US)
Física del Estado Sólido (Créditos: 5) Dra. Ángela Gallardo López | Dr. Diego Gómez García | Jhon Jairo Ipus Bados
Materiales con Funcionalidad Superficial (Créditos: 5) Dra. Leidy Marcela Martínez Tejada
Modelización Aplicada a la Caracterización Estructural de Medios Condensados (Créditos: 5) Dr. Carlos López Cartes (US) | Dra. Regla Ayala Espinar
Propiedades Magnéticas de Materiales (Créditos: 5) Dr. Víctorino Franco García

Procesado de Materiales Estructurales (Créditos: 5) Dr. Felipe Gutiérrez Mora | Dr. José Antonio Rodríguez Ortíz (US)
Propiedades Térmicas, Dieléctricas y Ópticas (Créditos: 5) Dr. Francisco J. Romero Landa
Química del Estado Sólido (Créditos: 5) Dr. Antonio Perejón Pazo | Dr. José Manuel Córdoba
Recuperación y Transformación de Materiales (Créditos: 5) Dr. Antonio Perejón Pazo | Dr. Leidy Marcela Martínez Tejada | Dra. Svetlana Ivanova
Síntesis de Materiales y Nanoestructuras (Créditos: 7) Dr. Luis Bobadilla Baladrón | Dra. Svetlana Ivanova
Técnicas de Caracterización de Materiales (Créditos: 8) Dra. Ana Morales Rodríguez | Dra. Anna Dimitrova Penkova | Dr. Joaquín Ramírez Rico | Dr. Juan Manuel Montes Martos (US)
Trabajo (Créditos: 10) | Dra. M. Dolorez Alcalá González | Dr. Francisco Javier Aparicio Rebollo | Dra. Regla Ayala Espinar | Dr. Luis F. Bobadilla Baladrón | Dr. Alfonso Caballero Martínez | Dr. José Manuel Córdoba Gallego | Dra. M. Isabel Domínguez Leal | Dr. Víctorino Franco García | Dr. Diego Gómez García | Dr. Felipe Gutiérrez Mora | Dra. Svetlana Ivanova | Dr. Víctor López Flores | Dra. Cristina López Pernía | Dra. M. Carmen López Santos | Dra. Leidy Marcela Martínez Tejada | Dra. Rocío Moriche Tirado | Dr. Manuel Oliva Ramírez | Dra. Esperanza Pavón González | Dra. Anna Dimitrova Penkova | Dr. Antonio Perejón Pazo | Dr. Tomás Ramírez Reina | Dr. Joaquín Ramírez Rico | Dra. Francisca Romero Sarria | Dr. Pedro Enrique Sánchez Jiménez

Asimismo, 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.

CONFERENCIAS INVITADAS IMPARTIDAS POR PERSONAL DEL ICMS
INVITED CONFERENCES BY PERSONNEL OF THE ICMS

13 Mayo | **Recubrimientos solares selectivos en forma de multicapas CrALN para colectores termosolares de concentración**
Dra. T. Cristina Rojas Ruiz
Lugar: Charla on-line, Universidad de SINU (Colombia)

30 Septiembre | **Hybrid light-matter states in molecular materials coupled to optical cavities**
Dr. Hernán Míguez
Lugar: ICIQ Auditorium. Institute of Chemical Research of Catalonia (Tarragona)

7 Octubre | **Lanthanide-Based Nanoparticles for Bioimaging applications**
Dr. Manuel Ocaña Jurado
Lugar: Facultad de Farmacia, Universidad de la Laguna (Tenerife)

11 Noviembre | **Functional applications of nanostructured surfaces developed by plasma and vacuum technologies: from energy harvesting to wetting**
Dra. Ana Isabel Borrás Martos
Lugar: Màsters Química de Materials Aplicada. University of Barcelona

5 Diciembre | **Luminophores persistants: des étoiles phosphorescentes aux nanodispositifs avancés pour la médecine**
Dr. Víctor Castaing
Lugar: Instituto Néel. Francia

CONFERENCIAS Y SEMINARIOS IMPARTIDOS EN EL ICMS
CONFERENCES AND SEMINAR IN THE ICMS

27 abril | **Materials for bioimaging and nanothermometry at IRCP Chimie-ParisTech, France; focus on the control of the kinetics**
Prof. Bruno Viana
PSL University IRCP Chimie-ParisTech

In bioimaging, the development of luminescent materials in various shapes (from nanoparticles to single crystals) requires perfect materials with high fluorescence intensity but also with careful control of the defects which could affect the kinetic of the luminescence. For instance, afterglow should be avoided in the scintillator domain in order to obtain clear and fast images. In that case the defects/traps must be carefully controlled to avoid room temperature detrapping and afterglow. Furthermore, on the opposite case, there is a large interest for materials with long afterglow or persistent luminescence. Several new applications are envisioned with these materials such as emergency signing, luminous painting, etc. Recently this concept was also proposed for the development of new optical imaging modalities. At nanoscale, deep red and near-infrared persistent luminescence nanoparticles enable highly sensitive in-vivo optical detection and complete avoidance of tissue autofluorescence [1].
Nanophosphors could also be used to measure thermometry at nanoscale and this appears to be the solution of choice to perform in-vitro and in-vivo temperature readings at cellular scale in real-time. This was the topic of the recent NanoTBTech EU2020 project [2]. Our study highlights that interaction between light and biological tissues is one main challenge to perform robust temperature readings with nanothermometry based on emission spectra. Surface functionalization of these photonic nanoprobes can be adjusted as well as the wavelength of the optical stimulation to favour multiple challenging biomedical applications.

References:
[1]B Viana et al., in “NIR-persistent luminescence nanoparticles for bioimaging, principle and perspectives” Book chapter in Near Infrared-Emitting Nanoparticles for Biomedical Applications, Nature Sringer, 163-197 (2020), D. Jaque et al. ed.
[2] http://nanotbtech.web.ua.pt/

26 septiembre | **Small scale high performance photonic devices for biomedical, agricultural, and environmental applications**
Prof. Ibrahim Abdulhalim
Department of Electro-Optics and Photonics Engineering and The Ilse Katz Institute for Nanoscale Science and Technology, ECE School, Ben Gurion University, Israel

Developments in nanotechnology, electronics, computing, algorithms, imaging, and fabrication technologies are assisting us in miniaturizing optical/photonic devices to become portable and suitable for point of care and field applications. During the last 10 years we have been working on different technologies for this purpose including full field optical coherence tomography, plasmonic sensors, and spectral/polarization control liquid crystal devices.
In this lecture I will review our miniaturized devices developed for these purposes including spectro-polarimetric imaging module based on unique liquid crystal devices demonstrated for skin cancer detection, plasmonic sensor with less than 1kg weight and small form factor demonstrated for detecting biomarkers, viruses, bacteria and other analytes, SERS sensors with ultrahigh enhancement, and more.

References:

1. Lior Graham, Yitzhak Yitzhaky and I. Abdulhalim, Classification of skin moles from optical spectro-polarimetric images, J. Biomed. Optics 18, 111403 (2013).
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21 octubre | **The road to flexible and sustainable nanomaterials-based energy storage devices**
Dr. João Carlos Mesquita Coelho
CENIMAT|i3N – NOVA School of Science and Technology (FCT-NOVA), Costa da Caparica, Portugal

In the last few years, a lot of interest has been shown in nanomaterials, which can exhibit enhanced or totally new properties when compared to their bulk counterparts.1–4 For instance, the confinement

of charge and heat in two dimensional (2D) graphene results in outstanding electrical, optical and mechanical properties. Not surprisingly, a wide range of nanomaterials has been suggested for several industrial applications.5–7 Special attention has been given to the role of nanomaterials in the energy sector due to the ongoing climate change and transition to greener energy sources. In addition, the advent of digital manufacturing technologies, such as 3D, inkjet printing and laser process/patterning demonstrated a huge potential to disrupt and create technologies such as wearable electronics and flexible, stretchable portable devices. A key technical constraint for the large-scale utilization of these devices is energy autonomy, which requires the development of flexible energy sources/storage systems, such as micro-supercapacitors and thin-film Li/Na-ion batteries. Inks based on conductive nanomaterials are promising material platforms for these flexible devices. For instance, due to their superior mechanical and electrical properties, carbon nanotubes (CNTs) and graphene, can be implemented as efficient current collectors, thus removing the need for bulky/heavy metallic components, while nanomaterials are responsible for the energy storage process.8,9 In order to maximize the exploitation of these material properties, optimized inks, formulations and depositions methodologies must be designed and characterized. Considering the wider societal awareness towards environmental issues and on-going legislations, energy storage devices of the future will have to be based in efficient, eco-friendly, and sustainable manufacturing processes.
In this talk, I will exhibit the advantages of 2D based energy storage devices along with approaches for their sustainable fabrication. A special attention will be given to green solvents, such as cyrene, and biodegradable substrates such as paper and cork. The combination of nanomaterials and efficient eco-friendly manufacturing technologies will open the avenue for the large-scale production of ultra-light and thin flexible energy storage devices. Additionally, by defining a smart integration approach based on hybrid electronics the pro-posed methodology will further close the gap between conventional and flexible electronics.

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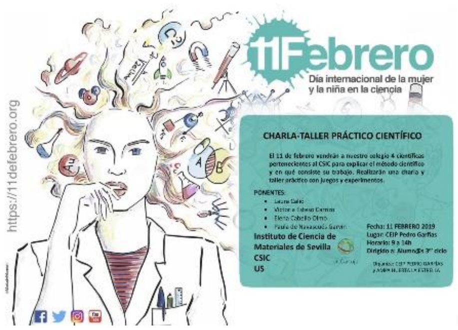
24 Noviembre | **Aerodynamic levitation, laser melting, and the synthesis of new functional ceramics**
Dr. Michael Pitcher
Laboratorio de Materiales en Condiciones Extremas (CEMHTI), Orleans, Francia

20 diciembre | **Smart acoustofluidic platform based on thin film acoustic wave technology**
Dr. Richard YongQing Fu
Faculty of Engineering and Environment, Northumbria University, Newcastle, UK

This talk will focus on acoustofludics platform and lab-on-chip applications based on piezoelectric thin film acoustic wave technology, which shows a broad range of functions such as biosensing, particle/cell concentrating, sorting/patterning, pumping, nebulisation, heating and jetting. Integrated acoustic wave sensing/microfluidic devices have been fabricated by depositing these piezoelectric films onto a number of substrates such as silicon, ceramics, diamond, quartz, glass, and more recently also polymer, metallic foils and bendable glass/silicon for making flexible devices. Such thin film acoustic wave devices have great potentials for implementing integrated, disposable, or bendable/flexible devices into various sensing and actuating applications, using portable, wireless, flexible and remotely controlled acoustic wave devices.

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:

Mujeres en nanotecnología y nanomedicina. Encarnación Arroyo Porriño. Colegio Salesiano Nuestra Señora del Águila, Alcalá de Guadaíra ,11/02/2022.

Nanomateriales y microscopía. Un dúo inseparable para un paradigma de energía sostenible. Gisela Mariana Arzac Di Tomaso. Biblioteca de San Jerónimo. 11/02/2022.

Mujeres en ciencia de materiales. T. Cristina Rojas. CDP Giner de los Rios, Montequinto. 11/02/2022 y Colegio San Alberto Magno de Montequinto 15/02/2022.

Nanopartículas luminiscentes para el diagnóstico de enfermedades. Ana Isabel Becerro Nieto. Colegio Salesianos de Trinidad. 11/02/2022.

Como convertir energía Mecánica en electricidad. Ana Borrás. Instituto San Juan Bosco de Jaén. 11/02/2022.

Charlas-Talleres

Plasmania: Carmen López Santos. 09/02/2022 en el IES Triana de Sevilla. 10/02/2022, IES Luis Vélez de Guevara de Écija (virtual). 11/02/2022 en el CEIP Maria Auxiliadora de los Palacios y Villafranca (virtual),

Nanotecnología para energía limpia. Lidia Contreras Bernal y Javier Castillo. 10/02/2022, IES Ibn Jaldún. Dos Hermanas, Sevilla. 17/02/2022 Colegio Adharaz. Altasierra, Espartinas.

¿Que hacen los científicos? Gloria Moreno, Laura Montes y Carmen López. CEIP La Salle Las Salesianas, 23/02/2022

Celebración 11F y presentación Sound of Ice y 3DScavengers . Grupo de nanotechnology on surfaces and plasma. Club de voleibol Las Flores. 06/02/2022

Mujeres Científicas – Taller celdas solares de frutos rojos: CEIP Pedro Garfias 11/02/2022

FESTIVAL DE NANOCIENCÍA Y NANOTECNOLOGÍA 10 A LA MENOS 9 / NANOSCIENCE AND NANOTECHNOLOGY 10 A LA MENOS 9

10ALAMENOS9
Festival de Nanociencia y Nanotecnología

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.

DIAS 22 Y 25 ABRIL: VISITA ALUMNOS DEL COLEGIO LAS SALESIANAS DE SEVILLA

PROGRAMA:

Charla “Bienvenidos al mundo de los nanomateriales”: Juan Ramón Sánchez Valencia.
Talleres: Fabricación de una celda solar de colorante: Mauricio Calvo. Carlos Romero y Laura Calio**. Superficies autolimpiables:** Mª Carmen Hidalgo y Nuria Núñez
Visita guiada a los laboratorios: Cómo preparamos y vemos los nanomateriales. Encarnación Arroyo. Jorge Gil, Juan Carlos Sánchez, Elena Cabello, Laura Calió, Mª Carmen Jiménez y T. Cristina Rojas

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: de la categoría A: Miguel Sánchez Liñán del Colegio San Juan Bosco de Sevilla, con su relato titulado “Nanoconocimiento”.
El jurado dejo desierta la categoría B al no reunir las obras presentadas un mínimo de calidad.

FERIA DE LA CIENCIA / FAIR OF SCIENCE

La 20 Feria de la Ciencia de Sevilla del 2022, 3ª Feria Virtual (del 12 al 14 de mayo de 2022), 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.
Las actividades realizadas en stand del ICMS, con título: Materiales Avanzados: Almacenando energía térmica, se centraron en dos de los ejes temáticos de la Feria: Ciencias para el Desarrollo Sostenible y Acción por el clima y fueron coordinadas por la unidad de Mecanoquímica y reactividad de Materiales.
Participantes: Luis Pérez Maqueda, Antonio Perejón y Pedro Sánchez, Juan Jesús Arcenegui, Virginia Moreno, Sandra Molina, Eva Gil, Nabil Mohamed, Alejandro Fernando Manchón, Juan Luis Martín, Guillermo Torres, Estela Ruiz, Sergio Carrasco, Gloria Moreno, Gisela Arzac, T. Cristina Rojas, Mª Carmen Hidalgo, Víctor Rico, Nuria Núñez, Encarnación Arroyo, Ana Isabel Becerro, Elisabet Gómez, Rosana Calderón, Mª Hiedra Acosta, Rosalía Poyato, Carmen Muñoz, Cristina López, Xavier García, Laura Montes, Javier Castillo, Elena Cabello, Clara Bujalance, Maria Morán.

The Fair of Science (12 to14 May 2022, 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. In this year, the ICMS stand were entitle: Materiales Avanzados: Almacenando Energia térmica.

PARTICIPACION EN LA NOCHE EUROPEA / EUROPEAN RESEARCHERS' NIGHT

LA NOCHE EUROPEA
DE L@S INVESTIGADOR@S
MUJERES Y HOMBRES QUE HACEN CIENCIA PARA TI

La Noche Europea de los Investigadores (#NIGHTspain. www.lanochedelosinvestigadores.es) celebrada el 30 septiembre de 2022 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:

- Luminiscencia y Nanociencia: Sus Interesantes Aplicaciones. Ana Isabel Becerro y Encarnación Arroyo
- La magia de los Materiales. Rosalía Poyato, Ángela Gallardo, Rocío Moriche, Carmen Muñoz, Felipe Gutiérrez y Elisa Guisado

- Ma-tch-teriales: Un torneo de rapidez visual ¿ Serás el primero en encontrar el símbolo común en la Ingeniería de Materiales? Rosalía Poyato, Ángela Gallardo, Rocío Moriche, Carmen Muñoz, Felipe Gutiérrez, y Elisa Guisado

SEMANA DE LA CIENCIA Y LA TECNOLOGÍA / SCIENCE AND TECHNOLOGY WEEK

La semana de la Ciencia (celebrada del 7 al 11 de noviembre de 2022) 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. El Plasma . El Rey Midas de los materiales. Dr. Juan Carlos Sánchez-López

MATERLAND / MATERLAND

MATERLAND

El ICMS ha participado y coordinado algunas de las actividades realizadas en el proyecto Bienvenidos a Materland: Acercándonos al maravilloso mundo de los materiales, proyecto financiado por la FECYT y donde han participado 100 personas de 22 centros distintos que cubren diferentes ámbitos de la Ciencia e Ingeniería de Materiales y con titulaciones en física, química, biología, ingeniería de materiales, mecánica, industrial, arquitectura, etc. de centros de investigación, universidades e institutos de secundaria

En el proyecto se han realizado 7 actividades englobadas en cuatros grandes áreas de trabajo:

A) Creación de material divulgativo para poner a disposición de centros educativos

B) Trabajos de investigación y experimentación

C) Otras actividades de divulgación

D) Congreso Nacional de Divulgación de Materiales (CNDMAT22D) y Exposición de Materiales

Las actividades y el material realizado pueden verse en la web (http://materland.sociemat.es/)

Participantes del ICMS: Carlos Romero, T. Cristina Rojas, Mª Carmen Hidalgo, Encarnación Arroyo, Rosalía Poyato, Carmen Muñoz, Javier Castillo, Elena Cabello, Gerardo Colón, J. Pedro Holgado, J. Carlos Sánchez-López, J Ramon Sánchez-Valencia, Lidia Contreras, Mauricio Calvo, Rocío Moriche

CIENCIA EN EL SUR

Ciencia en el sur: Participación en el **III Encuentro de comunicadores/as y divulgadores/as del CSIC Andalucía y Extremadura**, celebrado en Sevilla los días 22 y 23 de noviembre, con la ponencia: Bienvenidos a Materland: acercándonos al maravilloso mundo de los materiales. T. Cristina Rojas

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