BCMATERIALS
BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES
ehugroup

EUSKO JAURLARITZA
GOBIERNO VASCO

ikerbasque
Basque Foundation for Science

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

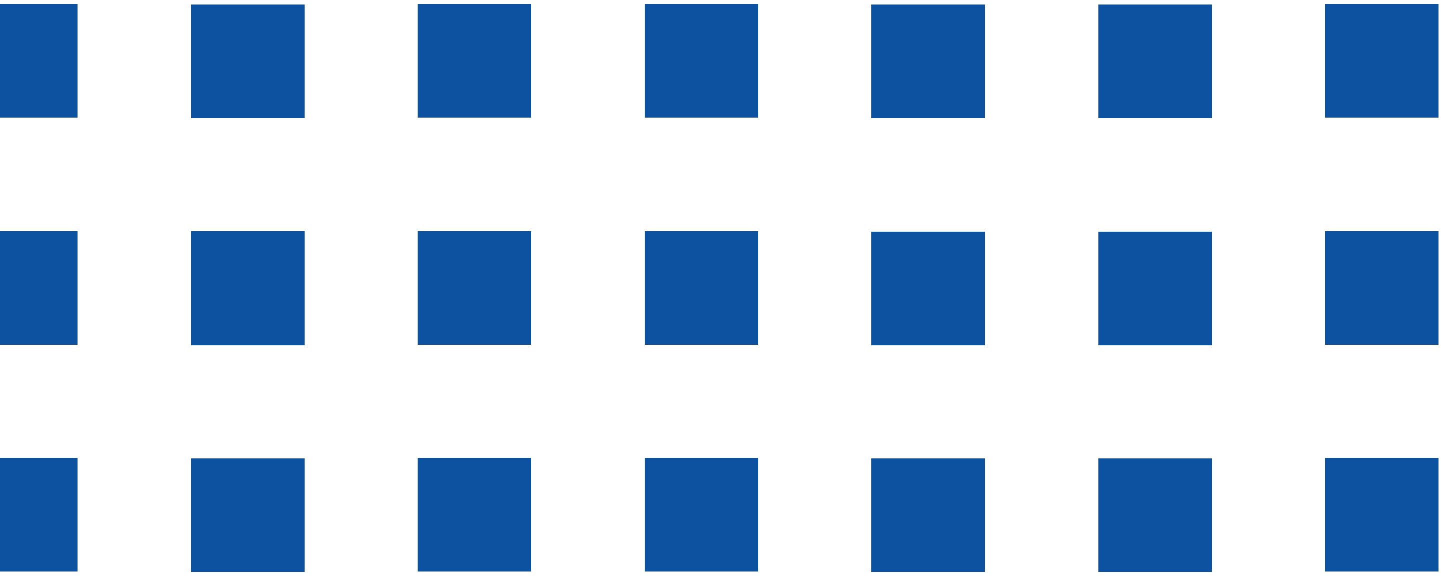
20
ANNUAL
REPORT
24

BCMATERIALS
BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES
ehugroup

EUSKO JAURLARITZA
GOBIERNO VASCO

ikerbasque
Basque Foundation for Science

Universidad del País Vasco
Euskal Herriko Unibertsitatea



20
ANNUAL
REPORT
24

CONTENTS

FOREWORD

2024 HIGHLIGHTS

THE CENTER 01

RESEARCH ACTIVITY 02

Research areas

Research lines

Transverse Research Lines

PROJECTS & TECH-TRANSFER 03

OUR SERVICES 04

OUTREACH ACTIVITIES 05

COMMITTED TO THE BENEFIT OF SOCIETY

Senentxu Lanceros-Méndez
Scientific Director

Dear colleagues and friends,

It is always one of the greatest pleasures of the year for the Director to write the forewords of our **annual report**. Since the first one in 2019 to the one I am writing right now, we have experienced an **impressive growth** in number of working colleagues, infrastructures, national and international collaborations, projects, outreach activities… and, mainly, in the excellent contributions we provide to advance in knowledge and technology for the benefit of the society and fulfil our mission to provide "new materials for a better life".

This growth has occurred in an **extremely dynamic contest** with profound and dramatic globally impacting events, from the pandemic to the burst of unjustifiable conflicts, that have placed science, technology and materials in the middle of the social attention.

Energy transition, environmental sustainability, digitalization and biomedical advances are just possible with new materials and materials technologies. Materials value chains, from providers to end uses and end of life strategies are at the center of social and political discussions… and geopolitical conflicts…

We, as a research center in **advanced materials**, are thus also at the middle of those strong efforts and development and must assume this position with ever evolving focus, ambition and responsibility, being aware on the potential of our contributions and the need of our commitment.

> **I am not afraid of storms, for I am learning how to sail my ship.**
>
> 'Little women' (1868)
> Louisa May Alcott (1832-1888)

We do publish, but the goal are not publications. We do get funding, but the goal is not to obtain money. We do participate in meetings, teaching and outreach activities, but the goal is not to show ourselves. The goal is plain and simple: **to generate knowledge and translate that knowledge in the best possible way for the benefit of society.** The rest are tools.

This relevant and noble goal can be only achieved with **focus, objectivity, commitment, collaboration** and addressing the **grand challenges** we are facing nowadays.

Over the years we have built up teams, conditions and abilities. We have defined areas, designed strategies and gained competence. We have been growing in impact and ambition, as well as in social responsibility and commitment.

The **2024 year report** you are about to read demonstrates the maturity of a center ready to tackle the most relevant challenges that materials and materials technologies present nowadays. A scientific report that demonstrates commitment with excellence, compromise with technology transfer, with the formation of young scientist and with society.

For the latter, it is particularly relevant the new activity **"Materials for Society"**, a forum of discussion of the intersection of materials science with art, philosophy, sociology, ethics and all other dimensions of human life.

No human activity is innocuous, and we must be well aware of the strong benefits but also on the multivalence implications of our activity and our research results.

We are in an uncertain historical moment with rapidly evolving priorities and potential game changing events. We must be prepared as a center and as individuals to maximize impact and contribution to positive development.

Maintain, refine or implement conditions for creative, collaborative and excellent atmosphere for relevant work, grow in local, national and international collaborations, focus on what really matters and contribute timely and properly with "materials for a better life" should not just be our goal and mission, but our reason to be and way of being as a research center.

Enjoy this this **2024 scientific report**, reflecting the excellent contributions of **BCMaterials members, colleagues and friends**. Contributions reflecting each person, each action and each interaction making possible the existence of BCMaterials as an excellence research center.

In this rapidly changing world and with many of the current challenges asking for next generation materials, **our best contribution** remains to believe in our ability to contribute to tackle those challenges that open the possibility of a more interconnected, sustainable, peaceful, healthier and efficient world, in which a "better life" is always possible.

> **The same night whitening the same trees.**
> **We, the ones then, are not the same.**
>
> 'Twenty Love Poems and a Song of Despair' (1924)
> Pablo Neruda (1904-1973)

2024 HIGHLIGHTS

93

ONGOING PROJECTS

A record figure for BCMaterials in terms of ongoing projects, with a total funding of 6,700,000 euros. 23 of these projects are funded by the European Union.

246

INDEXED PUBLICATIONS

In 2024, we produced 246 scientific publications, including 2 books and 15 book chapters. 85% of our papers were published in Q1 journals. An excellent scientific output.

NEW PATENT

In collaboration with the Gaiker technology centre, we obtained an important patent corresponding to a tactile actuator for robotic arms.

NEW LAB EQUIPMENT

In addition to the works to equip two new laboratories, BCMaterials acquired uniquely valuable equipment for its research, also open to use by those who require our services.

3 BIG EVENTS

2024 was a year in which BCMaterials put its capacity to organise scientific events to the test with three major conferences between July and November: the 44GERSEQ electrochemistry congress, the IMOH2024 neutron science conference and the annual New Materials for a Better Life! workshop.

01

THE CENTER

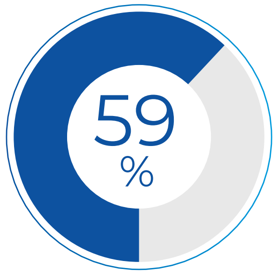
BCMaterials, Basque Center for Materials, Applications and Nanostructures, is an autonomous research center launched in June 2012 by Ikerbasque, the Basque Foundation for Science and the University of the Basque Country (UPV/EHU) as a research center for Materials, Applications and Nanostructures. The center is included in the BERC's (Basque Excellence Research Centers) network and its mission is to generate knowledge on next generation materials, turning this knowledge into (multi)functional solutions and devices for the benefit of society.

BCMATERIALS
IN NUMBERS

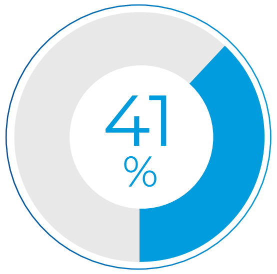
RESEARCH COMMUNITY

218

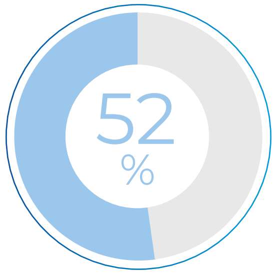
RESEARCHERS
Visitors included



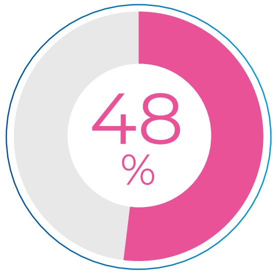
National= 130



International=88



Men= 112

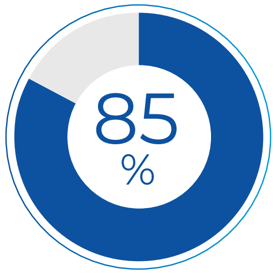


Women=106

RESEARCH OUTPUT

246

SCOPUS
Indexed Items



Q1 Publications

2

BOOKS

15

BOOK CHAPTERS

88

H INDEX

10997

CITATIONS

PROJECTS & FUNDING

93

ONGOING PROJECTS

= 6.700.000 €

FUNDING

TRAINING

14

PHD
Thesis Defended

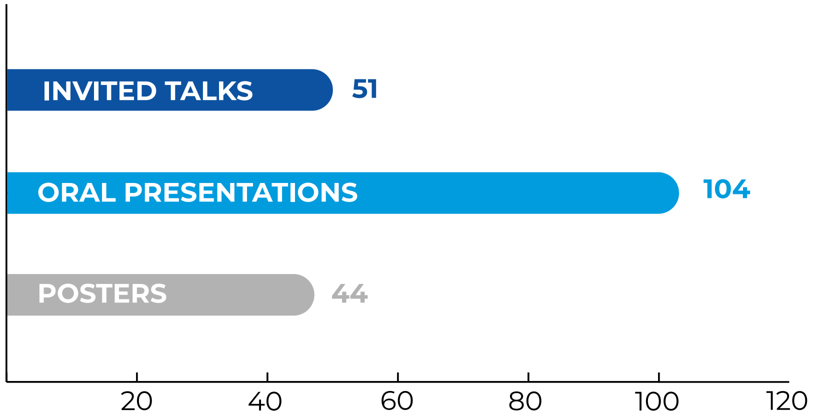
15

Master
Thesis Defended

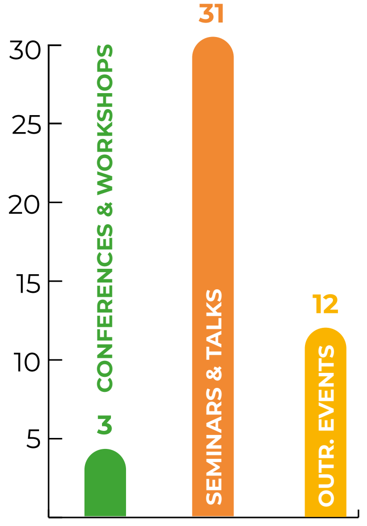
13

Final Degree
Projects Defended

OUTREACH

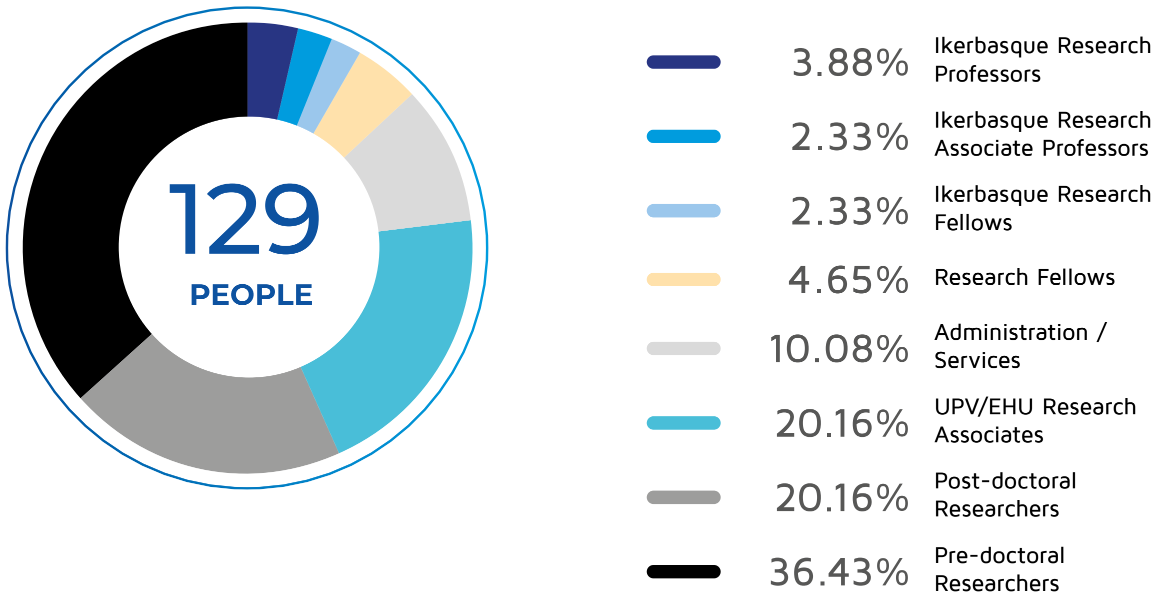


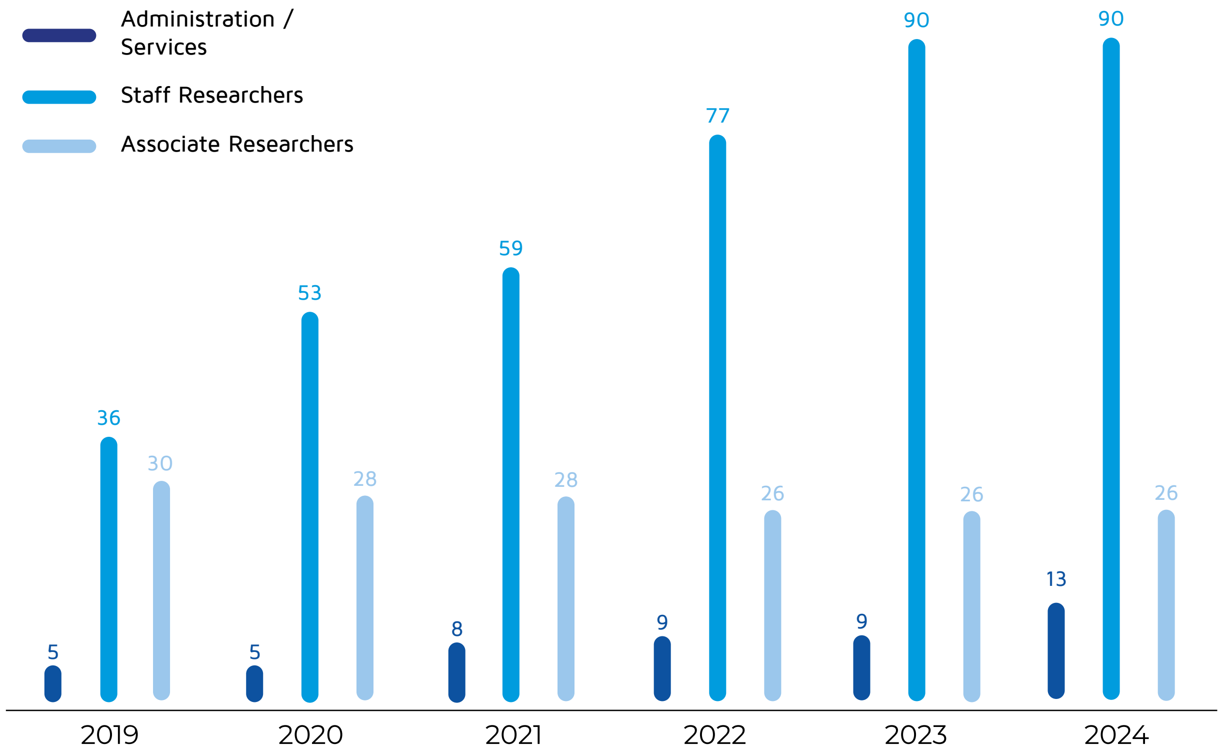
OUTSIDE BCMATERIALS



ORGANIZED BY OR WITH PARTICIPATION OF BCMATERIALS

BCMATERIALS COMMUNITY





INTERNATIONAL REPRESENTATION

Argentina		1
Belgium		2
Brazil		1
China	1	2
Colombia	5	10
Croatia		1
Czech Rep.	1	
Egypt		1
France		2
Greece		1
Hungary		3
India	6	4
Iran	1	
Italy	2	2
Kazahkstan		4
Mexico		1
Morocco	1	1
Pakistan	3	
Poland		1
Portugal	4	9
Russia	4	
Spain	81	49
Tunisia	1	6
Turkey		1
Ukraine	2	
UK	2	
USA	2	1
Venezuela	1	

116
STAFF & ASSOCIATE RESEARCHERS

102
VISITING RESEARCHERS

RESEARCH
NETWORK

>400
COLLABORATORS

>300
INTERNATIONAL

57
COLLABORATIONS IN SPAIN

66
REGIONAL COLLABORATIONS

39 RCVT | **7** CLUSTER | **20** PRIVATE

ARGELIA • ARGENTINE • AUSTRALIA • AUSTRIA • BELGIUM • BRAZIL • CANADA • CHILE • CHINA • COLOMBIA • CZECH REPUBLIC • DENMARK • EGYPT • FINLAND • FRANCE • GERMANY • GREECE • HOLLAND • INDIA • IRAK • IRAN • IRELAND • ISRAEL • ITALY • JAPAN • MALAYSIA • MOROCCO • NORWAY • PAKISTAN • PERU • POLAND • PORTUGAL • ROMANIA • RUSSIA • SERBIA • SLOVAKIA • SLOVENIA • SOUTH AFRICA • SWEDEN • SWITZERLAND • THAILAND • TURKEY • UAE • UNITED KINGDOM • UKRAINE • USA • VIETNAM

EXCELLENCE IN HUMAN RESOURCES

BCMaterials is fully committed to recruit the best scientists through transparent and fair processes, providing at the same time an estimulating environment for an excellent research. With this guidelines in mind our center applied in 2022 for the 'HR Excellence in Research' award. At the same time, we kept implementing the goals set on our 'Gender Equality Plan 2021-2025'.

HR EXCELLENCE IN RESEARCH

In March 2023 BCMaterials obtained the "HR Excellence in Research" award, based on the implementation of the Human Resources Strategy for Researchers (HRS4R) action plan.

The HSR4R accreditation is the culmination of the work of the European institutions started in the year 2000, when European Research Area (ERA) was established by the EU to strengthen the competitiveness of European institutions through closer research collaboration and better coordination of research infrastructure.

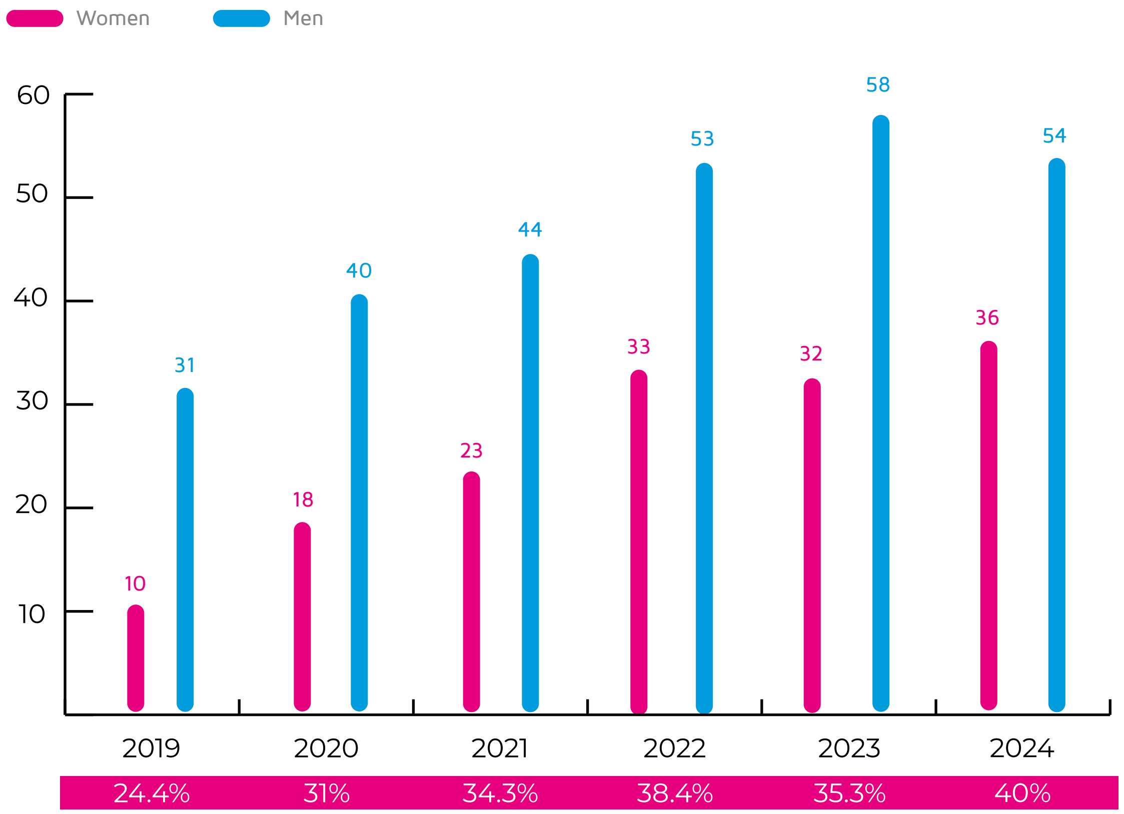
To contribute to the development of the European Research Area (ERA), The European Charter for Researchers and The European Code of Conduct for the Recruitment of Researchers (Charter and Code) were established by the European Commission in 2005. Charter and Code ensures open, **transparent and merit-based recruitment of researchers, safeguard good working conditions and focuses on professional development for researchers at all stages of their careers. It also highlights the importance of recognizing and valuing research mobility, internationally, inter-sectorial and interdisciplinary.** To implement Charter and Code at the individual institutions, the European commission has developed the Human Resources Strategy for Researchers HRS4R accreditation.

As part of its commitment to strengthen its competitiveness at the the European Research Area the Fundación BCMaterials endorsed in 2022 the European (Charter and Code) that sets out the rules and obligations of researchers, their employers and funders, as well as transparent and fair recruitment procedures. This was the first step to achieve the HSR$R accreditation, finally obtained in 2023.

GENDER EQUALITY

BCMaterials, in its commitment to guarantee gender equality in the institution, launched the '2021-2025 Equality Plan'. The Plan provides for specific measures in areas such as personnel selection and hiring processes, training in training in gender equality and work and family reconciliation...

Each action has compliance indicators that will allow its evaluation in order to comply with the provisions of the Law of Effective Equality between Men and Women.



NEW PERSONNEL

IKERBASQUE ASSOCIATE PROF.


REYES CALVO

MSCA POST-DOCTORAL FELLOW


MAIBELÍN ROSALES

RAMÓN Y CAJAL POST-DOCTORAL FELLOWS


DAVIDE SPIRITO


JORGE SAIZ

POST-DOCTORAL RESEARCHERS


CLARA ROJAS


LISA ALMONTE


DIMITRA DAS


EKATERINA CHERNOVA


SON SINGH

IKERBASQUE PROFESSOR & UPV/EHU ASSOCIATE


JOEL VILLATORO

PRE-DOCTORAL RESEARCHERS


STEPHANÍA RODRÍGUEZ


ÁLVARO CORTÉS


SHEHLA GUL


JUAN DAVID CORTÉS


VANESSA GALVÁN


MUHAMMAD USMAN


EUDOMAR HENRÍQUEZ

ADMINISTRATION & SERVICES


ELOIE GALLEGO


NEREA LOPATEGUI


OIHANE JIMÉNEZ


PAULA MARZANA

RULING & ADVISING BODIES

The Board of Trustees and the International and Local Advisory Committee are at the core of the progress of BCMaterials. They provide us with an external and objective vision and guidance that allows our center to grow not only with regards to research, which is essential, but also with the daily functioning itself of BCMaterials. These bodies share with us the will to make our center even more excellent and influential.

Board of trustees

ADOLFO MORAIS

Vice minister of Universities and Research, Basque Government

AMAIA ESQUISABEL

Director of Scientific Policy, Basque Government

FERNANDO COSSÍO

Scientific Director of Ikerbasque

INMACULADA AROSTEGUI

Vice Rector of Research. UPV/EHU

GUILLERMO QUINDÓS

Vice Rector of Scientific-Social Development and Transfer, UPV/EHU

AITOR ZURIMENDI

General Secretary of the UPV/EHU

International Advisory Committee

PROF. MARIA VALLET- REGÍ

Leader of the Smart Biomaterials Research Group. Group leader of the Biomedical Research Networking Centre in Bioengineering, Biomaterials and Nanomedicine (CIBER-BBN), and of the Research Institute of the Hospital 12 de Octubre, Madrid. Spain

PROF. OMAR M. YAGHI

James and Neeltje Tretter Chair Professor of Chemistry University of California, Berkeley

Co-Director: Kavli Energy NanoSciences Institute at Berkeley California Research Alliance by BASF

PROF. CAROLINE A. ROSS

Associate Head of the Department of Materials Science and Engineering

Toyota Professor of Materials Science and Engineering Massachusetts Institute of Technology (MIT), USA

PROF. GORDON WALLACE

Director ARC Centre of Excellence for Electromaterials Science (ACES)

Director ANFF (Materials Node)

Director Translational Research Initiative for Cellular Engineering and Printing (TRICEP)

PROF. SABETH VERPOORTE

Professor of microfluidics and miniaturized "lab-on-a-chip" systems Faculty of Science and Engineering University of Groningen, Netherlands

PROF. PHIL WITHERS FRS

Regius Professor of Materials at the University of Manchester, UK Chief Scientist of the Henry Royce Institute

Local Advisory Committee

PROF. TEÓFILO ROJO

Professor of Inorganic Chemistry at the UPV-EHU. Scientific director of CIC EnergiGUNE from 2010 to 2020 President of the Group pf Solid State Chemistry of the Royal Spanish Society from 2000 to 2010. National prize in Inorganic Chemistry of the Royal Spanish Society of Chemistry in 2013.

PROF. Mª ISABEL ARRIORTUA

Professor of Crystallography and Mineralogy at UPV/EHU, since 1992. Director of the UPV/EHU Advanced Research Facilities (SGIker) since its creation (2002-2021).Euskadi research award in Science and Technology in 2010.

PROF. LUIS MANUEL LEÓN

Professor of Physical Chemistry Founder of the Macromolecular group at the Department of Physical-Chemistry, University of the Basque Country. Member of the PhD commission and/or post-graduation of the UPV/EHU.

DR. ELENA GUEDE VÁZQUEZ

Cement & Roadstone Holding Corporative Quality Manager in the last two years and Plant Manager in Cementos Lemona, S.A for 6 years in previous ones. First woman appointed Cement Plant Manager in Spain and in the CRH Group.

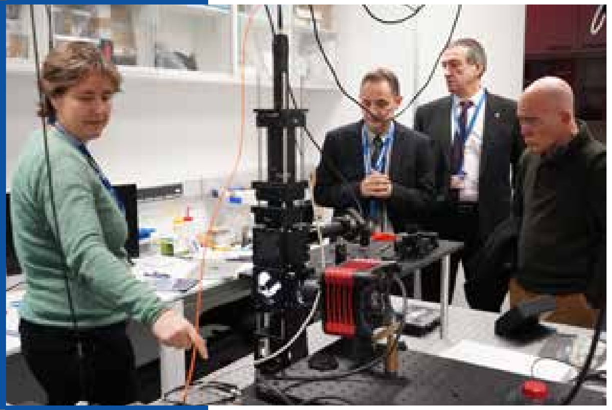
DR. ANTONIO PORRO

Former Chief Technology Officer and Business Development Director at TECNALIA Research & Innovation, BT Division. Former member of the Conseil Scientifique et Technologique of NOBATEK-INEF4 (France).

OFFICIAL VISITS

VISIT BY THE RECTOR OF THE UPV/EHU, EVA FERREIRA, *together with part of her dean's team: the vice-rector for Research, Inmaculada Arostegui, and the vice-rector for Scientific-Social Development and Transfer, Guillermo Quindós.*
January, 2024

VISIT BY THE BASQUE GOVERNMENT'S MINISTER OF SCIENCE, UNIVERSITIES AND INNOVATION, JUAN IGNACIO PÉREZ-IGLESIAS, *with the Deputy Minister of Science and Innovation, Adolfo Morais, and the Director of Scientific Policy, Amaia Esquisabel.*
November 2024



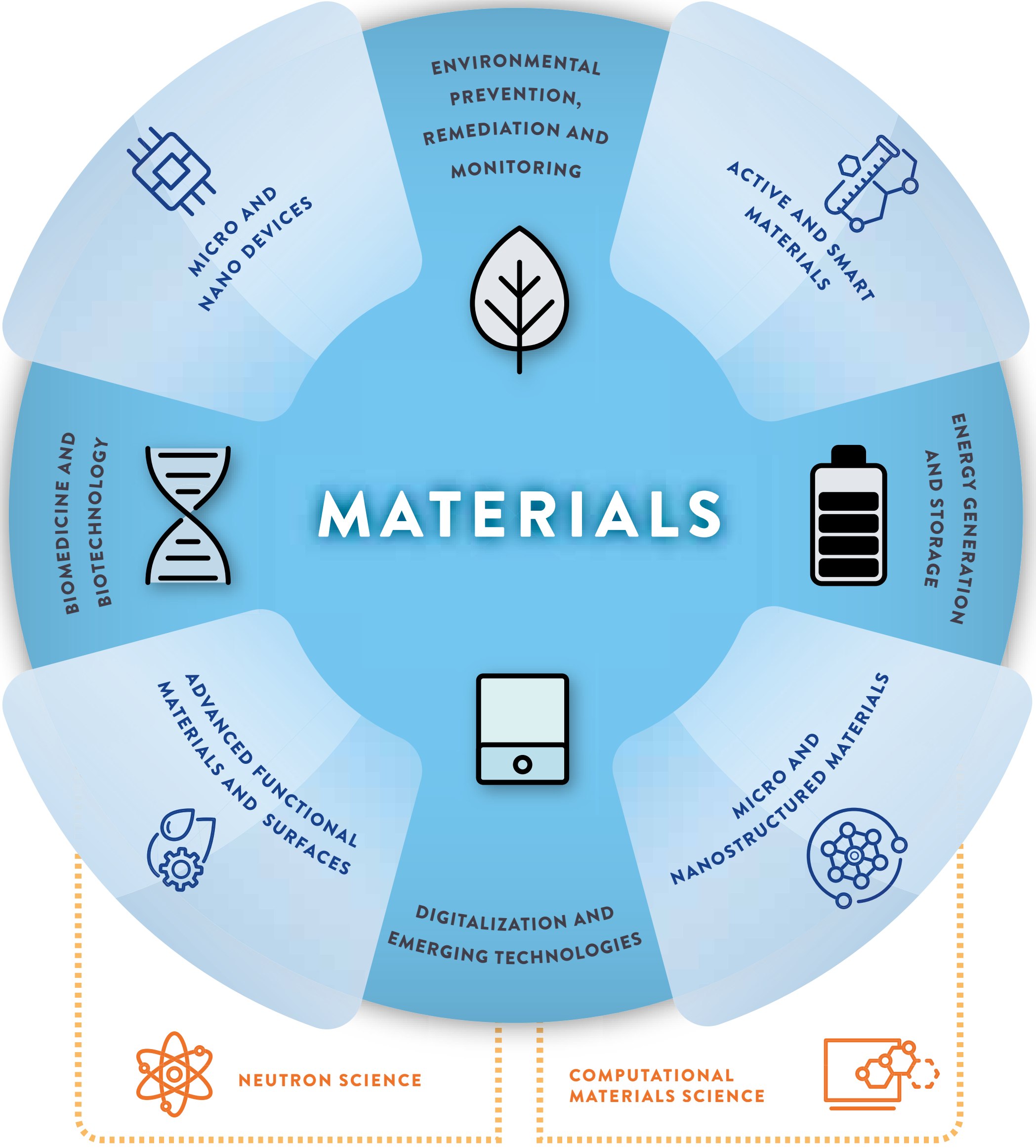
02

RESEARCH ACTIONS

BCMaterials organizes its activities into Research lines and Research areas. Research lines are designed to generate knowledge in the new generation of smart, active and multifunctional materials, to achieve excellence in the next generation of materials, to discover materials and effects and to transfer this knowledge to society. Research areas are designed to take advantage of the generated knowledge in advanced materials and to apply them to tackle the most relevant challenges of modern society, ranging from environmental prevention,monitoring and remediation, energy generation and storage, biomedicine and biotechnology as well as to provide the advanced materials required by the digitalization strategies.

RESEARCH LINES & AREAS

BCMaterials is structured into Research Lines, aiming to develop excellence science in the development of next generation materials, and Research Areas, designed to tackle, in a interdisciplinary way, the most relevant challenges of society. In this Research Lines and Areas, we develop, evaluate, understand and implement materials for sensors and actuators, which are critical for the digitalization of society and economy. We research on materials for advanced biological and biomedical applications, materials for environmental remediation and materials for energy (both generation and storage), among others, all at the core of the technological transitions shaping modern society.



Areas

Research areas are designed to take advantage to the generated knowledge in advanced materials and to apply them to tackle the most relevant challenges of modern society, ranging from environmental prevention, monitoring and remediation, energy generation and storage, biomedicine and biotechnology as well as to provide the advanced materials required by the digitalization strategies.

Lines

Research lines are designed to generate knowledge in the new generation of smart, active and multifunctional materials, to achieve excellence in the next generation of materials, to discover materials and effects and to transfer this knowledge to society. Within the research áreas, one or more of theses research lines work together in order to give answer to specific technological and society challenges.

Transverse lines

Neutron Science and Computational Materials Science are two research lines with strong impact in all the rest of the research lines and areas. These transversal lines support the desing of advanced and multifunctional materials as well as the understanding of their main physical-chemical and functional properties. Further, their are essential to determine their potential applications and application conditions.

RESEARCH
AREA 1

BIOMEDICINE & BIOTECHNOLOGY

Related to the aging of population and the strong needs on early detection of illnesses, advanced biomedical approaches are definitely needed. Advanced multifunctional materials, advanced manufacturing and nanoscience and nanotechnology are providing new tools in order to tackle those important challenges. In this context, BCMaterials is focusing, among others, on the development of materials and new approaches for nanoparticle based biomedicine, from hyperthermia to point of care devices, as well as on the development of active scaffolds and microenvironments for tissue engineering.

Drug-delivery and biological activity in colorectal cancer of a supramolecular porous material assembled from heptameric chromium-copper-adenine entities

Sandra Mena-Gutiérrez, Ekain Maiza-Razkin, Jon Pascual-Colino, Marcos J. Araúzo-Bravo, Garikoitz Beobide, Oscar Castillo, Ainara Castellanos-Rubio, Daniela Gerovska, Antonio Luque, Sonia Pérez-Yáñez. Journal of Material Chemistry B, Volume 12, 2024, 11156.

> “The supramolecular porous material, $[Cu_6Cr(\mu\text{-adeninato})_6(\mu_3\text{-OH})_6(\mu\text{-OH}_2)_6](SO_4)_{1.5}$ is used for drug controlled release. This compound efficiently captures 5-fluorouracil (5-FU), 5-aminosalicylic acid (5-ASA), 4-aminosalicylic acid (4-ASA) and theophylline (THEO) drug molecules. The use of pore-blocking molecules (cholesterol) increased the desorption $t_{1/2}$ of antitumoral 5-FU from 4.2 to 8.2 h. Cytotoxicity assays on human colorectal cancer cell cultures confirmed the more controlled release of 5-FU. RNA-seq transcriptomic studies were also carried out.

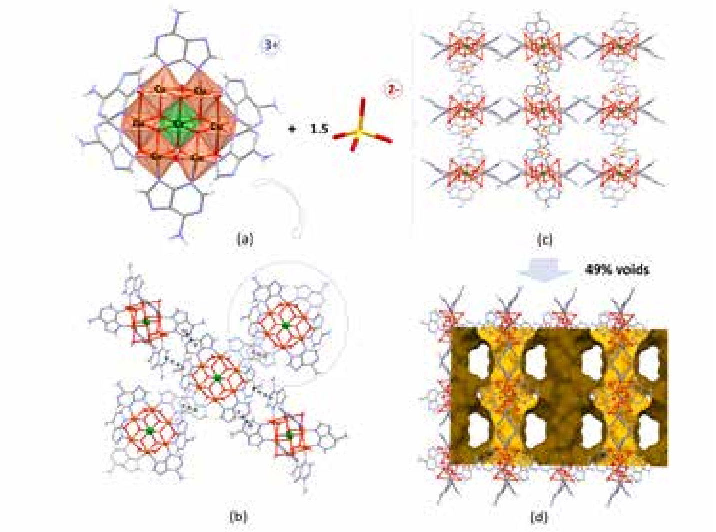


Fig 1
(a) The structural units of Cu_6Cr, (b) supramolecular interactions between cationic entities, (c) crystal packing of the compound and (d) voids in the crystalline building.

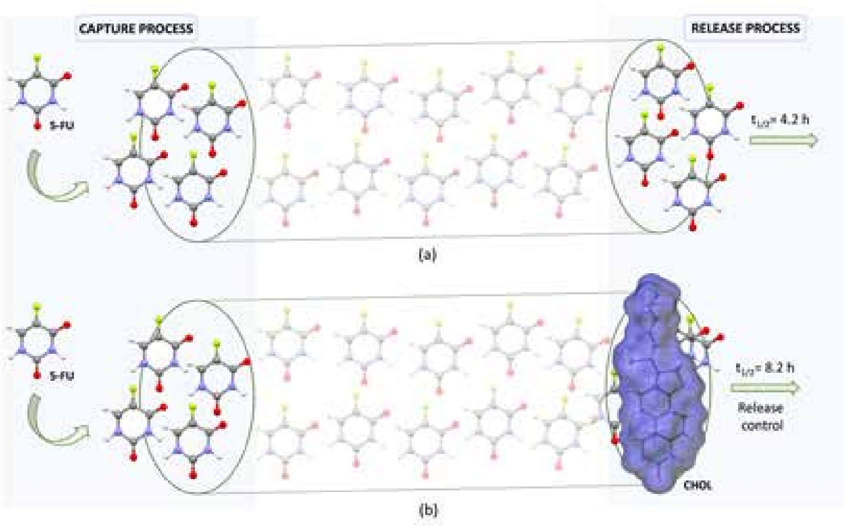


Fig 2
(a) Schematic representation of the capture and release processes without a capping molecule and (b) using cholesterol as a release controller of the ‘‘tap in a bottle’’ approach.

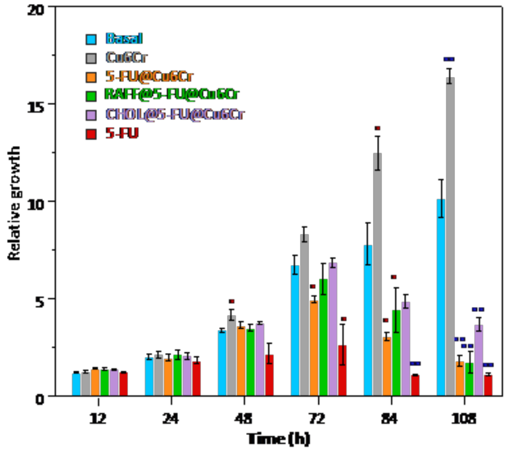


Fig 3
*Relative growth of the HCT116 cells measured with crystal violet at different time points. Cells were grown under basal conditions or after the different compounds were added. Data represent the mean and standard error of at least 4 independent experiments. *p o 0.05 (red); **p o 0.01 (blue) calculated by two-tail, paired Student’s t test against the basal condition.*

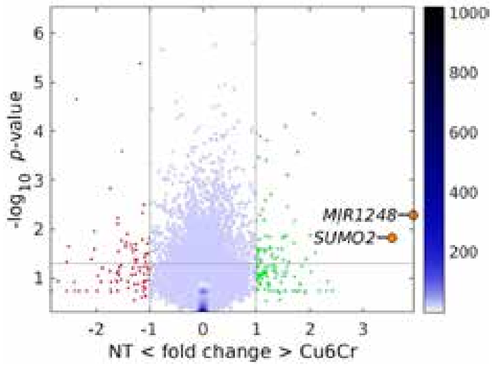


Fig 4
Pairwise volcano plot for Cu_6Cr cultured cells vs. the non-treated cultured cells (NT).

This study investigates a supramolecular metal-organic framework (SMOF), $[Cu_6Cr(\mu\text{-adeninato-}\kappa N3{:}\kappa N9)_6(\mu_3\text{-OH})_6(\mu\text{-OH}_2)_6](SO_4)_{1.5}\cdot nH_2O$ (Cu_6Cr) as a versatile platform for drug delivery. The Cu_6Cr framework, formed through hydrogen bonding and π-π stacking interactions, leads to a 3D network of interconnected pores which represents ca. 50% of the total volume (Figure 1).

Cu_6Cr proved capacity for adsorbing and releasing various drug molecules, such as the anti-tumoral drug 5-fluorouracil (5-FU), the antibiotics 5-aminosalicylic acid (5-ASA) and 4-aminosalicylic acid and the bronchodilator theophylline (THEO). Adsorption studies monitored by the novel magnetic sustentation technique showed mass adsorption capacities of 45.5% (5-ASA), 42.8% (4-ASA), 38.5% (5-FU) and 31.7% (THEO).

These results underline the material´s structural flexibility afforded by the sustaining supramolecular interactions to accommodate molecules of different sizes within its porous network. In addition, pseudo-first order desorption kinetics were observed with desorption half-lives ($t_{1/2}$) ranging from 2.2 to 4.7 h. Focusing on the application of 5-FU for the treatment of colorectal cancer, longer release times are desirable. Therefore, a ‘tap-in-the-bottle’ strategy was envisaged. The goal of this approach is to identify molecules that are small enough to interact with the outer particle apertures of the pores, but large enough to prevent their diffusion into the inner particle pore system. The molecules chosen are cholesterol (CHOL) and raffinose (RAFF). Their different chemical nature will probably affect to the discharge. Although both increase the $t_{1/2}$, CHOL covering the external surface of the particles, because of its hydrophobicity, achieved a greater increase in the desorption half-life of 5-FU from 4.2 to 8.2 h (Figure 2).

Cytotoxicity assays on colorectal cancer cells (HCT116) demonstrated a delayed cytotoxic effect of 5-FU when encapsulated within the Cu_6Cr framework, consistent with the extended release profiles (Figure 3). Furthermore, transcriptomic analyses revealed that Cu_6Cr exhibited a proliferative effect, potentially linked to overexpression of the MIR1248 and SUMO2 genes (Figure 4). These findings emphasize the SMOF’s dual role as both a controlled drug delivery system and a biologically active material, paving the way for innovative therapeutic applications.

The surface charge of electroactive materials governs cell behaviour through its effect on protein deposition

Rodriguez-Lejarraga P., Martin-Iglesias S., Moneo-Corcuera A., Colom A., Redondo-Morata L., Giannotti M.I., Petrenko V., Monleón-Guinot I., Mata M., Silvan U., Lanceros-Méndez S. (2024) Acta Biomaterialia, 184, pp. 201 - 209

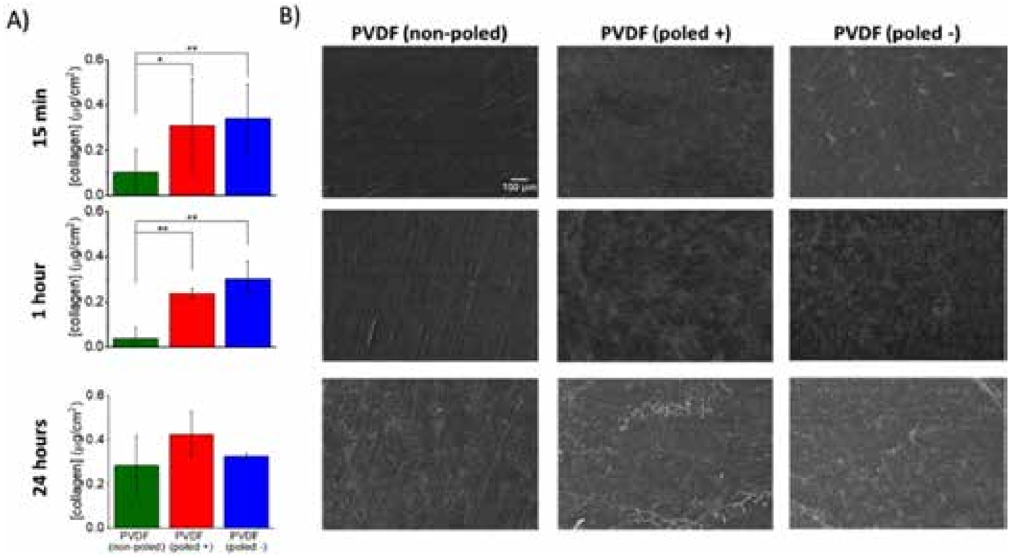


Fig 1
Quantification of deposited collagen and scanning electron (SEM) images images of collagen -coated PVDF.

Biomaterials, synthetic or natural, are often used to provide scaffolds that support cell attachment, growth, and differentiation, thereby facilitating tissue repair or regeneration. In this context, the development of new strategies for organ regeneration relies heavily on the understanding of how these biomaterials interact with biological tissues. While several factors that influence the cellular response, including surface chemistry, topography, and mechanical properties have been identified, the specific relevance and mechanism by which the surface potential affects cell behavior remains largely undescribed. In the present study, we have explored the interaction of collagen type-I, the most abundant extracellular protein in mammals, with poly(vinylidene fluoride) (PVDF), a synthetic electroactive polymer widely recognized for its potential in tissue engineering. The results of our study revealed significant differences in the adsorption of collagen depending on the surface potential of the PVDF substrates. In addition, mesenchymal stem cells (MSCs) adhering to the films exhibited distinct behaviors depending on their surface potential. Specifically, MSCs exhibited enhanced spreading on electrically charged surfaces and a reorganization of their focal adhesions, emphasizing the importance of surface charge in shaping the material–protein interface and, ultimately, the biological response. By shedding light on these differences, our work contributes to the broader understanding of how physical properties of biomaterials influence biological systems. While chemical and biological cues have traditionally been the focus of biomaterials research, there is growing recognition of the importance of physical properties in regulating cell behavior. This paradigm shift will enable the design of advanced biomaterials that better mimic the complex microenvironments of native tissues.

> “ In the present work, we have explored the interaction of collagen type-I, the most abundant mammalian extracellular protein, with poly(vinylidene fluoride) (PVDF). Our results reveal significant differences in collagen affinity, conformation, and interaction strength depending on the electric charge of the PVDF surface, which subsequently affects the behaviour of mesenchymal stem cells seeded on them. These findings highlight the importance of surface charge in the establishment of the material–protein interface and ultimately in the biological response to the material.

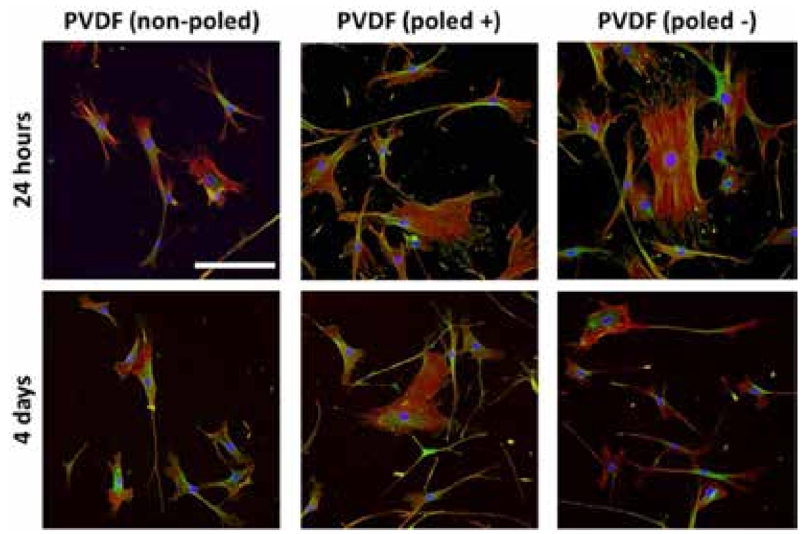


Fig 2
Fluorescence images of labelled MSCs after 24 h (upper row) and 4 days (bottom row) culture on PVDF of varying surface potentials. Cells were stained with NucBlue (nuclei in blue), anti-vinculin antibody (FA in green) and phalloidin (F-actin in red).

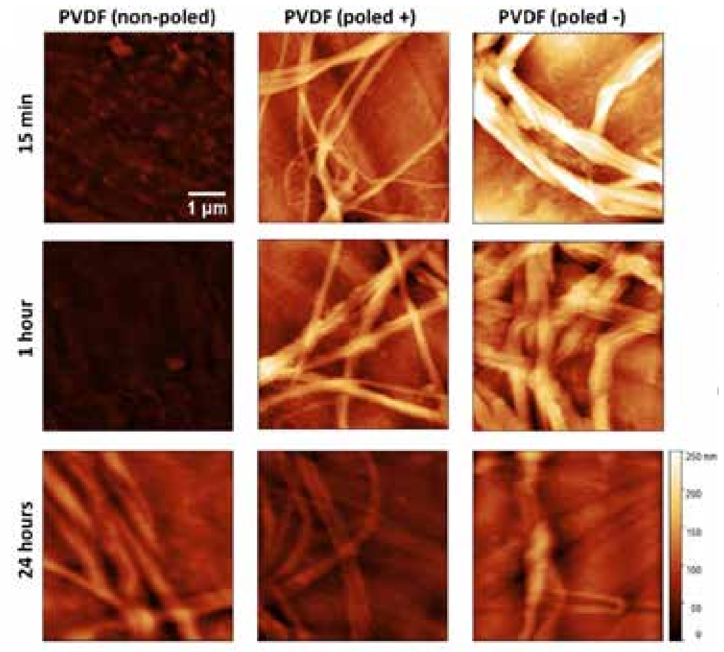


Fig 3
Atomic force microscopy (AFM) images of collagen deposited on PVDF.

Piezoelectric biomaterials with embedded ionic liquids for improved orthopedic interfaces through osseointegration and antibacterial dual characteristics

Carvalho E.O., Marques-Almeida T., Cruz B.D.D., Correia D.M., Esperança J.M.S.S., Irastorza I., Silvan U., Fernandes M.M., Lanceros-Méndez S., Ribeiro C. (2024) Biomaterials Advances, 164, art. no. 213970

> Combining piezoelectric materials with ionic liquids as interfaces for orthopedic implants presents an innovative approach to addressing both issues simultaneously. These films exhibited strong antibacterial properties, effectively reducing biofilm formation, thereby addressing implant-related infections. Furthermore, differentiation assays exposed the potential of these materials to induce osteogenesis. Our findings also revealed the upregulation of calcium channel expression as a result of electromechanical stimulation, pointing to a mechanistic basis for the observed biological effects.

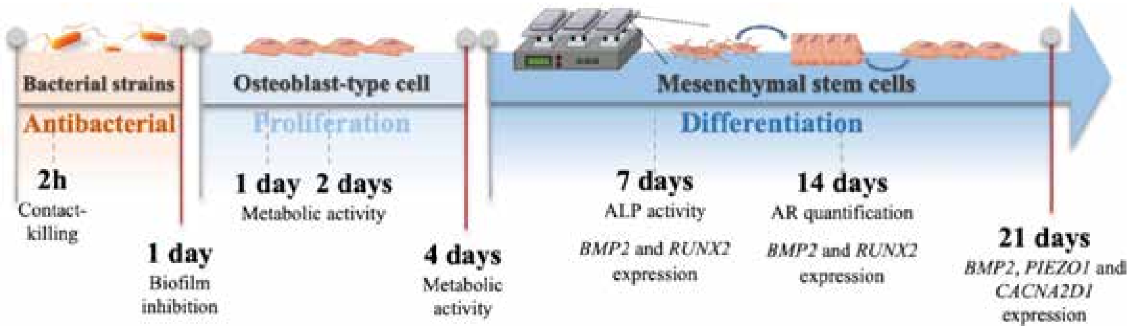


Fig 1
Timeline schematic illustrating the evaluation of antibacterial properties and osteogenic capabilities of the developed materials.

The failure of orthopedic implants, which is primarily attributed to aseptic loosening and implant site infections, poses significant challenges to patient recovery and frequently leads to revision surgeries. In this context, the combination of piezoelectric materials with ionic liquids (ILs) as interfaces for orthopedic implants presents an innovative approach to addressing both issues simultaneously. In the present study, films of poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)) incorporated with 1-ethyl-3-methylimidazolium hydrogen sulfate ([Emim][HSO_4]) IL were developed. These films exhibited strong antibacterial properties, effectively reducing the formation of biofilms, thereby addressing implant-related infections. To ensure that these films can be used for bone regeneration, the adhesion and proliferation of pre-osteoblastic cells were analyzed. The osteogenic potential was as well validated by analyzing several markers of osteogenic differentiation in stem cells adhering to the developed surfaces. In these experiments, to mimic the mechanical cues delivered by physical daily activities and ultimately simulate the bone piezoelectric microenvironment, the cell cultures were mechanically challenged using a custom-made bioreactor. Interestingly, our findings also revealed the upregulation of calcium channel gene expression as a result of the electromechanical stimulation, pointing to a mechanistic basis for the observed biological effects. Taken together, this work highlights the potential of piezoelectric materials with ionic liquids to improve the longevity and biocompatibility of orthopedic implants. Offering such dual-functionality for infection prevention and bone integration, these advancements hold significant potential for advancing orthopedic implant technologies and improving patient outcomes.

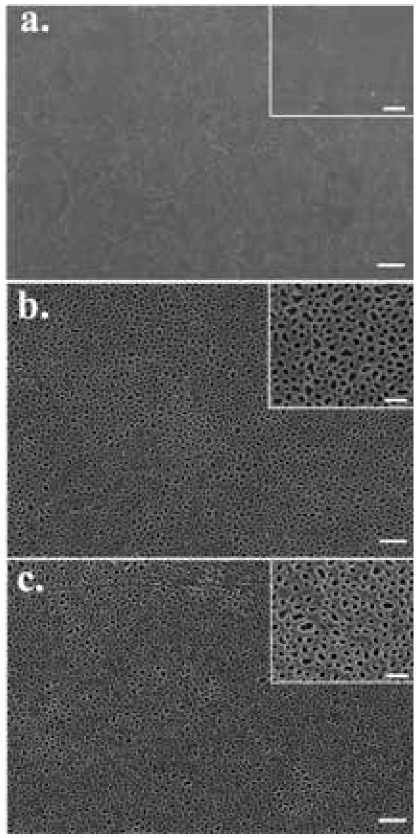


Fig 2
Scanning electron microscpy (SEM) images of (a) P(VDF-TrFE) and (b) P(VDF-TrFE)/10 %[Emim][HSO_4] and (c) P(VDF-TrFE)/20 %[Emim][HSO_4] films.

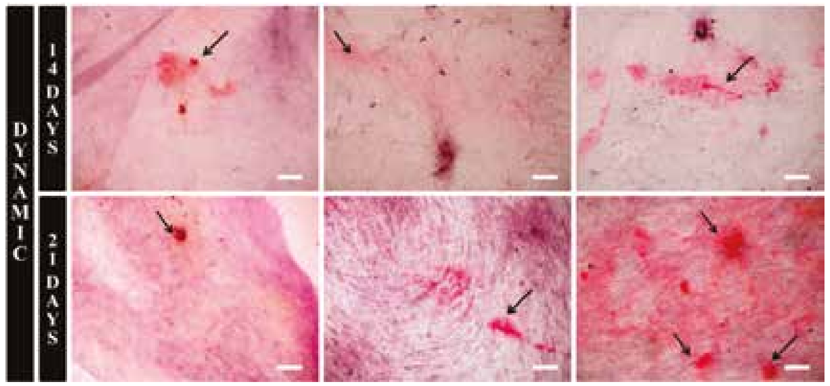


Fig 3
Alizarin red staining at 14 and 21 days of cultured hADSCs on P(VDF-TrFE) and P(VDF-TrFE)/[Emim][HSO_4] composite under dynamic stimulation. Calcified areas are stained in reddish pink.

RESEARCH
AREA 2

ENVIRONMENTAL PREVENTION, REMEDIATION & MONITORING

The strong technological advances of recent years are leaving important footprints in our environment. In this scope, three main issues must be solved in the near future: environmental friendlier technologies, sensors for environmental monitoring and remediation of contaminated scenarios. In these areas, BCMaterials is strongly focusing on the development of prevention (environmental friendly materials and processes), monitoring (environmental sensing) and remediation strategies for water and air.

Low Environmental Impact Magnetic Chitosan and Chitin Cryogels for PFAS Remediation

García-Castrillo M., Barandika G., Lizundia E. (2024) Advanced Functional Materials, 34 (46), art. no. 2405298

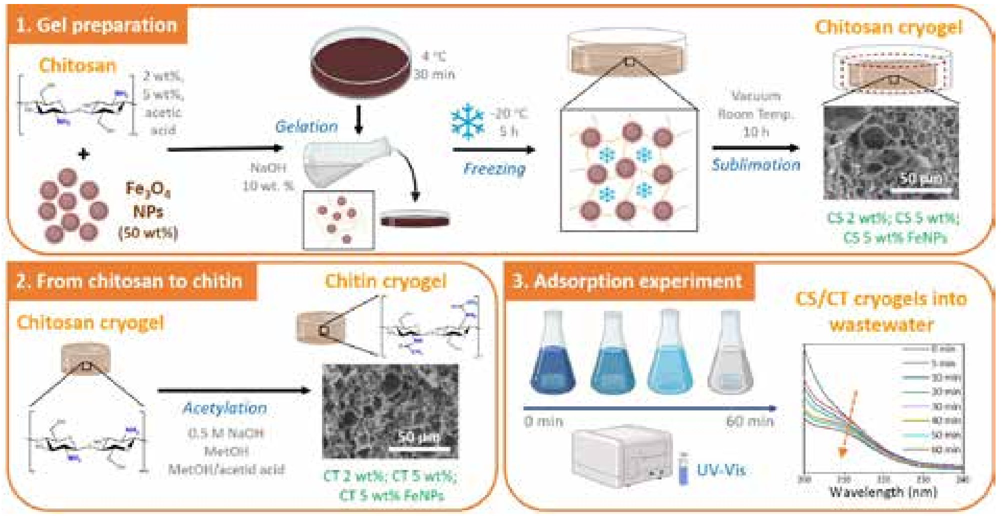


Fig 1
Schematic of the fabrication of magnetic chitosan and chitin cryogels.

Solely 0.036% of the world´s 2% of freshwater is accessible for use, with the rest found in aquifers, underground wells and polar ice caps. With the environment increasingly at risk and the world population potentially reaching 9.7 billion by 2050, the 2030 Agenda for Sustainable Development has identified water conservation and treatment as a top priority. A significantly relevant group of water contaminants are per- and polyfluoroalkyl substances (PFAS). Due to the fully fluorinated methyl or methylene groups in PFAS, these substances persist over very long time scales. Natural polymers offer a unique combination of chemical functionalities, mechanical stability, water affinity and potential recyclability, essential requirements for environmentally sustainable water remediation. Chitin and chitosan, are highly effective in water remediation due to their abundance of hydroxyl and amine groups, which facilitate hydrogen bonding and electrostatic interactions. For additional functionalities, magnetite nanoparticles were incorporated into chitosan cryogels fabricated by dissolution in acetic acid, coagulation and freeze-drying (Figure 1). Chitosan cryogels were acetylated upon immersion in an acetic anhydride/methanol solution to obtain highly porous chitin cryogels.

The potential to remove dyes, pharmaceuticals, and PFAS from contaminated water by simple adsorption was tested, showing a clear affinity towards PFAS (Figure 2). With a maximum removal capacity of 451 mg·g-1, the amount of exposed chitin and chitosan surfaces in the cryogels was found to be determinant. The results suggest that anionic materials with a high number of nucleophilic sites and a low number of electrophilic sites are strongly attracted to chitosan and chitin cryogels.

A cradle-to-gate life cycle assessment was conducted to evaluate whether the applied strategy results in materials with a low environmental footprint. The disaggregated global warming potential in Figure 3 shows global warming potential values of 42.6-77.4 kg CO2 equiv.·kg-1, while its acetylation to magnetic chitin cryogel adds 15.1–75.8 kg CO2 equiv.·kg-1. In comparison, the production of starch aerogels by supercritical drying has a footprint of 1060-3840 kg CO2 equiv.·kg-1. The combination of biobased nature, ease of processing, functional performance, small footprint, and recyclability offers unique competitive advantages for chitin and chitosan in the development of sustainable environmental remediation materials.

> Renewable polymers will play a key role in the transition to a sustainable circular economy by replacing conventional fossil carbon materials. Utilizing the abundant hydroxyl and amine groups of chitin and chitosan, that facilitate hydrogen bonding and electrostatic interactions, we developed chitin and chitosan cryogels for the rapid removal of per- and polyfluoroalkyl substances (PFAS). We achieved capacities of 451 mg·g-1, offering competitive performance against state-of-the-art materials. The materials are recyclable, and the environmental sustainability of the materials has been confirmed by Life Cycle Assessment (LCA).

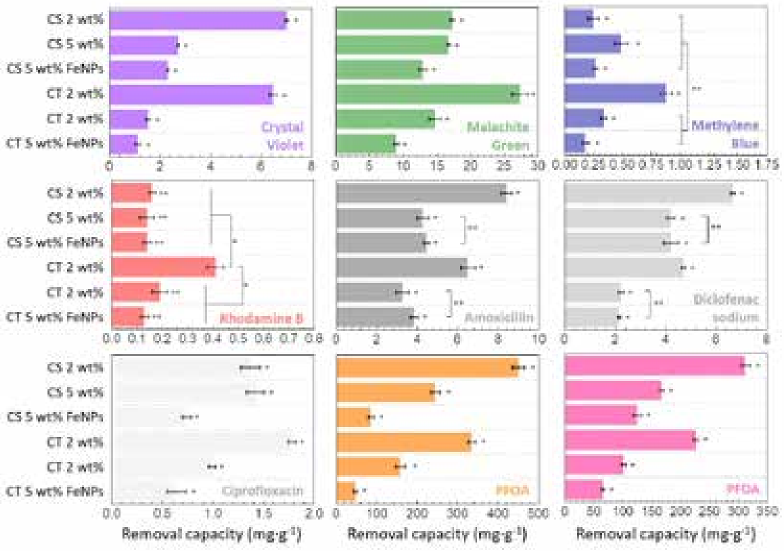


Fig 2
Summarized pollutant removal capacity of chitosan and chitin cryogels for multiple contaminants.

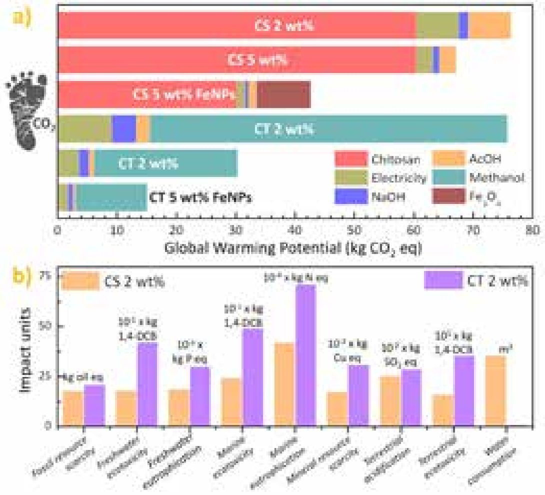


Fig 3
a) Disaggregated global warming potential for the fabrication of all chitosan and chitin cryogels;
b) Environmental impacts for different categories.

Hexavalent chromium dual water remediation and sensing based on hybrid polymer/metal-organic framework composites

Brito-Pereira R., Queirós J.M., Celaya-Azcoaga L., de Luiz R.F., Martins P., Lanceros-Mendez S. (2024)
Journal of Environmental Chemical Engineering, 12 (5), art. no. 113839

> The environment hosts various chemical pollutants, including hexavalent chromium (Cr(VI)), a global threat requiring efficient monitoring and remediation. This study developed multifunctional membranes by immobilizing Metal-Organic Frameworks int PVDF-HFP polymer, forming Cr(VI) sorbents in different morphologies. Electrospun membranes with 10 wt. % of MOFs showed the highest adsorption (2.32 mg/L in 300 minutes). Integrated into a portable system, they achieved ~50% adsorption efficiency and high colorimetric sensitivity ($R^2 = 0.990$) at 0.085 ppm, offering a novel solution for Cr(VI) detection and removal.

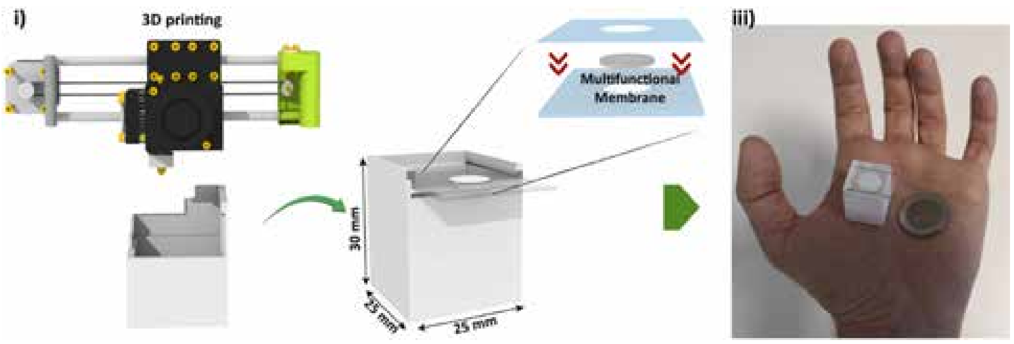


Fig 1
i) FDM 3D printing process of the PLLA reservoir and the device assembly with the insertion of the multifunctional membrane between a two-layer support. ii) Dimensions of the final portable sensing 3D device compared to a 2 euros coin.

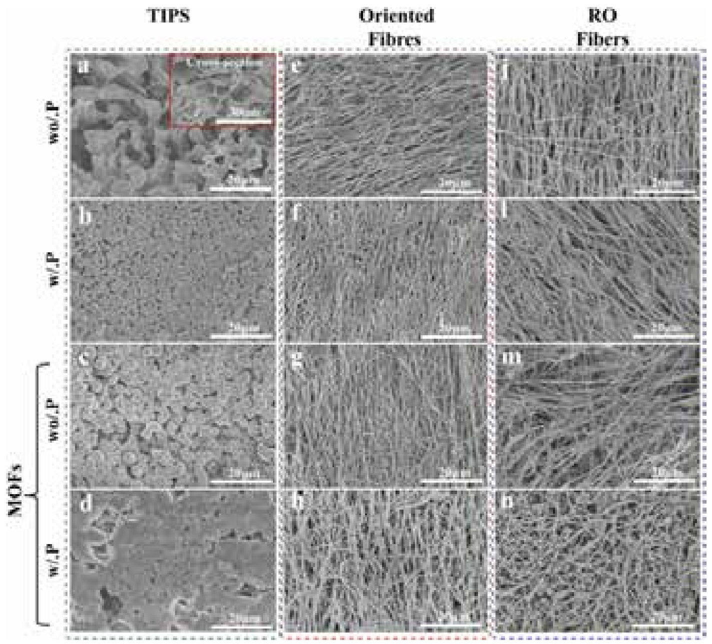


Fig 2
Representative SEM images of the non-oriented and oriented PVDF-HFP/MOF membranes processes by electrospinning and O2 plasma.

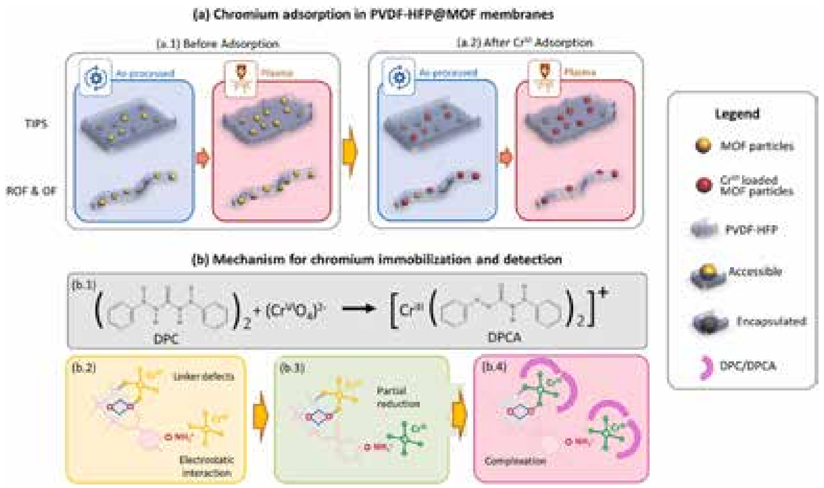


Fig 3
a) Schematic 3D representation of the portable filtration and detection system for Cr(VI). b) Adsorption efficiencies of Cr(VI) (0.5, 1, 2.5, 5 mg/L) by oriented membranes (10 %OF-P) inserted in the portable device; c) Colorimetric calibration curves of different Cr(VI) concentrations in the membranes; d) Representative images of the portable device and the tested membranes after Cr(VI) assays.

This work introduces a novel, avant-garde approach in which a multifunctional portable-printed system integrates a remediation and sensing solution. This portable system can simultaneously measure chromium concentration in water samples using colorimetry and carry out remediation to levels that meet the safety standards set by the World Health Organization (WHO) (Figure 1).

To optimize remediation and sensing performance, poly (vinylidene fluoride-co-hexafluoropropylene), PVDF-HFP, has been employed as a robust matrix to integrate Metal-Organic Framework (MOF) particles able to capture and sense by colorimetry Cr(VI). PVDF-HFP is a fluorinated polymer with outstanding chemical, thermal, mechanical and radiation resistance. The PVDF-HFP matrix has been combined with an amino functionalized zirconium-based MOF (i.e. UiO-66-NH2) to obtain a composite system that has demonstrated efficacy in capturing and separating both inorganic and organic contaminants. PVDF-HFP@UiO-66-NH2 composite membranes have been processed in a variety of different morphologies from (i) oriented and (ii) randomly-oriented electrospun fibres, as well as (iii) porous membranes obtained via thermally induced phase separation technique (TIPS). UiO-66-NH2 has been selected as an active component because it has already been proven as an outstanding adsorbent and photocatalyst for chromate oxyanions. Further, to overcome the hydrophobicity of the membranes, surface post-treatments with oxygen plasma were performed (Figure 2).

These PVDF-HFP/MOF composite platforms were designed and tested for holds the ability to remediate and quantify chromium in water. In fact, when a chromium solution was passed through the PVDF-HFP/MOF membrane, this heavy metal was mostly retained within it giving rise a significant colour change (Figure 3).

Last but not least, the structure of the membranes before and after the Cr(VI) uptake, and the mechanism of the Cr(VI) colorimentric detection in the this composite system was explained (Figure 4). This work represents the first example of a portable system that integrates detection and remediation simultaneously, a feature with significant potential for diverse environmental applications.

Metal-Organic Framework Functionalized Chitosan/Pectin Membranes for Solar-Driven Photo-Oxidation and Adsorption of Arsenic

Salazar H., Rosales M., Zarandona I., Serra J., Gonçalves B.F., Valverde A., Cavalcanti L.P., Lanceros-Mendez S., García A., de la Caba K., Guerrero P., Martins P.M., Fernández de Luis R. (2024) Chemical Engineering Journal, 497, art. no. 154417

> Arsenic contamination in water is a global challenge requiring efficient remediation of As(III) and As(V) species. This study introduces CHIPEC@UiO-66-NH2 membrane, which combines chitosan/pectin biopolymers with the porous and photoactive UiO-66-NH$_2$ metal-organic framework. The membrane demonstrates exceptional performance, with adsorption capacities of 254 mg g^{-1} for As(III) and 335 mg g^{-1} for As(V) in groundwater. Its ability to photo-oxidize As(III) to As(V) and effectively adsorb both species establishes it as a cost-effective, environmentally friendly solution for arsenic detoxification.

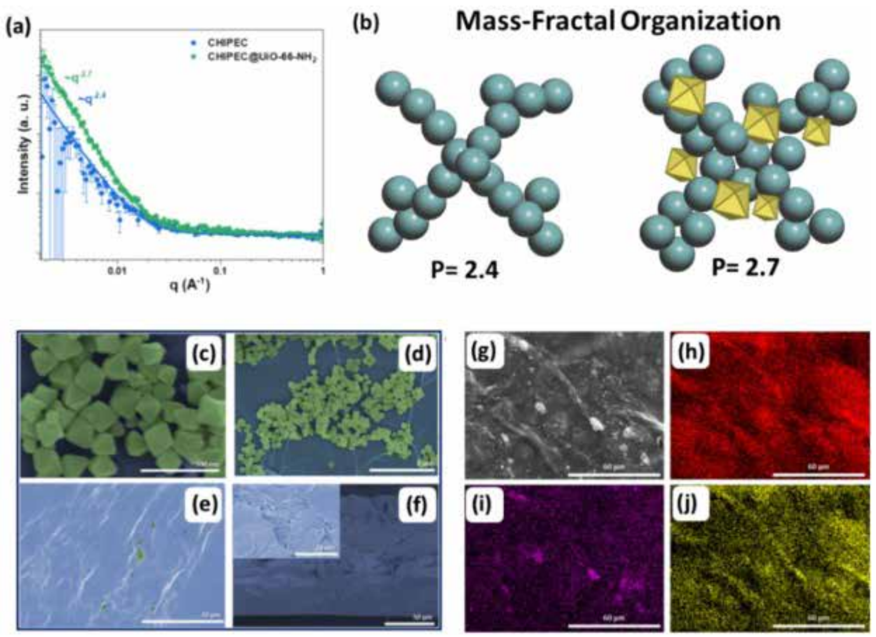


Fig 1
(a) SANS data and fitting for CHIPEC and CHIPEC@UiO-66-NH$_2$ membranes; (b) Illustration of the Fractal structuration of CHIPEC and CHIPEC@UiO-66-NH$_2$; (c-j) SEM images of (c–d) UiO-66-NH$_2$ nanoparticles; (e) surface and (f) cross-section SEM images of CHIPEC@UiO-66-NH$_2$ composite membrane; (g) EDX mapping of CHIPEC@UiO-66-NH$_2$ membrane; (h) carbon, (i) zirconium and (j) oxygen contents.

Thus, the aim of the present work is to demonstrate to which extent the outstanding efficiency of UiO-66-NH$_2$ for the dual photooxidation and adsorption of arsenic is maintained when the nanoparticles of the active porous photocatalyst are immobilized into a composite CHIPEC@UiO-66-NH$_2$ Biopolymer/MOF membranes. To achieve this end, several intermediate objectives has been staidly achieved. First, the synthesis and functional characterization of UiO-66-NH$_2$ nanoparticles with a narrow size distribution was achieved. Second, the MOF nanoparticles were homogeneous integrated into the polymeric CHIPEC matrix to assemble a highly permeable and hydrophilic membrane like technology (Figure 1).

In the third step, the capacity of the active MOF material and of the membrane can eliminate arsenic species from in synthetic and real water matrixes was evaluated. And last but not least, the adsorption and photocatalysis performance of the MOF and MOF@CHIPEC membrane system was duly evaluated (Figure 2a-d), and the immobilization of the arsenic species in the free and immobilized MOF particles quantified (Figure 2e).

In order to unravel the underlying mechanisms leading to the arsenic photo-transformation and fixation, the individual components and the composite membranes were deeply characterized to understand their chemistry, porosity, nanostructure, and specially the synergic photocatalytic and adsorptive performance when integrating MOF and CHIPEC components in the same system (Figure 3).

Last but not least, the portable membrane was tested both in ideal laboratory conditions (i.e. pH, scavengers, ...) and for surface and underground waters obtained from the field. All in all, the CHIPEC@UiO-66-NH$_2$ membranes have been revealed as an outstandingly efficient and portable technology that can be easily delivered to isolated regions, and applied without the need costly facilities or devices by non-technical users.

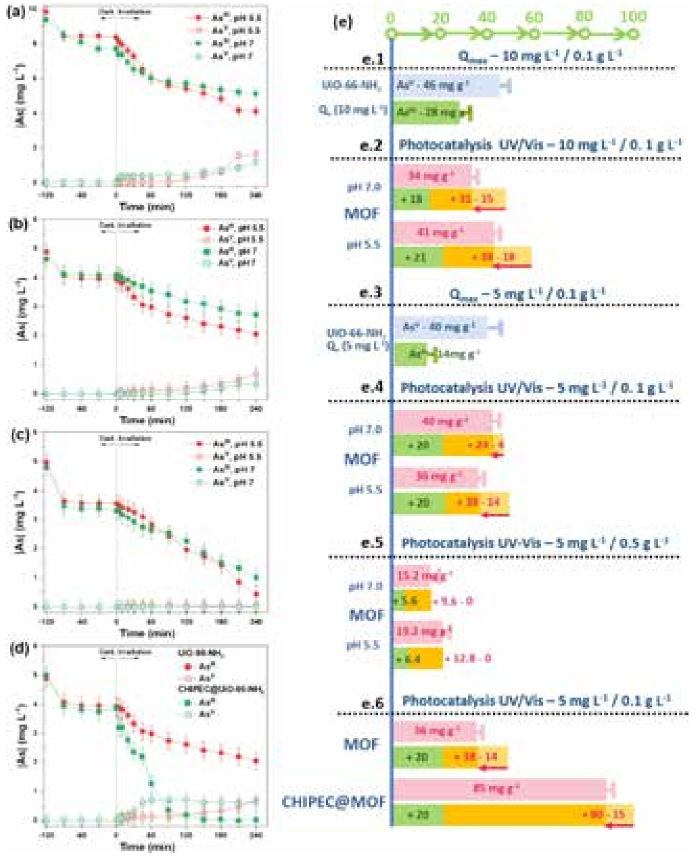


Fig 2
(a–c) Photooxidation kinetics of As(III) to As(V) by UiO-66-NH$_2$ under irradiation at different pH values: (a) photocatalyst loading: 0.1 g/L, [As(III)]: 10 mg/L; (b) photocatalyst loading: 0.1 g/L, [As(III)]: 5 mg/L; (c) photocatalyst loading: 0.5 g/L, [As(III)]: 5 mg/L; (d) comparison of As(III) photooxidation by UiO-66-NH$_2$, CHIPEC, and CHIPEC@UiO-66-NH$_2$ (pH:5.5; photocatalyst loading: 0.1 g/L, [As(III)]: 5 mg/L); (e) Summary of the MOF-arsenic adsorption capacity under adsorption and photocatalysis experiments (blue bar: As(V) adsorption; green bar: As(III) adsorption; pink bar: overall arsenic retention in the MOF during photocatalysis; dark orange bars: As(V) generated during the illumination and retained in the MOF; light orange bars: As(V) generated during illumination and released to the media).

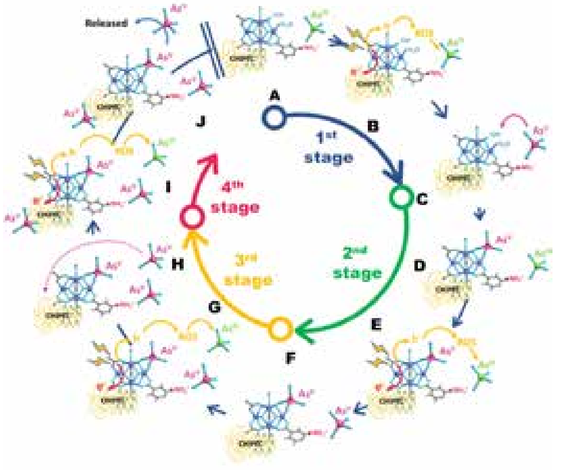


Fig 3
Photooxidation and adsorption mechanisms in CHIPEC@UiO-66-NH$_2$ membrane.

RESEARCH
AREA 3

ENERGY GENERATION & STORAGE

One of the grand challenges facing humankind is related to energy. Energy generation and storage are among the key issues of modern society, increasingly dependent on mobility. BCMaterials specifically focus on solar energy conversion in applications such as perovskite and kesterite based solar cells. We also work on the development of energy harvesting systems, mainly based on mechanoelectric (piezoelectric and triboelectric) and thermo-electric systems for self-powered and wearable sensors. Finally, materials and concepts are being developed for Li and Na batteries, as well as new approaches for solid electrolytes and printable batteries.

Designed-by-purpose power sources: A cardboard primary battery for smart packaging

M. Navarro-Segarra, O. A. Ibrahim, I. Martin-Fernandez, C. Tortosa, J. M. Ormaetxea, M. Baumann, M. Weil, J. P. Esquivel. Energy & Environmental Science 17 (2024) 5639-5652

“Electronic devices demand portable energy sources with high performance, but they should also consider environmental sustainability and social responsibility. In this work, smart packaging is selected as a blooming sector to present a designed-by-purpose battery to power IoT devices. The article provides a concise view of the energy needs of increasingly digitalized products and services, the environmental concerns of current portable power sources and how the proposed technology broadens the edges of portable power solutions in terms of sustainability combined with useful performance metrics, offering a profitable design approach to address future society's technological needs from a just and safe space.

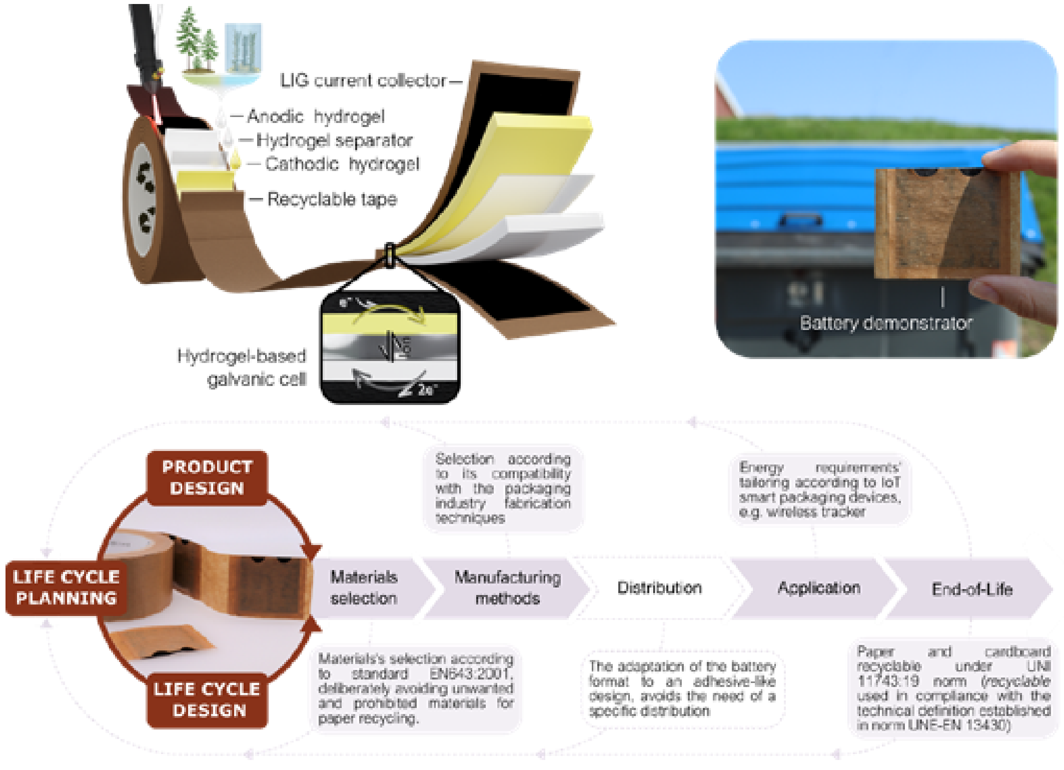


Fig 1
Prototype evolution from holistic envisioning to the functional battery in an adhesive label format. The battery design enhances the demonstrator compatibility with smart packaging industry and allows a fit-for-purpose energy format, which allows it to be recycled along with cardboard boxes at its end-of-life. The systematic methodology followed for the life cycle planning is shown in the bottom.

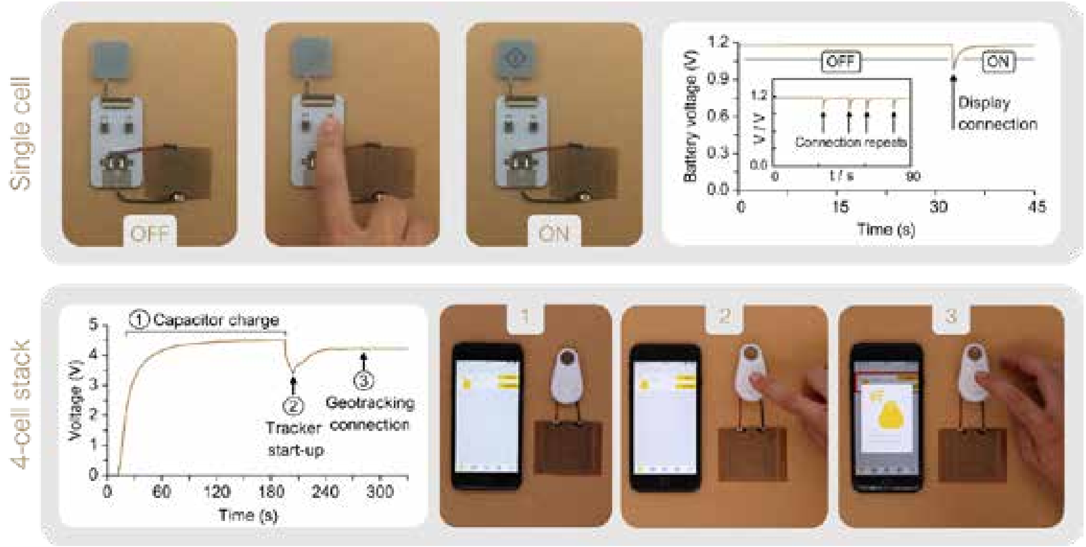


Fig 2
Proof of concept of the battery energy adaptability demonstrating the capability of powering an electrochromic display (single-cell battery) and the start-up, idle mode and Bluetooth connection of a tracker device (4-cell stack battery).

Internet-of-Things (IoT) is considered one of the primary enablers of the next digital transformation wave. Generating and exchanging data between the increasing number of delocalized sensors comes with the need for high-performance portable power sources that also meet environmental and social responsibility standards.

This article presents a ‘fit-for-purpose’ battery approach to meet the energy requirements of IoT devices in the smart packaging sector that has been designed-by-purpose in an ecologically benign way since the early development stage.

To minimize the environmental impact throughout its life cycle, the battery follows the value chain of paper and cardboard, from materials sourcing to disposability. Naturally abundant materials, such as cellulose derivates and alginate biopolymers, are prioritized to create the separator and contain the redox species. Manufacturing techniques, easily implementable in the packaging industry, are used to fabricate an adhesive label-like battery (based on layered components) and engrave the current collectors, via Laser-Induced Graphene. The prototype's energy adaptation capability is demonstrated by directly powering two applications particularly appealing for smart packaging, i.e., a printed electrochromic display and a wireless tracker device. Once depleted, the battery is compatible with paper and cardboard recycling standardized processes used in the industry. This unconventional End-of-Life for a battery represents an alternative solution for ensuring the power source's correct management, preventing potential environmental risks while overcoming the need for separate collection and treatment routes which cause high efforts and environmental impacts.

The presented methodology considers relevant aspects that facilitate the industrial scale-up of a technology from an early conceptual stage, including criteria to define the materials and product design based on environmental sustainability considerations, economic viability and manufacturability. The reconceptualization of the whole battery life cycle leads to the generation of a disruptive power source concept that aims to be an enabler of a sustainable digitalization of society.

Wool/soy protein isolate membranes as separators toward more sustainable lithium-ion batteries

J.P. Serra, J.C. Barbosa, M.M. Silva, R. Gonçalves, J. Uranga, C.M. Costa*, P. Guerrero, K. De la Caba, Lanceros-Mendez, S. 2024. Journal of Energy Storage, 75, 109748

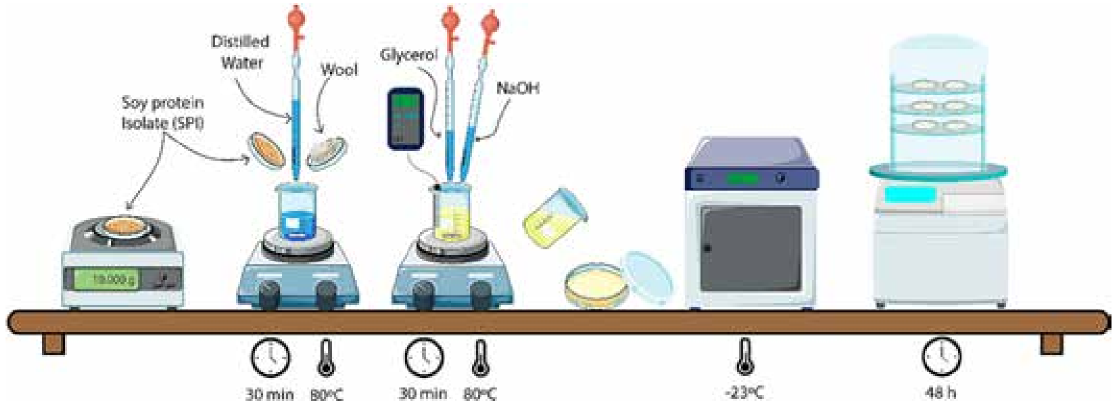


Fig 1
Schematic representation of membrane preparation and conditions.

The development of sustainable batteries based on products of natural origin, such as soy protein isolate and wool, for LIB separators is essential and subject of great interest.

In this work, soy protein isolate membranes were prepared with different amounts of wool up to 25 wt.% content using the freeze-drying method (Figure 1). Once the separator performance is strongly influenced by the movement of ions and this movement is closely related to the separator pore size and distribution, these properties were assessed (Figure 2). The results show that the control membranes revealed more defined and uniform pores, whereas wool containing samples had randomly distributed pores of varying sizes and shapes, increasing tortuosity with wool content increase. The membranes calculated porosity revealed a value of 83 % for all samples.

A critical property of separator membranes is the electrolyte uptake, with the membranes revealing a rapid absorption of the electrolyte and reaching equilibrium in <1 min; however, a higher concentration of wool affects the wettability of the membrane by the electrolyte solution. Moreover, it is verified that the addition of wool does not affect the structure or the thermal properties of the soy protein membranes, maintaining their thermal stability. Hence, the addition of wool gives the SPI membranes a superior mechanical resistance.

The electrochemical stability of the materials is also a relevant parameter for battery applications. Cyclic voltammetry tests show that none of the membranes presents any anodic or cathodic peak, demonstrating the membranes stability in the normal operating voltage range of batteries with LFP as cathode (2.5 to 4.2 V).

Regarding the electrochemical data, ionic conductivity and lithium transfer number presented values between 1.22 and 1.93 mS.cm^{-1} and 0.42 and 0.67, respectively, for the samples with different wool content. The developed samples were tested as separators of LIBs. All cathodic half-cells show an excellent electrochemical performance at different C-rates with particular emphasis on the membrane with 15 wt% wool content, that presents a higher discharge capacity value when compared with other samples. Cycle life performance at 2C rate is also verified with a discharge capacity value of 28 mAh.g^{-1} for SPI15W and 130 mAh.g^{-1} at C/10 after 100 cycles (Figure 3). This study demonstrates that it is possible to develop sustainable lithium-ion batteries separators based on soy protein isolate and wool.

“ In this study, wool and soy protein isolate (SPI) are proposed to develop separator membranes for lithium ion batteries (LIBs), aiming toward a new generation of sustainable batteries. The developed membranes show suitable wettability by the electrolyte solution and are characterized by a porous morphology that becomes more irregular with the addition of wool with respect to the distribution and size of the pores. The physicochemical properties of the membranes are not strongly affected by the addition of wool, excepting for the low mechanical resistance of the SPI membranes, which is improved with the presence of wool. With respect to lithium-ion battery applications, the ionic conductivity is larger than 10^{-4} S.cm^{-1} and the lithium transference number ranges between 0.42 - 0.67, leading to excellent battery performance with a discharge capacity up to ~150 mAh.g^{-1} at C/10 rate.

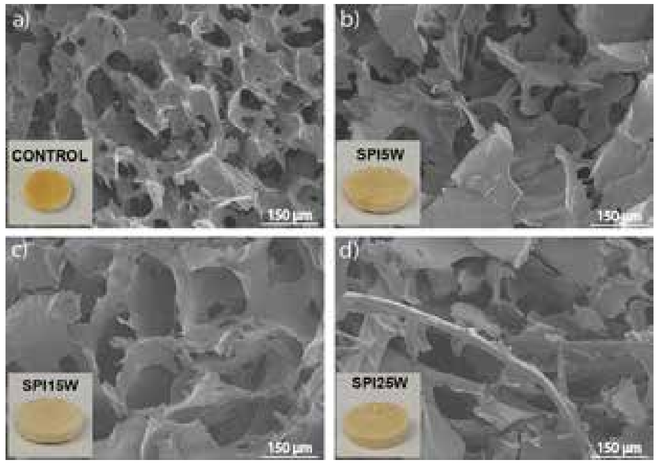


Fig 2
SEM images for wool/SPI membranes.

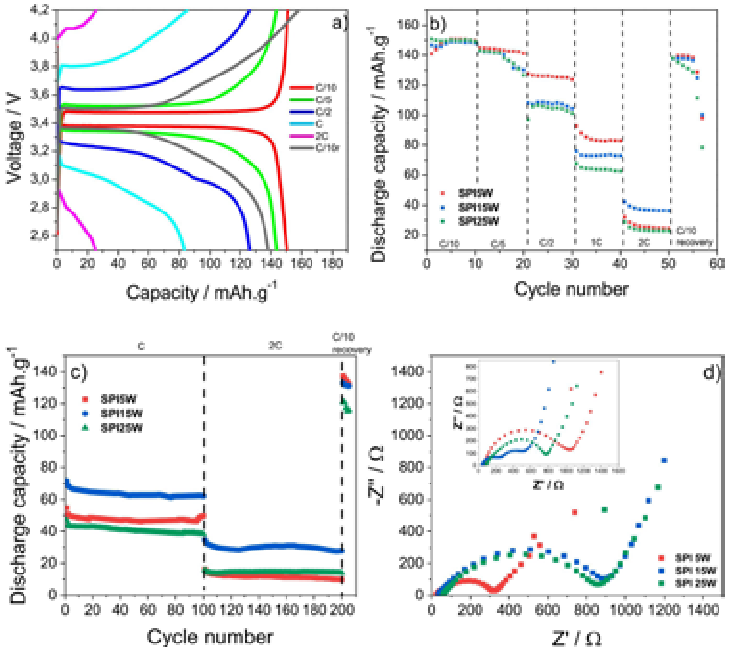


Fig 3
a) Charge/discharge profiles for the cathodic half-cells for the wool/SPI membranes (SPI5W), b) rate performance as a function of the cycle number with the different wool/SPI membranes, c) discharge capacity value at C and 2C rate for 100 cycles for wool/SPI half-cells and d) electrochemical impedance spectroscopy: before and after (inset) cycling of the half-cell batteries prepared with the wool/SPI membranes as separator.

Multifaceted Design of Surface Passivator for Upgraded Charge Extraction in Perovskite Solar Cells

Gassara M., Kazim S., Ahmad S. (2024) Solar RRL, 8 (19), art. no. 2400438

> Surface passivation of the perovskite is endorsed as an effective method to mitigate nonradiative recombination losses and to boost the photovoltaic properties of perovskite solar cells. So far, a range of organic materials, as passivators, have been employed in perovskite thin films to reduce defect formation and defect density through molecular interaction with undercoordinated metal cations or halide anions. We uncover the role of Cyanoguanidine diiodide (DYI) as a radical surface passivator for perovskite solar cells.

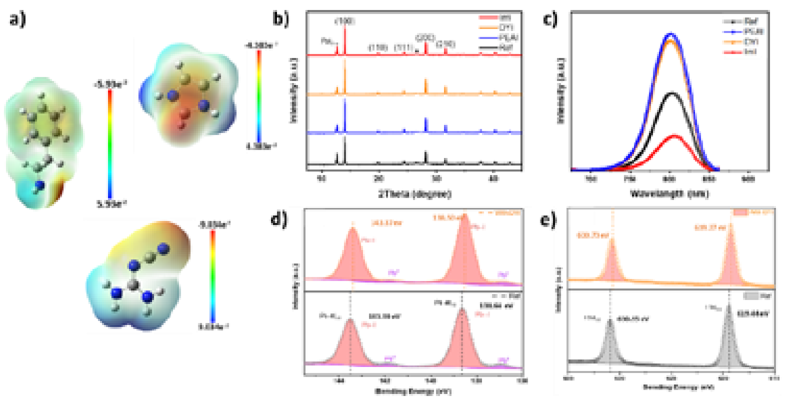


Fig 1
a) Electrostatic potential (ESP) analysis of PEAI, ImI, and DYI, b) XRD pattern of perovskite films with different passivators, c) Steady-state PL of perovskite and passivated perovskite thin films (PEAI, ImI, and DYI), d) XPS-spectra of Pb 4f, and e) I 3d of perovskite and DYI-passivated perovskites thin films.

Cyanoguanidine diiodide (DYI) stands out as a radical surface passivator for perovskite solar cells (PSCs), offering significant improvements in both efficiency and stability. DYI's amino and cyano functional groups enable robust chemical bonding with undercoordinated Pb^{2+} ions on the perovskite surface, reducing the presence of Pb° defects that commonly degrade device performance. Compared to traditional passivators like phenyl ethyl-ammonium iodide (PEAI) and imidazolium iodide (ImI), DYI exhibits superior electrostatic surface potential. The strong dipole interactions of DYI's C≡N and C═NH groups generate a higher negative potential, which optimally coordinates with the perovskite Pb^{2+} ions. This effect reduces surface trap densities more effectively than other passivators, enabling enhanced defect passivation. As a result, DYI-treated PSCs achieve a power conversion efficiency (PCE) of 23.04%, surpassing the 20.44% recorded for control devices. This improvement is attributed to a higher fill factor (80.65%) and an open-circuit voltage (Voc) of 1119 mV. Moreover, the chemical interaction between perovskite and DYI, promotes the crystallinity, a dense grain growth in perovskite films, minimizing ion migration pathways and improving charge carrier mobility. These structural enhancements lead to smoother charge extraction at the interface between the perovskite and the hole transport material (HTM).

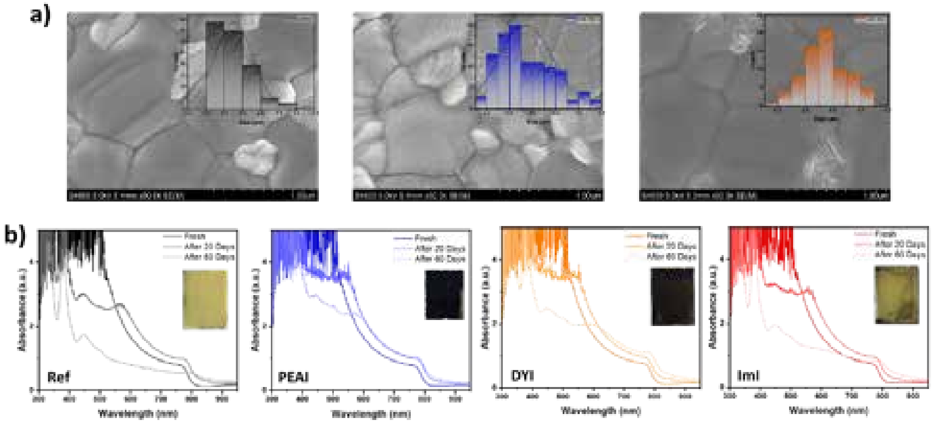


Fig 2
Surface (top view) scanning electron microscopy image for pristine perovskite, perovskite with PEAI, and perovskite with DYI, b) Absorption spectra of fresh and aged perovskite only and with different passivators. The inset shows the perovskite thin film after 60 days of storage (stored in the dark under ambient air conditions).

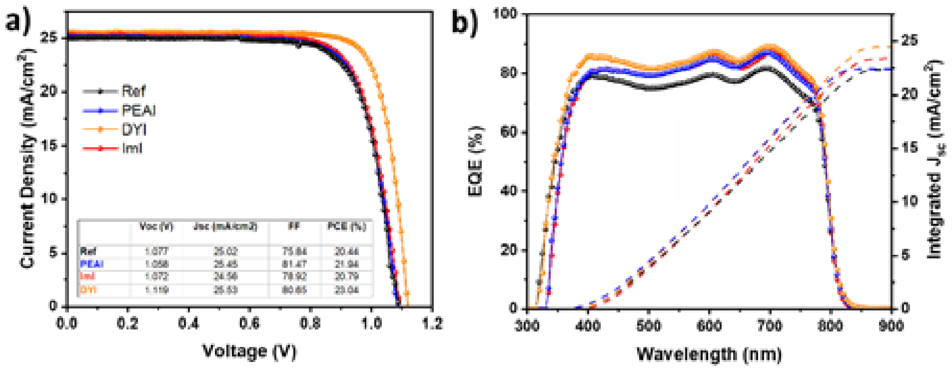


Fig 3
a) J–V characterization and b) EQE spectra of the corresponding PSCs along with the integrated current (Jsc) obtained from the EQE for control, PEAI, ImI, and DYI respectively.

PSCs treated with DYI retain over 83% of their initial efficiency after 60 days of storage in dry air, significantly outperforming the 77% retention observed in control devices. Additionally, the black-phase stability of DYI-passivated perovskite films resists degradation caused by moisture and oxygen, ensuring prolonged operational integrity.

To conclude, DYI offers superior passivation through its enhanced electrostatic potential and strong interactions with Pb^{2+} ions, by simultaneously addressing surface defects and improving device stability.

RESEARCH
AREA 4

DIGITALIZATION & EMERGING TECHNOLOGIES

Technological advances rely on both new materials and processing/manufacturing technologies. BCMaterials is working on the development of smart and multifunctional materials with improved processability and integration through advanced manufacturing processes, including additive manufacturing. Self-sensing, self-cleaning and self-repairing materials will be developed for printing technologies. Data providing and data management are at the core of the digitalization of society. Materials for sensors and actuators are therefore being developed and integrated in a variety of applications, including smart cities, smart interiors, industry 4.0 and wearables, among others.

Self-sensing magnetic actuator based on sustainable collagen hybrid nanocomposites

Mireia Andonegi, Carmen R. Tubio, Nelson Pereira, Carlos M. Costa, Senentxu Lanceros-Mendez, Koro de la Caba, Pedro Guerrero. (2024) International Journal of Biological Macromolecules, 277, art. no. 134364

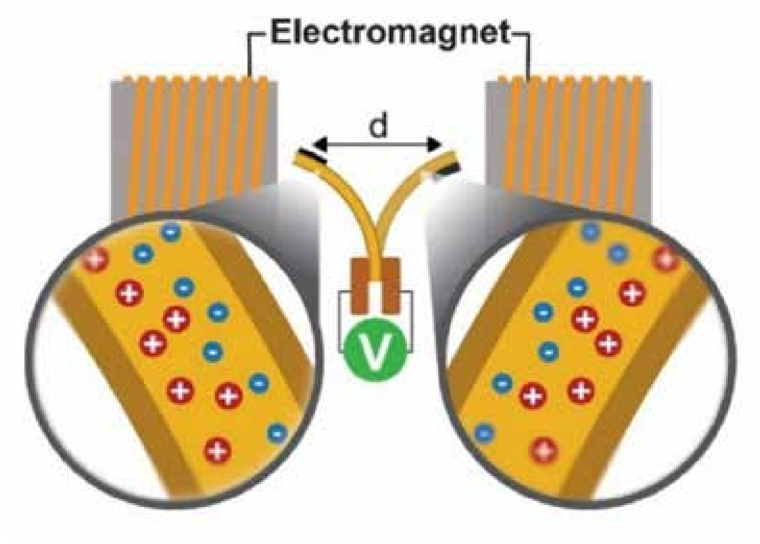


Fig 1
Electromagnetic diagram of the self-sensing actuator.

Sustainable collagen composites have been developed for applications in self-sensing magnetic actuator devices. These composites were prepared by varying the ferrite type, Fe_3O_4 NPs, Fe_3O_4 NRs and $CoFe_2O_4$ NPs, for a given filler concentration. It is shown that the magnetic filler type has no bearing on the morphology, physical-chemical, and thermal characteristics of the composites, whereas the mechanical properties are determined by the magnetic filler, leading to a reduction in tensile strength, with values of 4.95 MPa (Fe_3O_4 NPs), 9.20 MPa (Fe_3O_4 NRs) and 5.21 MPa ($CoFe_2O_4$ NPs) samples. However, the highest magnetization saturation is obtained for Fe_3O_4 NPs (44 emu/g) and the higher coercive field for $CoFe_2O_4$ NPs (2062 Oe). Finally, in order to prove functionality of the developed composites, a self-sensing magnetic actuator device has been developed. Due to the hysteresis loop of the samples containing the $CoFe_3O_4$ NPs, the self-sensing magnetic actuator has been developed with the piezo-ionic sensing element being an ionic liquid (IL)/collagen composite. The response of the sensor to variations in the magnetic field was demonstrated, with the sensor accurately detecting changes in direction and position of the cantilever in response to applied magnetic fields of approximately ±120 mT. The maximum bending was achieved with an angle of 55° when a positive magnetic bias was applied and 40° when a negative field was applied. The sensor can function as a magnetic position sensor, specifically a magnetic encoder, by detecting the rotational movement of a motor by the inclusion of a magnet in the motor rotor. The fluctuation of the magnet creates a fluctuating magnetic field, which causes the sensor to bend and stimulates the flexoelectric action of the IL collagen. Therefore, the viability of creating sustainable nanocomposites for the upcoming generation of electronic devices is confirmed by this work.

> Taking into account that natural polymers are renewable and biodegradable, hybrid materials based on natural polymers are required for advanced technological applications with reduced environmental footprint. In this work, sustainable composites have been developed based on collagen as a polymeric matrix and different magnetic fillers, in order to tailor magnetic response. Various magnetic fillers were used, including magnetite (Fe_3O_4) nanoparticles (NPs), Fe_3O_4 nanorods (NRs) and cobalt ferrite ($CoFe_2O_4$) NPs. The thermal, physical-chemical, morphological, mechanical, electrical and magnetic properties of the composites were analyzed. In addition, a self-sensing magnetic actuator was developed to demonstrate the applicability of the developed materials.

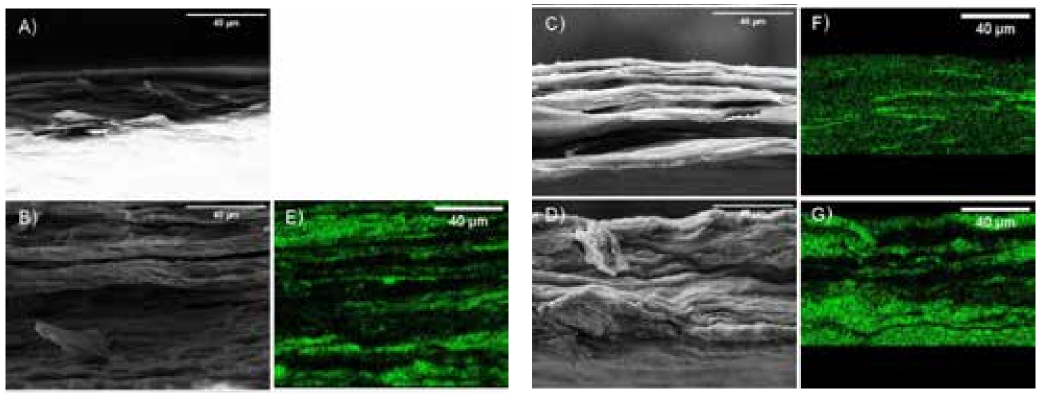


Fig 2
SEM images of the cross-section of a) Control, b) MNPs, c) MNRs and d) CFO NPs samples, and EDX mapping images of Fe for e) MNPs, f) MNRs and g) CFO NPs samples.

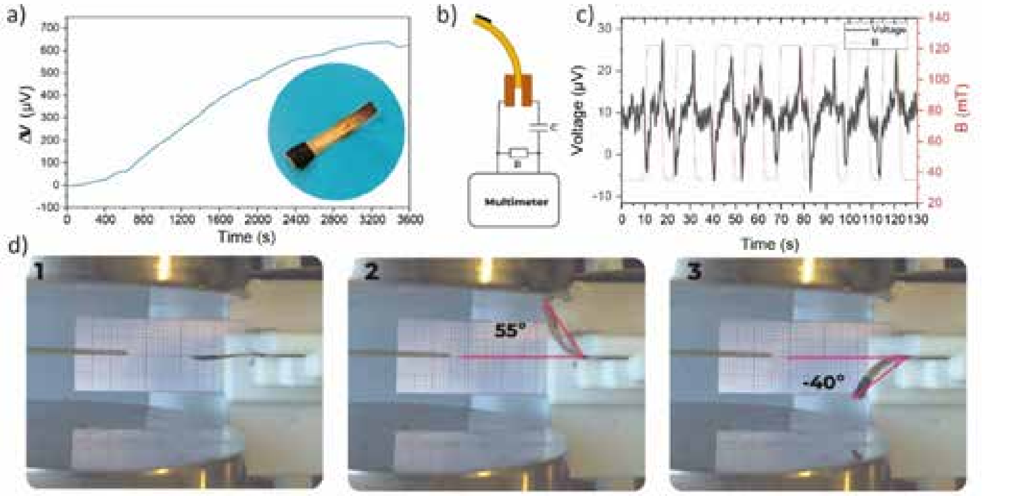


Fig 3
a) Stability of the IL/collagen film over 1 h (inset of the self-sensing actuator), b) schematic of the high-pass filter connected to the IL/collagen film, and c) signal from the IL/collagen film after filtering. d) Frames taken from the video in support information for a bending of the IL/collagen film when a magnetic field is applied. (1) B = 0 mT, 2) B = 120 mT, and 3) B = - 120 mT).

Dual-Mode Comb Plasmonic Optical Fiber Sensing

Villatoro E., Loyez M., Villatoro J., Caucheteur C., Albert J. (2024) ACS Sensors, 9 (6), pp. 3027 - 3036

> A partially coated tilted fiber Bragg grating is proposed for plasmonic sensing. The architecture of the proposed device enables the generation of dual-comb resonances, encompassing sensitive (TM/EH modes) and insensitive (TE/HE modes) components in unpolarized transmission spectra. This new sensing platform brings the following important practical assets: (1) a simpler fabrication process, (2) no need for polarization control, (3) limited bandwidth interrogation, and (4) maintained refractometric accuracy, which makes it a true game changer in the ever-growing plasmonic sensing domain.

Fig 1
(a) Schematic view of fiber cross section with the single-sided metal deposited layer. P and S are the orientation of the linear polarizations of the input light in the fiber core needed to excite cladding modes. (b) Side view of the optical fiber (not to scale) with the tilted Bragg grating in the core and single-sided metal coating.

Tilted fiber Bragg gratings (TFBG) enable coherent and wavelength selective excitation of a large number of cladding modes that show up as narrowband transmission resonances. It was demonstrated that TFBGs uniformly coated with a thin metal layer can excite a surface plasmon resonance (SPR) due to selective coupling to “TM-like” cladding modes. However, when a single-sided metal deposition is performed on a TFBG, as shown schematically in Figure 1, the layer thickness is highly nonuniform around the fiber cross section, and a degradation of the SPR response can be expected.

The approach followed in the present work removes the requirement of linear polarization of the interrogation light propagating in the fiber core. We demonstrate a new paradigm resulting from the combination of nonuniformly gold-coated TFBGs and unpolarized interrogation. In this precise case, the resulting transmission spectrum is made up of two well separated interleaved resonance combs as shown in Fig. 2. One comb comprising radially polarized modes (P modes) and another comprising azimuthally polarized modes (S modes).

It is demonstrated that the P resonances in the spectrum retain outstanding sensitivity to surrounding refractive index (SRI) changes, while the S resonances in the same measurement is nearly totally insensitive to SRI. Furthermore, it was observed that both sets of resonances shift equally with temperature, see Fig. 3. Hence, a multiresonant sensing methodology can be implemented to combine the responses of several resonances into a single measurement (thus improving the accuracy through statistical averaging) to provide a simultaneous measurement of temperature (which is important for grating-based and interferometric sensors) and input power level. The feasibility and sensing accuracy of our approach are demonstrated experimentally by measurements of small SRI changes (3x10^{-4}) in water solutions at different temperatures. By combining the responses of SPR-active and SPR-insensitive modes in a multiresonant approach, the refractometry accuracy is shown to be equal to or better than that obtained with conventional SPR-TFBG sensors, which require more complex fabrication and interrogation.

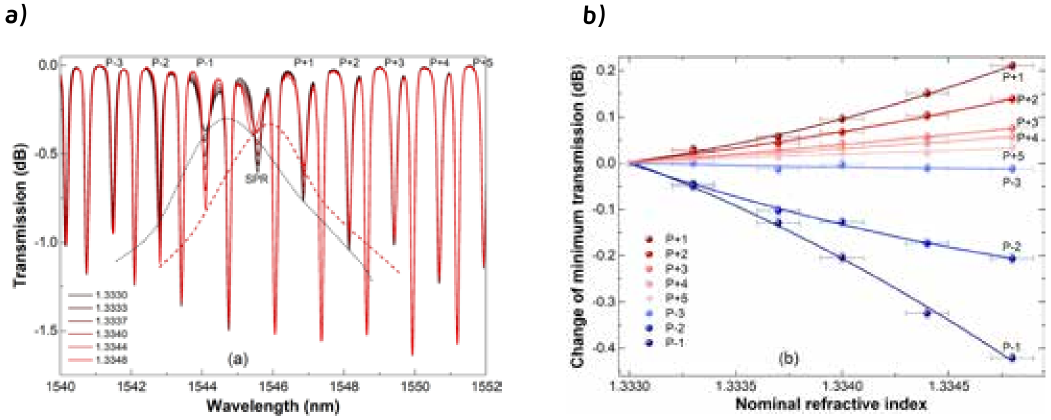


Fig 2
(a) Unpolarized spectra at constant temperature (20°C) for single-side-coated TFBG in six different ethanol-water solutions (with nominal refractive indices measured with a commercial Abbe refractometer). The SPR signature is sketched. (b) Changes of the minimum transmission of the P resonances surrounding the SPR dip, adjusted for power level changes. The horizontal and vertical error bars correspond to the nominal RI uncertainty and the standard deviation of successive measurements on the amplitude of an S resonance, respectively. The P-3 resonance is clearly very insensitive to refractive index changes.

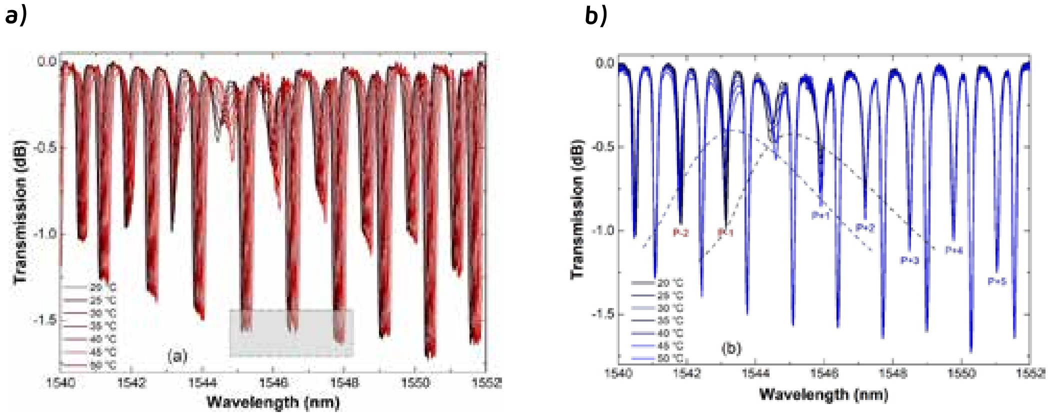


Fig 3
Temperature dependence of the cladding modes of a half coated TFBG in DI water, measured with unpolarized light: (a) as acquired data and (b) spectra corrected by removing the average shifts of the three S resonances highlighted with a shaded rectangle in (a). In spite of this correction, changes in the P resonance amplitudes indicate a clear SPR shift toward shorter wavelengths, now due solely to the negative thermo-optic coefficient of water.

Towards a REASSURED reality: a less-is-more electronic design strategy for self-powered glucose sensing

S. K. Sailapu, S. Liébana, I. Merino-Jimenez, J. P. Esquivel, N. Sabaté

Biosensors and Bioelectronics 243 (2024) 115708

Sensing strategies adopting minimal electronic systems help in realizing REASSURED diagnostic tests. However, the challenge in developing such strategies escalates with demand in power and electronics during pursuit of reliable and accurate sensing. Herein, we present an electronic design strategy using a smart strip, operating with power generated from 3.5 μL of serum sample, to reveal glucose concentration. The design strategy uses only four components – two resistors, diode, and capacitor - of simple architecture likely transferable to printed technologies to deliver advanced self-powered sustainable devices.

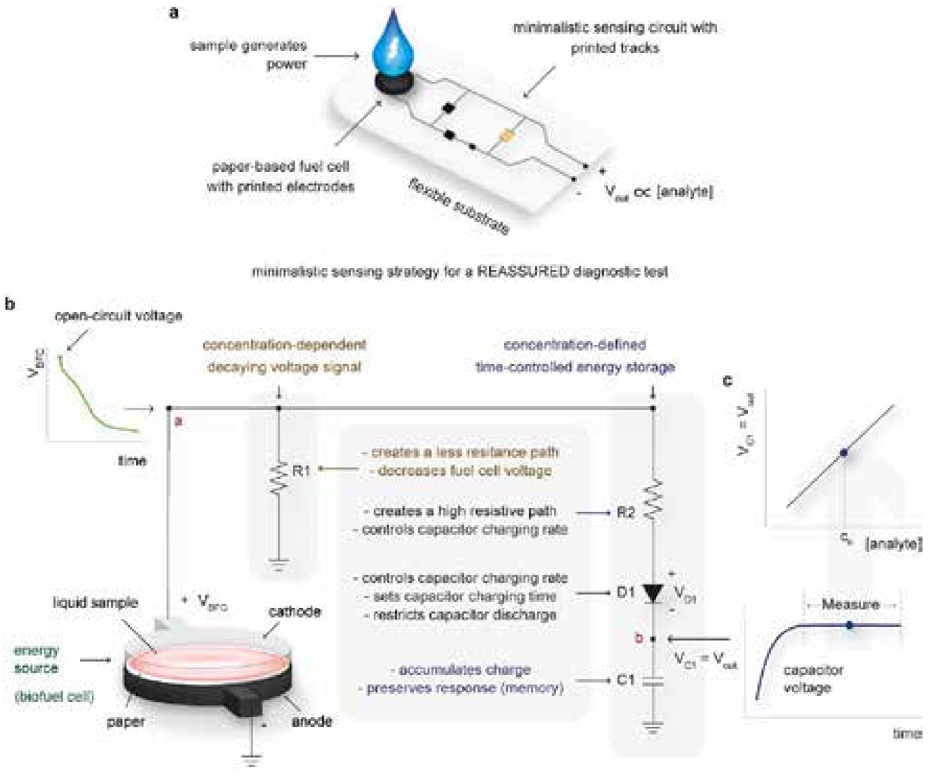


Fig 1
A minimalistic strategy for REASSURED implementation of a diagnostic test. (a) Scheme illustrating self-powered quantification of analyte using a fuel cell and minimalistic sensing circuit hosted on a flexible substrate. The circuit operates with the power generated from sample and delivers an output voltage revealing analyte concentration. (b) The sensing strategy involves operating the fuel cell in a diffusion-controlled process. (c) A quantitative information of analyte concentration is then achievable by relating the capacitor voltage to a pre-established calibrated curve.

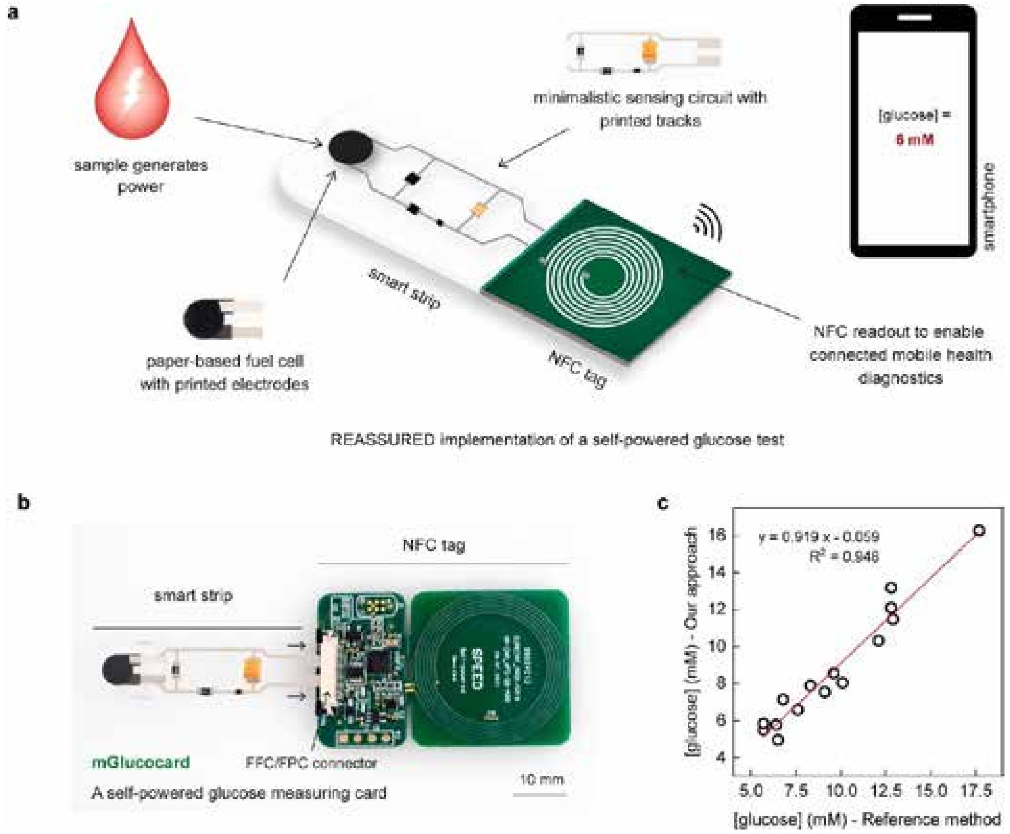


Fig 2
Self-powered glucose test with clinical samples. (a) Illustration of the REASSURED implementation of a self-powered glucose test. (b) Picture of the assembled mGlucocard. (c) Comparison of mGlucocard response against a colorimetric reference method with commercial device using serum samples.

Efforts to develop point-of-care (POC) diagnostics remain crucial for early detection and personal management of chronic diseases like diabetes. Advances in approaches enabling large-scale and low-cost rapid development of POC glucose sensing platforms - abiding the REASSURED (Real-time connectivity, Ease of specimen collection, Affordable, Sensitive, Specific, User-friendly, Rapid and robust, Equipment free or simple and Environmentally friendly, Deliverable to end-users) criteria and support by mobile devices for connected diagnostics, as defined by World Health Organization (WHO) - allow widespread diagnosis to improve health care. Unlike lateral flow tests, amperometric glucose sensing solutions have not fulfilled the ASSURED criteria. They require a dedicated power source and complex circuit implementation, that render them pricey and pollutant.

Herein, we propose a radical minimalistic strategy of circuit implementation for self-powered quantification of analyte with a paper-based biofuel cell to achieve a sustainable solution that fits well within the framework of a REASSURED diagnostic test. To demonstrate the minimalistic self-powered strategy of circuit implementation, we developed a smart strip to measure glucose concentration in human serum. For enabling 'connected mobile-health diagnostics', we further devised a CR80 card-sized portable self-powered glucose measuring card, mobile-glucocard (or mGlucocard) that consists of a reusable and battery-free NFC tag alongside the smart strip to retrieve the digital result using a smartphone in an easy manner. In this way, a measurement that typically requires a potentiostat with a microcontroller and a battery is performed with a minimalistic and battery-less circuit that fits well within the footprint of a commercial glucose strip and supposes a radical decrease in cost and electronic waste.

Here, the compact size of mGlucocard, involved low-cost, potential transferability to printed technologies, and sustainable approaches with paper-based design, no batteries and minimum sensing electronic components are highly advantageous to POC application for on-demand use and disposal akin to colorimetric strips but with ability for logging accurate quantitative digital readings.

RESEARCH
LINE 1

ACTIVE & SMART MATERIALS

Active and smart materials are at the core of the on-going rapid technological development. Shape memory, magnetocaloric and elastocaloric materials, piezoelectric, magnetoelectric and self-healing materials as well as multifunctional hydrogels are being developed. A deep understating on the structural and molecular modifications behind the active responses allows tailoring materials responses.

Anisotropic nanoparticle-based magnetorheological elastomers: Effect of shape and orientation on the magnetorheological performance

Ander Garcia Díez, Carmen R. Tubio, Ainara Gómez, Joanes Berastegi, Maite Insausti, José S. Garitaonandia, M. Mounir Bou-Ali, Jon Gutiérrez Etxebarria, and Senentxu Lanceros-Méndez. (2024) Polymer, 295, art. no. 126776

Magnetorheological elastomers (MREs) respond to applied magnetic fields with a change in their mechanical properties. Within this work, iron oxide nanorods (IONRs) have been synthesized and the suitability of anisotropic nanoparticles to obtain highly responsive isotropic and anisotropic MREs has been demonstrated. Electron microscopy images show that the IONRs are well distributed inside the styrene-ethylene-butylene-styrene (SEBS) polymeric matrix and can be successfully oriented. Magnetization loops show a difference in the orientations, with variations of the anisotropy field from 39.2 to 67.7 kA/m. Magnetorheology measurements show that the relative MRE effect experiences a twofold increase for the anisotropic MREs, from 8.3 to 17%. This, along with the improved mechanical properties of the anisotropic MREs, offers excellent possibilities for the design of high performance MREs that work optimally in the elastic region with improved applicability.

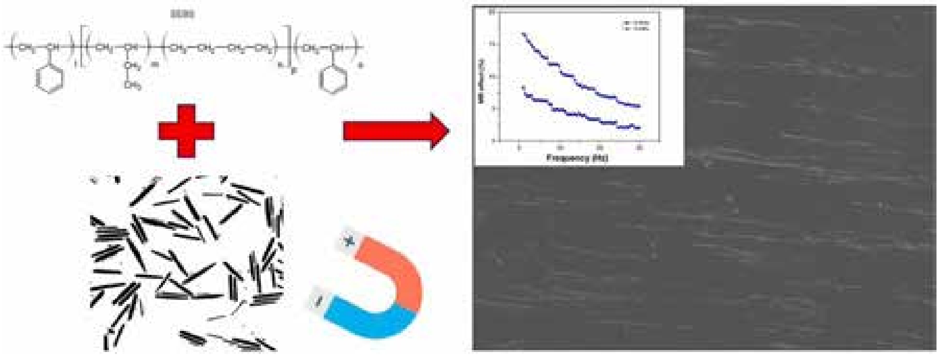


Fig 1
Covert art

A comprehensive study of how shape and orientation of magnetic nanofillers affect the properties of MREs has been performed. In particular, the suitability of anisotropic nanoparticles to fabricate non-oriented (isotropic) and oriented (anisotropic) MREs has been demonstrated. For that, iron oxide nanorods (IONRs) have been synthesized with approximately 112 nm in length and 12 nm in width (AR = 10) and introduced within a SEBS polymer matrix. Composites were produced applying a magnetic field during processing to obtain a preferential orientation of the fillers (anisotropic composites) and without the application of the magnetic field, leading to a random orientation of the anisotropic fillers (isotropic composites). As a result, the influence of the shape and orientation of the magnetic particles on the morphological, thermal, mechanical, magnetic, and MR characteristics of the magnetoactive materials has been determined. SEM images confirmed that the fillers are well distributed within the polymeric matrix, without significant alterations in the microstructure. Magnetic measurements also confirm these results, where the magnetic properties of the fillers are retained. The main difference is in the anisotropy field, which increases from 39.4 to 67.7 kA/m between parallel and perpendicular orientations, demonstrating the anisotropy of the composites. Mechanical properties also exhibit significant anisotropy. The elastic modulus of the bare polymer was 0.7 MPa but, for the anisotropic MRE, the modulus was just enhanced when the loading is applied parallel to the orientation of the fillers, reaching 1.3 MPa. Meanwhile, the isotropic composite also showed and twofold increase in the Young's modulus. Due to the geometric and magnetic anisotropy of the composites, the MR effect was also enhanced for the anisotropic MRE, exhibiting a relative increase of 104 % with respect to isotropic MRE. This relative increase in the MR effect is larger when compared to other studies that featured anisotropic composites or anisotropic nanoparticles. Considering these results, it can be concluded that the use of high aspect ratio nanofillers with shape and magnetic anisotropy leads to MREs with unique features such as higher elastic modulus and higher response to magnetic fields when the particles are adequately aligned. Additionally, the use of nanoparticles instead of microparticles opens new possibilities in the fabrication of high-resolution devices by using additive manufacturing techniques.

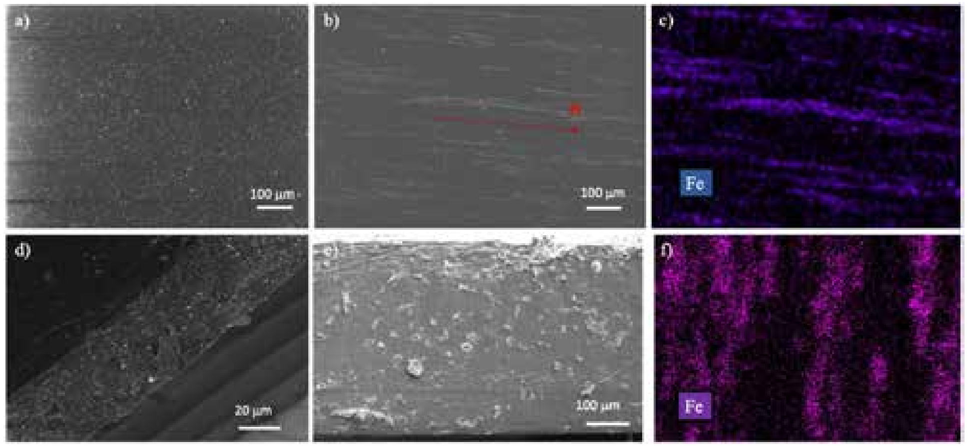


Fig 2
Surface and cross-sectional images of the randomly oriented (R), R-NRs (a, d) and oriented (O), O-NRs (b,e) samples, respectively. Iron (Fe) EDS mapping on the oriented samples: surface (c) and cross-section (f) images.

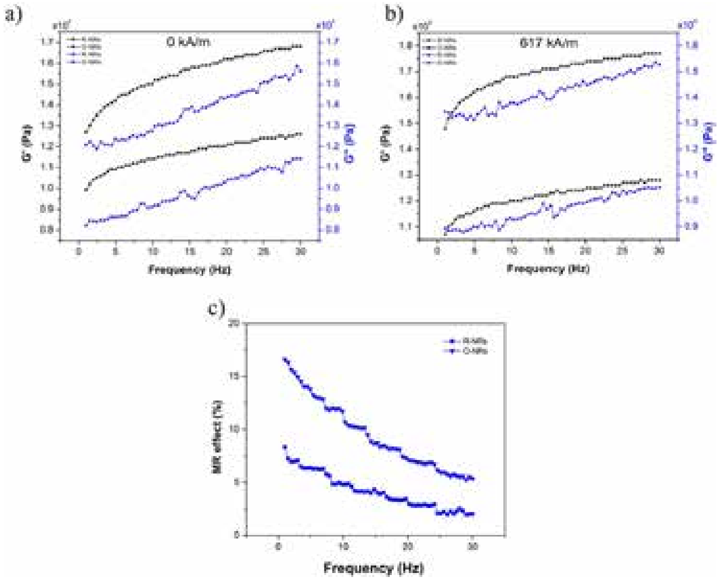


Fig 3
Storage and loss moduli measurements of the composites containing NRs in the off-field (a) and on-field (b) states. Magnetorheological effect of the samples (c).

Design of acrylated epoxidized soybean oil biobased photo-curable formulations for 3D printing

Matilde Porcarello, Cristian Mendes-Felipe, Marco Sangermano, Senentxu Lanceros-Méndez.

Sustainable Materials and Technologies 40, e00927, 2024.

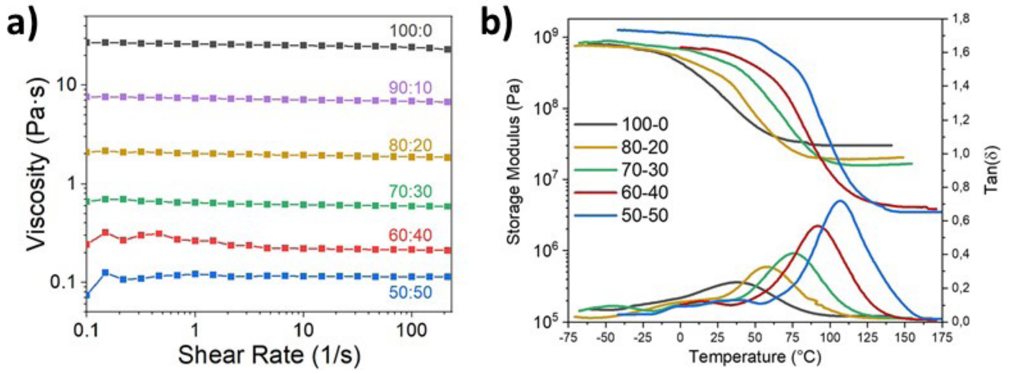


Fig 1
Viscosity as function of shear rate for the photocurable formulation AESO-LA (a) and DMTA results for AESO-IBOMA printed specimens (b).

Additive manufacturing (AM) has revolutionized production by employing a layer-by-layer approach, reducing waste, and enabling rapid prototyping, versatility, and precision across industries like aerospace, construction, and biomedical sectors. VAT polymerization (VP), a key AM technique, utilizes photocurable liquid resins to create high-resolution 3D objects. However, its reliance on fossil-based photopolymers underscores the need for sustainable alternatives. Vegetable oils, particularly acrylated epoxidized soybean oil (AESO), have emerged as promising bio-based options due to their abundance, biocompatibility, and photopolymerization potential. Challenges like AESO's high viscosity are addressed by incorporating reactive diluents to improve printability.

This study develops AESO-based photo-curable formulations for digital light processing (DLP) 3D printing, using reactive diluents such as lauryl acrylate (LA) and methacrylate (LMA), and isobornyl acrylate (IBOA) and methacrylate (IBOMA). These diluents reduce viscosity and influence photopolymerization reactivity, making the formulations suitable for DLP processes. Experimental procedures included rheological and photo-rheological assessments, mechanical and thermal characterizations, and printability tests, emphasizing mechanical precision and resolution.

The findings show that formulations with 20–50 wt% diluent achieved optimal viscosity and curing behaviour. Acrylate diluents like LA and IBOA enhanced curing rates and reduced gelation times, while methacrylates like LMA and IBOMA raised glass transition temperatures (T_g) due to their structural rigidity. Mechanical testing revealed that IBOA- and IBOMA-containing samples exhibited increased tensile strength and stiffness at higher diluent concentrations, whereas LA- and LMA-based formulations retained softer, more elastic properties. Key results are highlighted in figures like viscosity and DMTA curves (Fig. 1) and stress-strain analyses (Fig. 2).

Complex 3D structures, such as hollow cubes and gyroids, were printed and assessed for accuracy using 3D scanning (Fig. 3), confirming the precision and feasibility of AESO-LA and AESO-IBOA formulations for intricate designs. This study demonstrates AESO-based biobased resins as sustainable alternatives to petroleum-based materials, advancing environmentally friendly additive manufacturing and providing a foundation for further innovations in bio-renewable materials for high-performance 3D printing.

> “ The development of bio-based polymeric materials has gained importance due to environmental concerns and declining oil availability. Vegetable oils, especially soybean oil (SO), offer cost-effective, abundant alternatives. SO can be functionalized to produce photocurable acrylate epoxidized soybean oil (AESO) used in this study for Digital Light Processing (DLP). To reduce its viscosity, reactive diluents like lauryl (meth)acrylate and isorbornyl (meth)acrylate were added. Formulations with appropriate viscosities were 3D printed and analyzed for mechanical and thermo-mechanical properties.

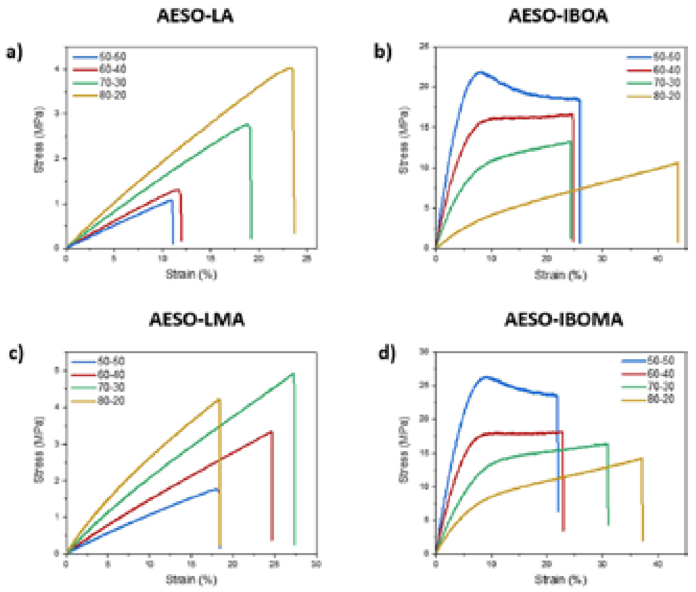


Fig 2
Stress-strain curves of 3D printed specimens for AESO-LA (a), AESO-IBOA (b), AESO-LMA (c) and AESO-IBOMA (d) formulations.

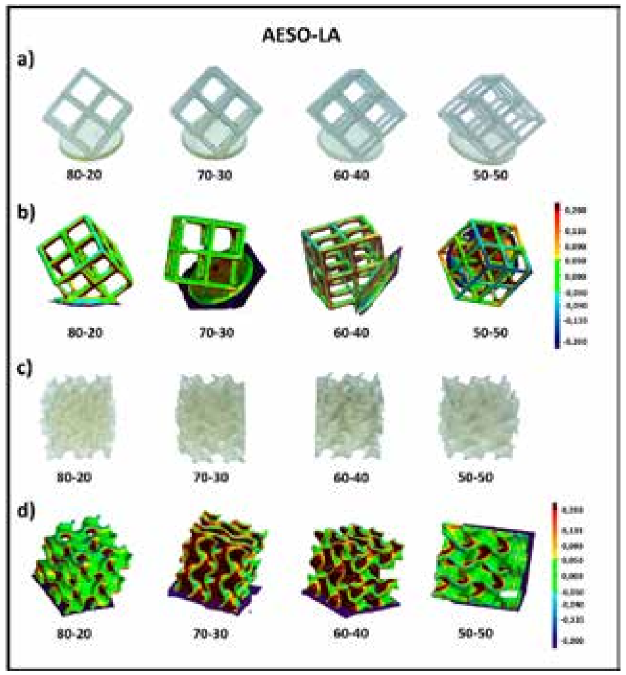


Fig 3
Pictures of 3D printed cubes (a) and gyroids (c), compared to their 3D scanner evaluation images of the differences between the CAD project and the real printed object (b) and (d) respectively, for AESO-LA formulations.

Stretchable Conductive Inks with Carbon-Based Fillers for Conformable Printed Electronics

Lia Campos-Arias, Nikola Peřinka, Pedro Costa, José Luis Vilas-Vilela, Senentxu Lanceros-Méndez.

(2024) Advanced Engineering Materials, 26 (21), art. no. 2400354

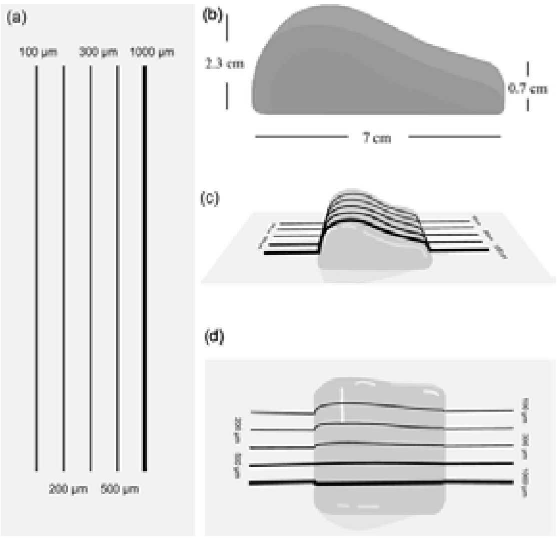


Fig 1
Scheme of samples a) before and c,d) after thermoforming and b) the mold used for thermoforming with its dimensions.

> “The global need for sustainable materials boosts development of novel functional composites for additive manufacturing. Combined with other processes, such as thermoforming, printed electronics can be transformed to a 3D shape. Herein, conductive inks made of styrene-ethylene/butylene-styrene and different aspect-ratio carbon-based materials for conformable electronics were developed. The inks are prepared with carbon black (CB), carbon nanotubes (CNTs), and reduced graphene oxide (rGO), showing electrical conductivity up to 141 S m^{-1} and compatibility with the thermoforming process.

The evolution of industry 4.0 has raised concern about increasing amount of electronic waste (e-waste). Therefore, development of electronics with fewer components and more environmentally friendly materials and processes is essential. One way to reduce e-waste is by developing materials that can be functional and structural at the same time, reducing assembling parts to its minimum. Printing, being an additive manufacturing technique, allows materials and device customization from small to large areas of flexible and conformable systems. Combining printed electronics with thermoforming and molding processes, in-mold electronics (IME) emerges. The IME product comprises an electronic circuit embedded in a piece that can be structural, being in its final 3D shape. To ensure enough stretchability and thermal stability, the conductive inks for IME need to be based on elastomeric binders, such as polystyrene-b-(ethylene-co-butylene)-b-styrene (SEBS). In this study, the effect of using different aspect-ratio carbon-based conductive materials as fillers in an elastomeric matrix (SEBS) has been evaluated for the development of conductive traces to be subjected to a thermoforming process. The inks were prepared with carbon black (CB, 0D), multiwalled carbon nanotubes (CNTs, 1D), and reduced graphene oxide (rGO, 2D), printed onto a flexible substrate and thermoformed to a 3D shape using a mold with different levels of curvature (Figure 1). The stress–strain measurements showed different mechanical behaviour of each composite prepared with different concentrations of each filler (Figure 2).”

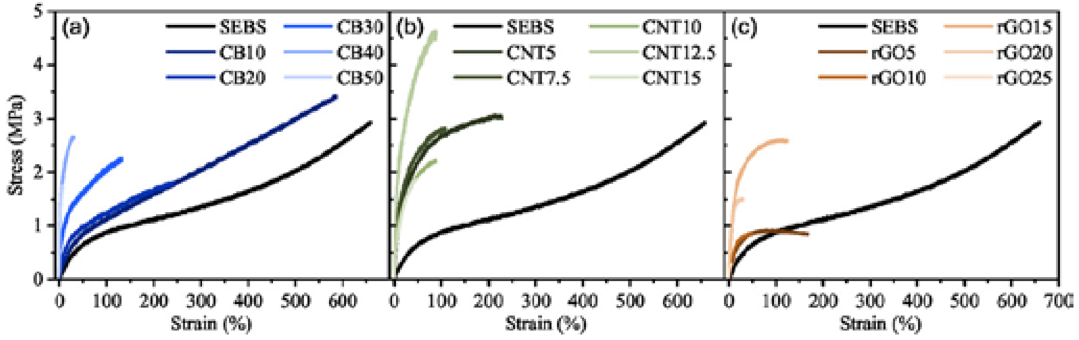


Fig 2
Stress–strain mechanical characteristics of the samples with a) CB, b) CNT, and c) rGO.

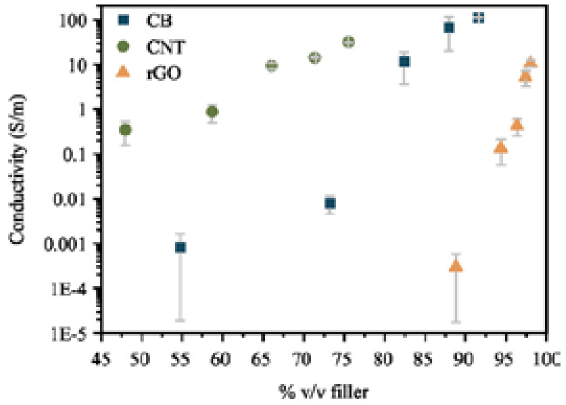


Fig 3
Electrical conductivity and standard deviation of bulk materials as a function of filler content in % v/v.

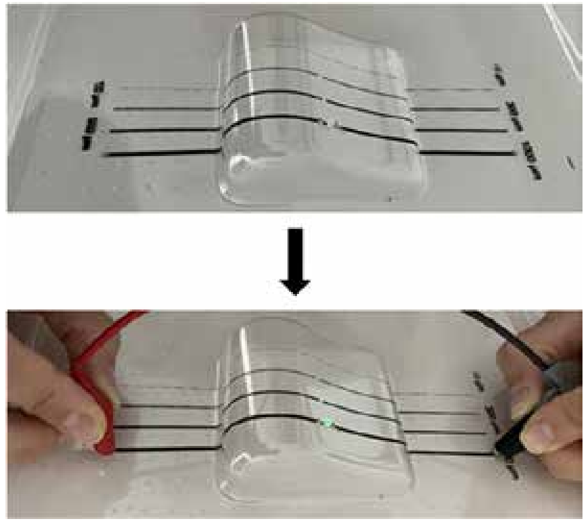
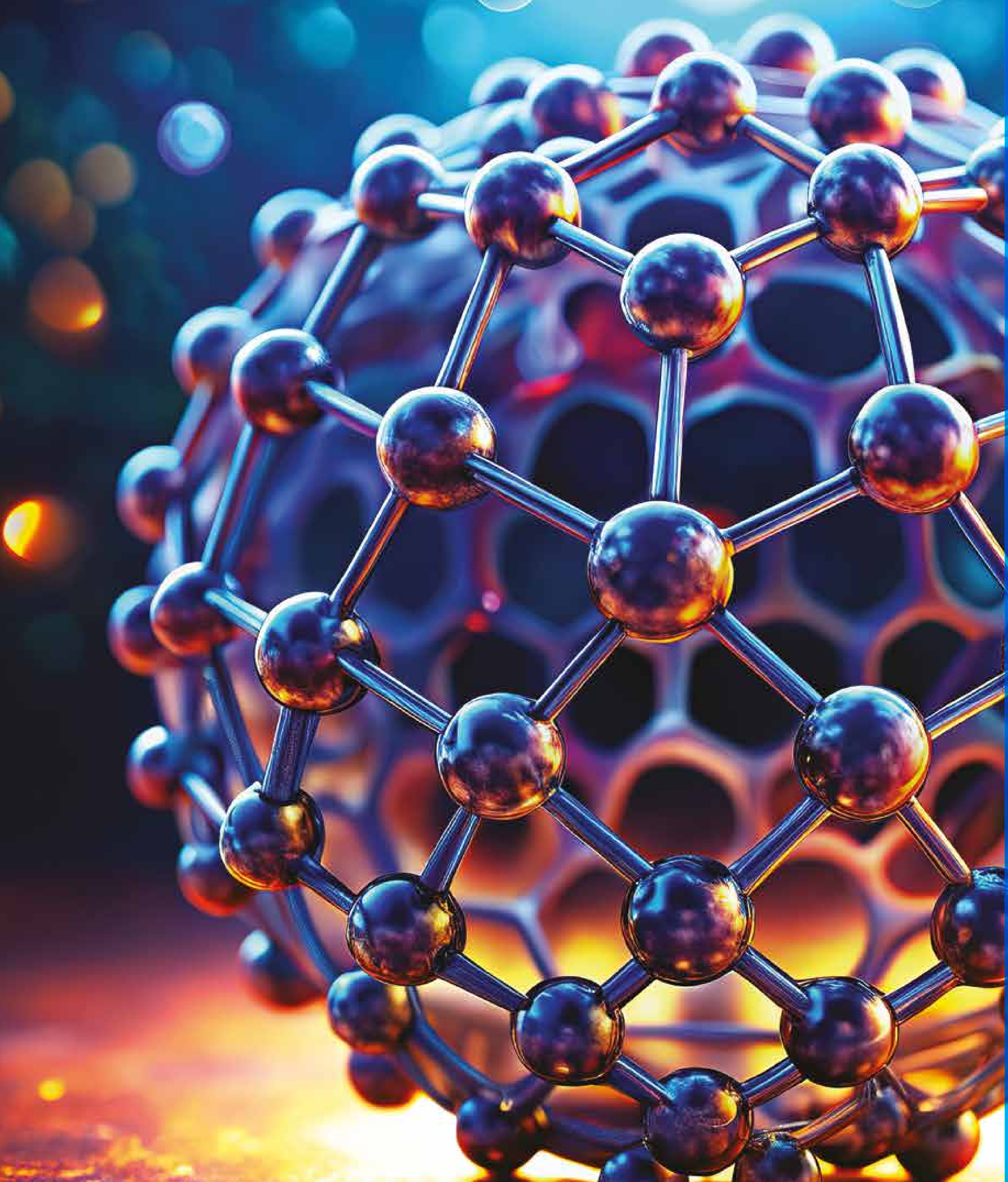


Fig 4
CNT sample with the green LED mounted on the printed track (top) and with an applied bias of 3.5 V (down).

. The SEBS strain–stress curve shows a maximum deformation of 655%, while the addition of fillers induces a shift in the mechanical response by increasing the brittleness of the samples. For instance, by adding even a small amount of CNT filler a huge change in SEBS mechanical properties and its elasticity is disrupted. The electrical conductivity of the printed films with different fillers as a function of filler volume content shown in Figure 3 indicates the filler contents for each filler to achieve suitable conducting properties. Thus, to obtain 1 S m^{-1}, it is necessary to add almost 80% v/v (<30 wt%) of CB and around 98% v/v (<20 wt%) of rGO to the mixture, but it is enough with 60% v/v (>7.5 wt%) of CNT. Finally, a green-light-emitting diode (LED)-mounted thermoformed samples demonstrated the feasibility of the developed materials for screen-printable conformable electronics applications (Figure 4).



RESEARCH LINE 2

MICRO & NANO-STRUCTURED MATERIALS

Nanostructures are being developed in order to take advantage of their specific tailored properties and to support the development of multiresponsive hybrid materials. Magnetic and metallic nanoparticles produced by bacteria and plants, single and hybrid magnetic, plasmonic and photocatalytic nanoparticles are being developed, among others. We devote special attention will be devoted to mesoporous materials, mainly metallic organic frameworks and zeolites, which are being investigated based on their tuneability and specific intrinsic properties for sensing, energy, environmental and biomedical applications. In particular, strong efforts are being developed in the area of hierarchical materials out of MOFS as well as to molecular materials such as molecular magnets.

Effect of the heteroatom on the magnetic and luminescence properties of hybrid lanthanide-substituted Keggin-type polyoxometalates

Janire Bustamante-Fernández, Estibaliz Ruiz-Bilbao, Corina Rodríguez-Esteban, Mathieu Gonidec,
José A. García, Luis Lezama, Juan M. Gutiérrez-Zorrilla, Itziar Oyarzabal and Beñat Artetxe;
Dalton Trans., 2024,53, 13330-13334.

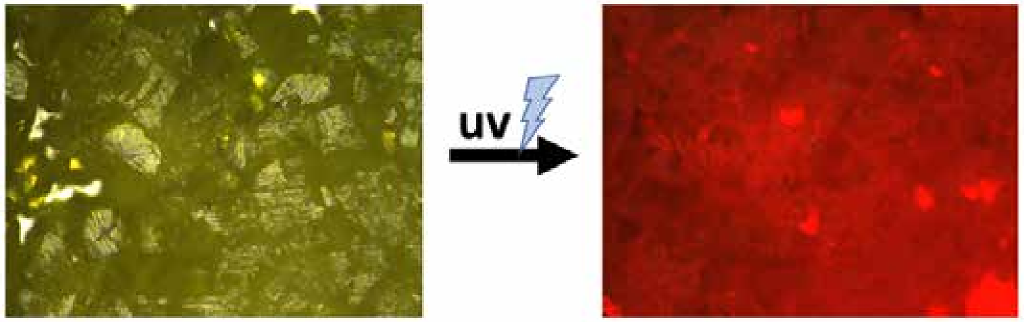


Fig 1
Photographs of bulk crystalline samples of 1Si-Eu before and after irradiation with UV light.

Combination of lacunary polyoxometalates (POMs) with lanthanide ions constitutes a powerful tool to design architectures with applications in fields like catalysis, luminescence or magnetism. In a similar way, the use of compartmental organic ligands has proved to be effective to prepare 4f- or 3d/4f-based dual magneto-luminescent materials. However, the simultaneous coordination of both organic and inorganic ligands remains almost unexplored.

The recently reported reaction between mid-to-late LnIII salts, the N,N'-dimethyl-N,N'-bis(2-hydroxy-3-formyl-5-bromobenzyl)ethylenediamine (H2L) ligand and the monolacunary Keggin-type POM $[\alpha\text{-SiW}_{11}O_{39}]^{8-}$, leads up to ten isostructural compounds with the formula $K5[Ln^{III}(H_2L)(\alpha\text{-SiW}_{11}O_{39})]\cdot 14H_2O$ (1_{Si}-Ln, Ln^{III} = Sm–Lu).[1] Among these species, 1_{Si}-Gd and 1_{Si}-Yb display slow relaxation of the magnetization below ~5-6 K after the application of an external magnetic field, whereas photoluminescent emission is displayed by 1_{Si}-Sm and 1_{Si}-Eu in the visible region and 1_{Si}-Er and 1_{Si}-Yb in the NIR region (Fig. 1). In order to evaluate the effect of the heteroatom on the magnetic and luminescent properties, the Si centre was replaced by Ge, resulting in nine additional hybrids; $K_5[Ln^{III}(H_2L)(\alpha\text{-GeW}_{11}O_{39})]\cdot 14H_2O$ ($1_{Ge\text{-}Ln}$, Ln^{III} = Sm–Yb).

The larger size of the heteroatom in 1_{Ge}-Ln allows 4f ions to be better incorporated into the lacunary site, in such a way that the distances to central O atoms are shortened in 0.2 Å (Fig. 2). The slight modifications in the local geometry of the Ln ions lead to a shift of the frequency dependent ac susceptibility signals of the Gd and Yb derivatives towards higher temperatures (from ~5-6 K to ~8-9 K) (Fig. 3). Regarding the photoluminescent properties, a clear colour shift to orange in 1Ge-Sm upon irradiation is observed, whereas the Yb-derivatives represent the first lanthanide-containing POM-based systems able to exhibit simultaneous slow magnetic relaxation and NIR emission, and more interestingly, NIR emission at room temperature in the case of 1_{Ge}-Yb (Fig. 4). It is noteworthy that these compounds present some advantages compared to those emitting in the UV range, such as their use as luminophores to create bioimages with higher sensitivity as well as in the field of optical communication. Therefore, this work nicely exemplifies the importance of the heteroatom in lanthanide ion/lacunary POM/aromatic multidentate organic ligand systems to construct molecular materials with interesting optical and magnetic properties.

> Replacement of the heteroatom from Si to Ge has a strong influence on the luminescence properties of a series of hybrid sandwich-type $K5[Ln(\alpha\text{-GeW}_{11}O_{39})(C_{20}H_{22}Br_2N_2O_4)]\cdot 14H_2O$ (1_{Ge}-Ln, Ln = Sm to Lu) anions. Interestingly, the Gd and Yb derivatives retain their ability to display slow relaxation of magnetisation.

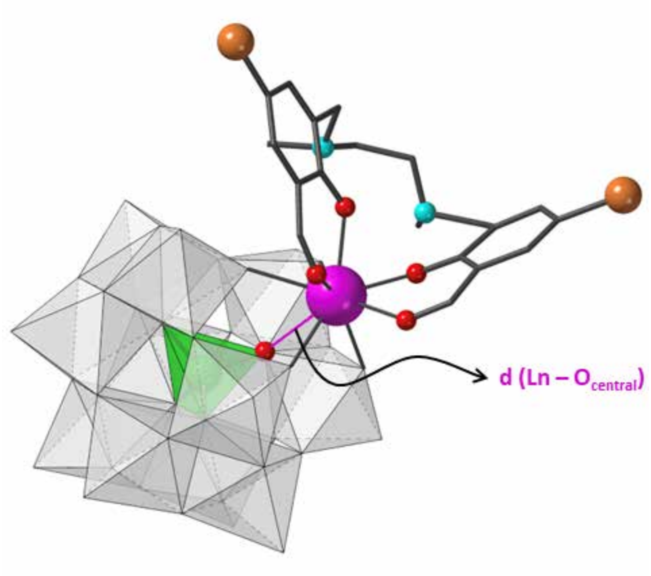


Fig 2
Molecular structure of hybrid $[Ln(H_2L)(\alpha\text{-GeW}_{11}O_{39})]^{5-}$ anions in 1Ge-Ln. The Ln… $O_{central}$ bond is represented as a purple line and discussed in the text. Colour code: WO_6, grey; GeO_4, green; Ln, purple; C, black, O, red; N, blue; Br, orange. H atoms have been omitted for clarity.

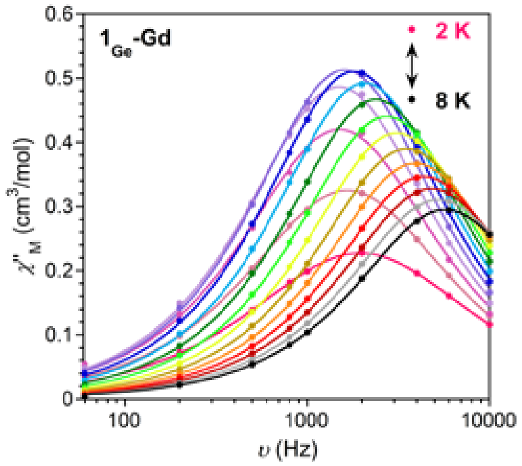


Fig 3
Frequency dependence of the out-of-phase component of the ac susceptibility at H_{dc} = 2500 Oe for 1_{Ge}-Gd. The experimental data are denoted by circles; solid lines represent the best fit to the data.

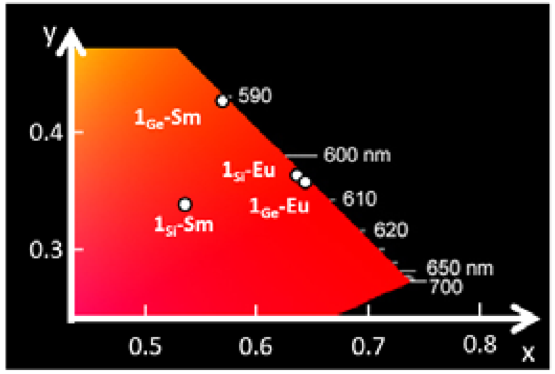


Fig 4
CIE 1931 x, y chromaticity coordinates as a function of the emission wavelengths for 1_{Si}-Sm, 1_{Ge}-Sm, 1_{Si}-Eu and 1_{Ge}-Eu.

Identifying synthetic variables influencing the reproducible microfluidic synthesis of ZIF nano- and micro-particles

Dutta S., Sinelshchikova A., Andreo J., Wuttke S. (2024) Nanoscale Horizons, 9 (6), pp. 885 - 899

> Reproducible synthesis of nano- and microparticles is crucial to their application, as their morphology directly impacts physicochemical properties. Using a coiled tube microfluidic reactor, we explored the interplay between mixing dynamics, modelled via Dean flow, and key synthetic parameters. By varying reagent concentration, stoichiometry, aging time, and nine modulators, we identified critical factors influencing the synthesis of ZIF-7, ZIF-8, ZIF-9, and ZIF-67. Our findings offer strategies to address reproducibility challenges and enhance control in microfluidic particle synthesis.

Reproducible synthesis of nano- and microparticles is essential for developing materials with tailored properties. This study explores the microfluidic synthesis of four ZIFs—ZIF-8, ZIF-67, ZIF-7, and ZIF-9—chosen to evaluate the influence of different metal-linker combinations on particle size, shape, and morphology. We examine key synthetic parameters, including reagent concentration, stoichiometry, reaction aging time, and various chemical modulators (e.g., pH-altering agents, surfactants, and polar polymers), alongside the role of Dean flow mixing and its interaction with these variables.

Dean flow mixing is critical in microfluidic systems, with mixing strength directly affecting particle formation. As the Dean number (De) increases, the mixing undergoes three phases: no vortex formation at low De, stable vortex formation at high De, and an unstable range in between, which can result in strong particle size variations between otherwise identical synthesis.

We find that reagent concentration correlates with particle size, with larger particles formed at higher concentrations. Stoichiometry also impacts particle size, with deviations from ideal ratios leading to smaller particles, though the effect of mixing strength varied between materials. Aging time influenced the morphology of ZIF-8 and ZIF-67 particles, but ZIF-7 and ZIF-9 required extended aging times (6 and 2 hours, respectively) to form crystalline structures. The role of nine different modulators was also explored, with TEA significantly reducing the size of ZIF-8 and ZIF-67 particles. Interestingly, polymer molecular weight strongly influenced particle size, with longer polymer chains leading to size reductions at high De.

Finally, the reproducibility challenges related to Dean flow mixing were identified, particularly in the unstable De range. At De 50, the presence or absence of vortices can result in large discrepancies in particle size. This variability emphasizes the need for precise control over the microfluidic setup, as inconsistencies in mixing behaviour compromise reproducibility.

This work provides valuable insights into the microfluidic synthesis of ZIF nanoparticles, highlighting key parameters and the critical role of Dean flow mixing in controlling particle size and morphology. Our findings offer guidance for improving the reliability and control of microfluidic synthesis, aiding future researchers in the development of advanced materials and synthesis methodologies.

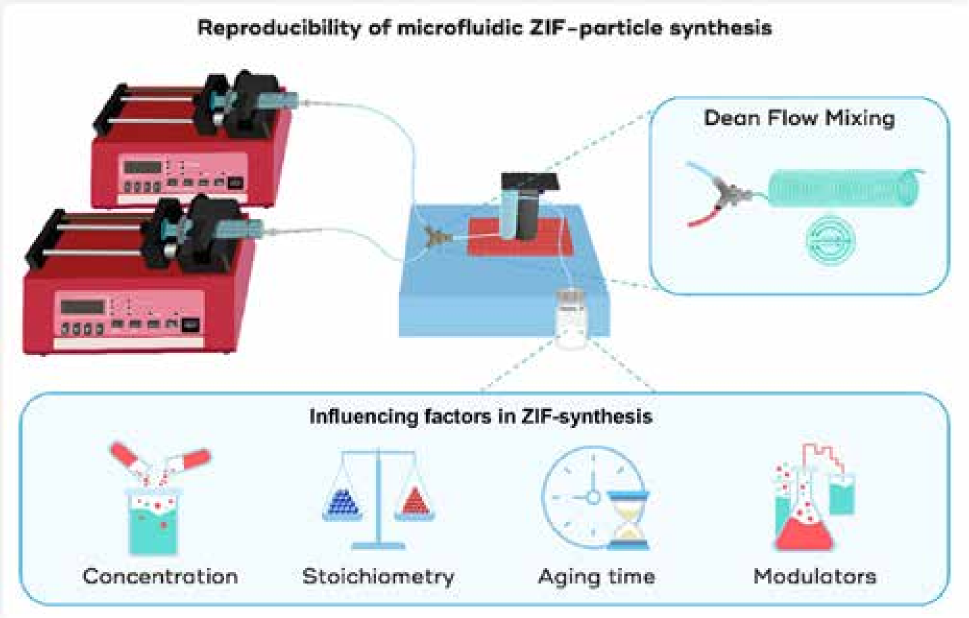


Fig 1
Schematic representation of the experimental setup used for ZIF synthesis and the synthetic variables investigated in this work.

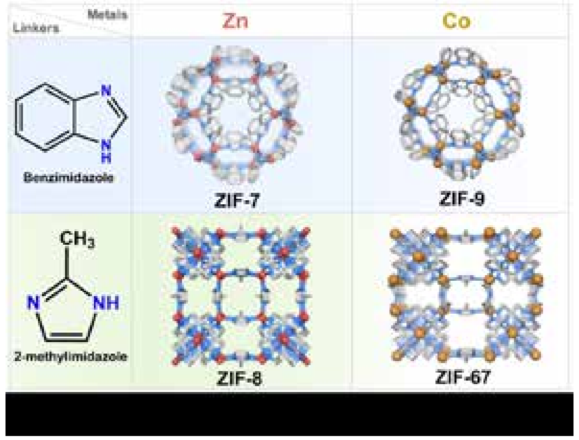


Fig 2
Structural representation of the ZIFs used in this work and their constituents.

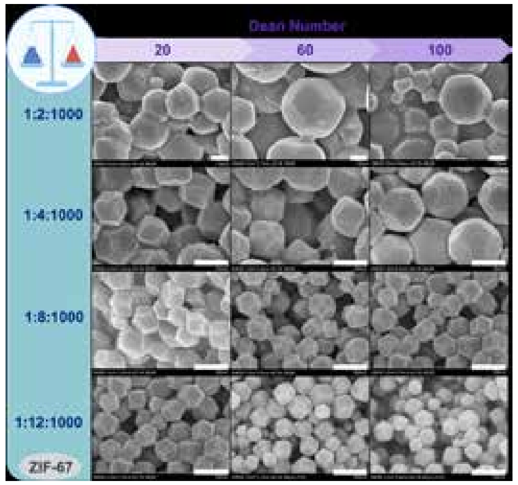


Fig 3
SEM images of ZIF-67 particles showing the influence of different dean numbers and stoichiometric ratios of the precursors on particle size and morphologies.

Unravelling co-catalyst integration methods in Ti-based metal–organic gels for photocatalytic H_2 production

Maite Perfecto-Irigaray, Garikoitz Beobide, Oscar Castillo, Michael G. Allan, Moritz F. Kühnel, Antonio Luque, Harishchandra Singh, Ashok Kumar Yadav, Sonia Pérez-Yáñez. Dalton Transactions, Volume 53, 2024, 9482.

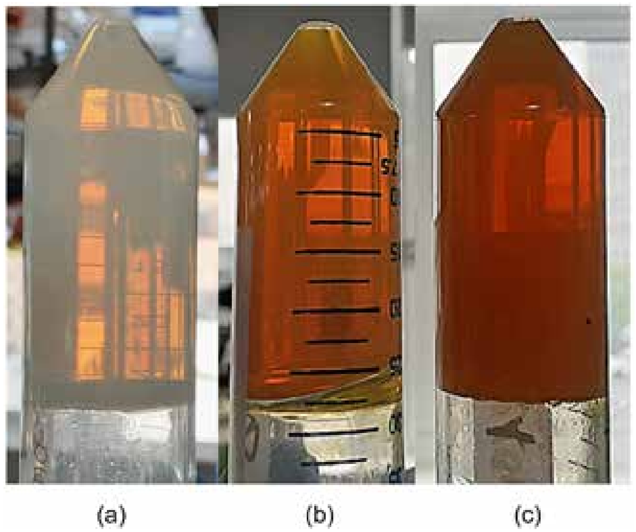


Fig 1
Appearance of as-synthesised (a) B100, (b) B50A50 and (c) A100 gels.
A = benzene-1,4-dicarboxylic acid (H_2BDC);
B = 2-aminobenzene-1,4-dicarboxylic acid (H_2NH_2BDC).

In this work, we describe the synthesis, comprehensive characterization, and HER performance of a series of MOGs related to the MIL-125 MOF that are constructed by the assembly of Ti-oxo clusters and dicarboxylato linkers (benzene-1,4-dicarboxylato and 2-aminobenzene-1,4-dicarboxylato; Figure 1). The chemical characterization reveals a similar local structure to that of MIL-125 MOFs, but highly defective in comparison and with no long-range ordering. All the systems exhibit similar microstructure, comprised of nanoscopic metal–organic particles (<5 nm) intertwined into a highly porous structure. However, only the BDC-based system has demonstrated activity for H_2 production under simulated solar irradiation when using TEOA as a hole scavenger.

Therefore, to enhance the H_2 production, the defective sites and highly porous structure of the MOGs were utilised to anchor platinum as co-catalyst.

Platinum is introduced as a co-catalyst by either adding in-situ H_2PtCl_6 to the HER media or ex-situ, through a post-synthetic metalation of the MOG structure (Figure 2). In both cases, the H_2 production is significantly enhanced (Figure 3). Although the in-situ addition of the co-catalyst resulted in slightly higher H_2 production rates (because of a higher Pt amount), it also led to greater Pt waste compared to the ex-situ modified Pt(IV)-doped MOGs. These differences appear to be attributed to the final amount of co-catalyst in contact with the metal–organic network (forming a heterostructure) and the size of co-catalyst nanoparticles. Specifically, when normalized with respect to the amount of Pt anchored to the MOG, the H_2 production rate of the ex-situ metalated MOG surpassed that of the in-situ addition, despite presenting 20% less platinum. The smaller nanoparticle size and thus, the better distribution of Pt along the matrix in Pt-doped MOGs implies more co-catalyst/metal–organic gel contacts, resulting in a more efficient utilization of the metal. This finding bears significance for maximizing the efficiency of precious-metal co-catalysts in other photocatalytic systems. Additionally, these materials exhibit an increase in activity when a 400 nm cut-off filter was used to eliminate UV radiation from simulated solar light irradiation (Figure 4).

> Metal–organic gels (MOGs) constructed from Ti^{IV}-oxo clusters and dicarboxylato linkers were prepared for their application as light absorbers for the sacrificial photocatalytic HER under simulated solar light irradiation using a platinum co-catalyst by either: (1) in-situ photodeposition or (2) ex-situ post-synthetic metalation. The in-situ approach led to greater HER rates (227 vs 110 $\mu molH_2\ gMOG^{-1}\ h^{-1}$ for in-situ and ex-situ), but the ex-situ modification provided a finer distribution of platinum nanoparticles and a more efficient utilization of the co-catalyst (45 vs 110 $mmolH_2\ gPt^{-1}\ h^{-1}$).

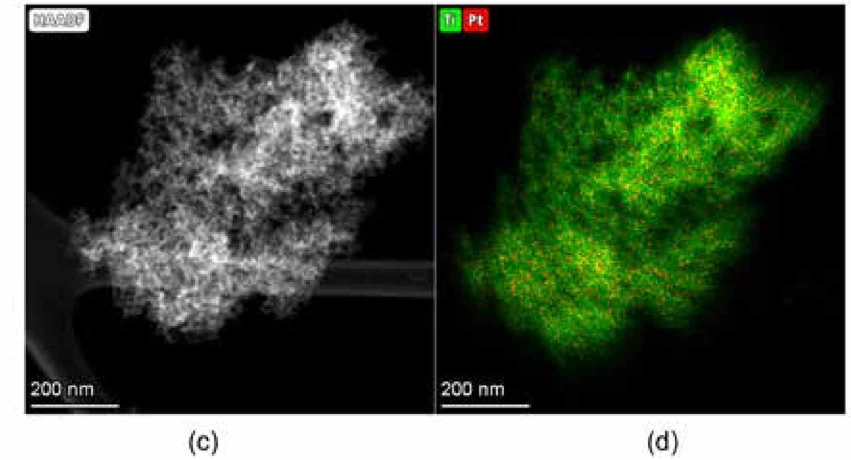


Fig 2
HAADF-TEM micrograph and left: Ti and Pt element mapping of Pt@ B100 aerogel.

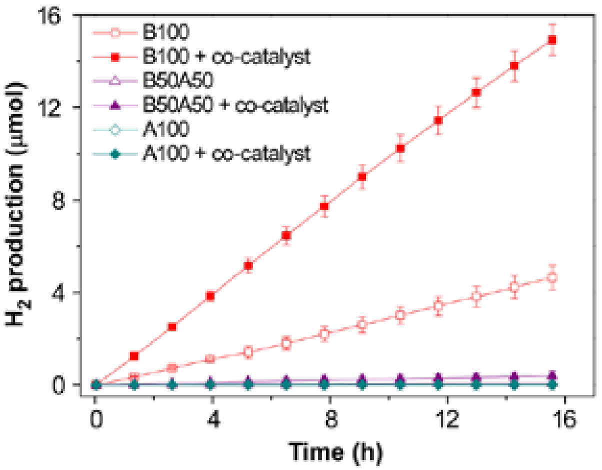


Fig 3
(a) Photocatalytic H_2 generation in neat MOGs with and without 1% wtPt/wtMOG of H_2PtCl_6 as co-catalyst.

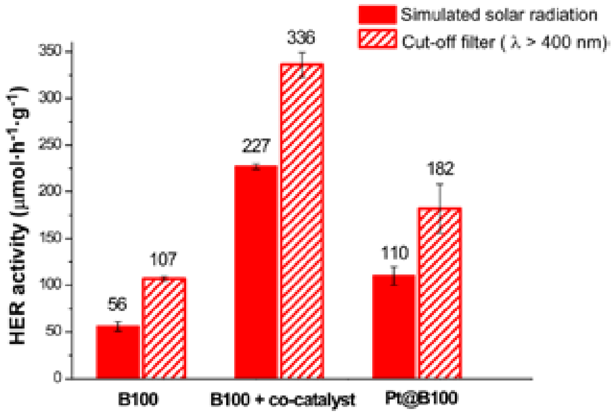


Fig 4
Photocatalytic HER activity per MOG mass for neat and doped BDC-based MOGs under simulated solar light or visible (400 nm cut-off filter) irradiation.

RESEARCH
LINE 3

ADVANCED FUNCTIONAL MATERIALS & SURFACES

This research line is devoted to the development of materials for specific technological needs. BCMaterials covers the synthesis, development and scale-up of a wide range of materials for fuel cells and batteries, photovoltaic materials or permanent magnets. Further, to provide surfaces with additional functionalities beyond the traditional decorative or protective ones is a key issue in science and technology. BCMaterials is working on sensing, self-cleaning, self-healing and antibacterial surfaces, following a wide variety of methods, including chemical and physical deposition and printing techniques.

Impact of magnetic, atomic and microstructural ordering on the magnetocaloric performance of powdered NiCoMnSn metamagnetic shape memory ribbons

Rodríguez-Crespo B., Río-López N.A., Lázpita P., Ceballos S., Ríos M., Domenech D., Rodriguez-Velamazán J.A., López-García J., Chernenko V., Porro J.M., Salazar D. (2024) Advanced Energy Materials, 14 (44), art. no. 2402469

Co-doped NiMnSn Heusler-type metamagnetic shape memory alloys (MMSMAs) are promising for next-generation solid-state refrigeration due to their tuneable magnetocaloric performance near the martensitic transformation. Powders of Mn-rich NiCoMnSn MMSMAs were obtained from ribbons, minimizing residual stresses and defects. Structural analysis via neutron diffraction revealed that heat treatments improve martensitic transformation, enhancing magnetisation change, isothermal entropy change, and refrigeration capacity by reducing structural stress and ensuring phase purity.

We have incorporated a technologically simple method of preparation and heat treatment of the Heusler-type magnetocaloric Ni43Co7Mn39Sn11 (at. %) powders through intermediate stage of obtaining melt-spun ribbons from the master bulk alloy. This method allowed minimizing the content of residual stresses, defects or segregations in the material alongside getting micro-sized grain structure suitable for easy disintegration into powder. The transformation behavior, crystal structure, and magnetic and magnetocaloric properties of the powders were studied systematically using calorimetry, neutron powder diffraction, and magnetic measurements.

Atomic site occupancy analysis showed Mn atoms increasingly occupy Sn sites, while Co atoms distribute across all sites in samples with dual heat treatments (1173 K + 723 K), causing unit cell disorder due to Mn displacement to Ni sites. In samples with a single heat treatment (1173 K), Co atoms move to Ni sites, increasing Mn occupancy of proper sites and reducing Mn displacement from Sn sites. Despite these changes, ferromagnetic coupling is retained. Heat-treated samples exhibit increased magnetisation saturation and Curie temperature (TC), driven by enhanced ferromagnetic interactions associated with higher Mn content. Non-heat-treated powders from as-received ribbons exhibited significant internal stresses. Heat treatment at 1173 K relieved these stresses, while additional annealing at 723 K showed no further effect. Structural analysis revealed the 3M modulated monoclinic martensite in heat-treated samples, while non-heat-treated samples exhibited coexisting martensite and cubic austenite phases at 123 K. Complete martensitic transformation in heat-treated samples enhanced saturation magnetisation of austenite and its change at MT. Heat-treated NiCoMnSn powders achieved high values of magnetic field-induced isothermal entropy change and refrigeration capacity. Magnetic, atomic, and microstructural order, as well as transformation and magnetic transition temperatures, were strongly influenced by heat treatment and composition. Magnetocaloric performance was linked to atomic, magnetic, and microstructural order, influenced by $L2_1$ austenite phase formation, ferromagnetic interactions, and residual stresses. A peak magnetisation changes of 110 Am^2kg^{-1} was achieved near the martensitic transformation at a low applied field of 1.5 T.

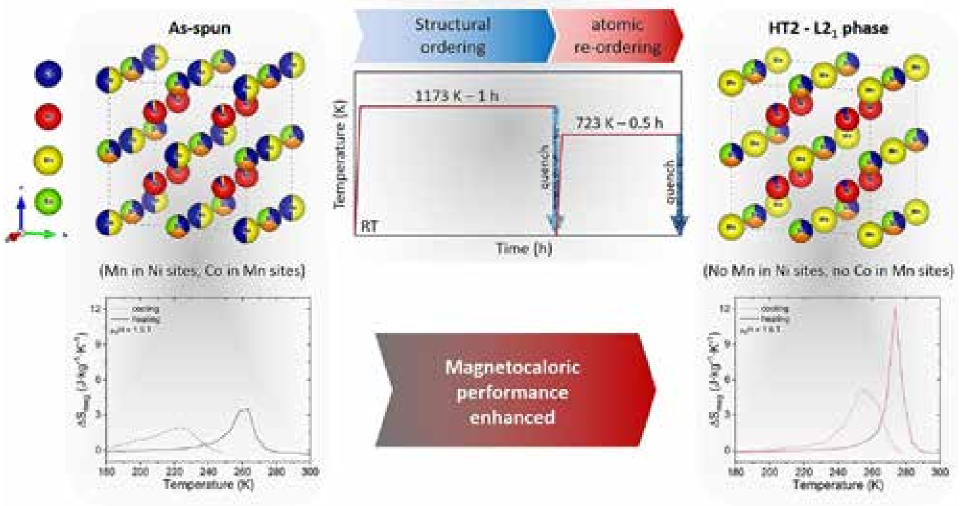


Fig 1
Structural and atomic unit cells of metamagnetic shape memory alloys before and after heat treatments, along with their respective magnetocaloric performance under a 1.5 T applied field.

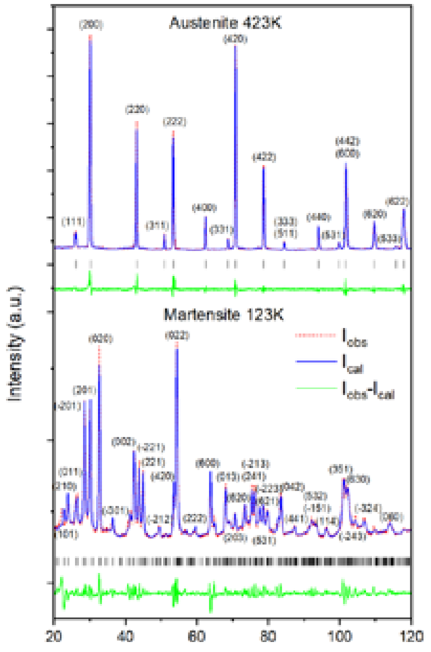


Fig 2
Lebail refinements of the neutron diffractograms of the A1 HT2 powder in the austenitic (at 423 K) and martensitic (at 123 K) phases. All the samples present a Fm-3 m cubic symmetry in the austenitic phase and a 3 M modulated P2/m monoclinic structure in the martensitic one.

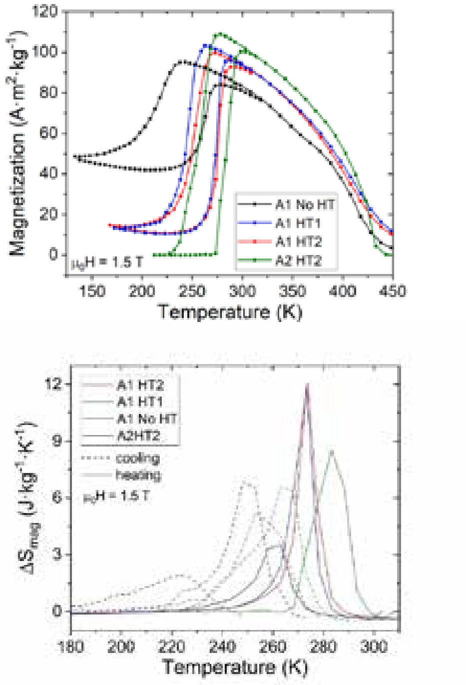


Fig 3
Up) Magnetisation versus temperature dependences for the studied powders measured under 1.5 T magnetic field. The magnetization jump at MT, M, is critically affected by the heat treatments.
Down) Magnetic entropy change at 1.5 T for the four powders studied as a function of temperature.

Enhancing Single-Layer WSe_2 Light Emission in Perylene-Doped Polymer Films **through Efficient Energy Transfer**

Gadea M., Asaithambi A., Bernabeu-Cabañero R., Farrando-Pérez A., Ramos M., Sancho-García J.C., Kriegel I., Díaz-García M.A., Calvo M.R. (2024) Advanced Functional Materials, 34 (36), art. no. 2401896

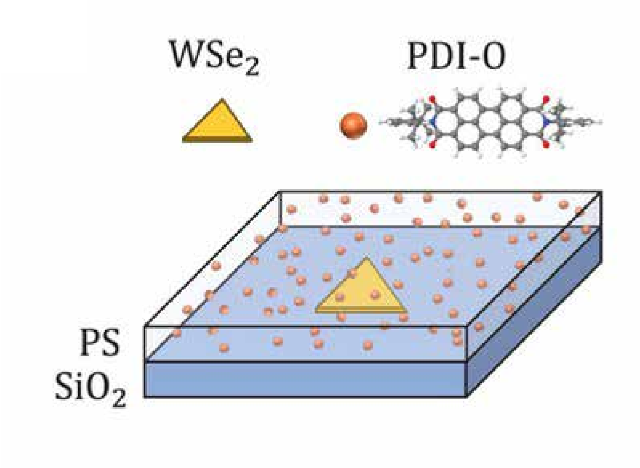


Fig 1
Sketch illustrating a single-layer WSe_2 flake (1L-WSe_2) deposited onto a SiO_2/Si substrate, and integrated beneath a polystyrene (PS) film containing a dispersed molecular dye, perylene orange (PDI-O).”

Two-dimensional (2D) semiconductors like single-layer WSe_2 are promising materials for flexible optoelectronic applications due to their robust light emission and their outstanding resilience to mechanical deformation. A major challenge in using 2D materials in plastic light-emitting devices is their relatively modest quantum yields compared to, for instance, molecular dyes. However, this limitation can be addressed by leveraging the inherent tunability of 2D materials, enabling optimization of their optical properties through functionalization or environmental control. Charge and energy transfer interactions with molecular systems present an effective strategy to increase the light emission efficiency of 2D materials. Despite the extensive exploration of molecular dyes embedded in polymer films and the recent efforts to integrate 2D materials with polymeric waveguides, the combination of both systems in polymeric structures – to potentially tune their properties based on their interplay – remains largely unexplored.

This work reveals the enhancement of photoluminescence (PL) in single-layer WSe_2 (1L-WSe_2) when integrated into a polystyrene (PS) matrix doped with perylene orange (PDI-O) molecules. The enhancement scales with the concentration of PDI-O in the PS matrix and occurs exclusively upon excitation of the PDI-O, while the emission intensity and lifetime of PDI-O decrease. These observations suggest that Förster resonance energy transfer (FRET) from PDI-O molecules to 1L-WSe_2 is highly efficient compared to other systems involving molecular donors and single-layer acceptors, significantly boosting the light emission of the 2D material.

Our results hold promise for the development of flexible plastic optoelectronics devices incorporating active 2D materials, where the polymeric matrix can provide physical support and serve as a functional element, such as a waveguide. Beyond mere structural roles, the polymer film can host molecular dopants, enabling the fine-tuning of the properties of 2D materials through tailored interactions. In particular, our results demonstrate that this approach has the potential to enhance the light emission of 2D semiconductors, with the capacity to overcome their limitations toward their application as active materials in plastic light-emitting devices. There is ample opportunity for further improvement in emission by exploring alternative combinations of 2D and molecular compounds. Furthermore, energy transfer with molecular systems could enable flexible devices with improved efficiency, leveraging the unique properties of 2D materials, such as flexible photodetectors, excitonic light emitters, or strain sensors.

> “The optical and mechanical properties of 2D semiconductors make them ideal active materials for plastic optoelectronics. Single-layer WSe_2 (1L-WSe_2) integrated into a polystyrene (PS) film containing perylene orange (PDI-O) molecules shows a notable light emission enhancement. This increase coincides with PDI-O emission quenching, pointing to efficient long-range energy transfer between PDI-O (donor) and 1L-WSe_2 (acceptor). These findings highlight the potential of flexible optoelectronics integrating active 2D materials with the polymeric matrix serving as physical support and hosting for dopants that can optimize the light emission properties of the 2D semiconductor.

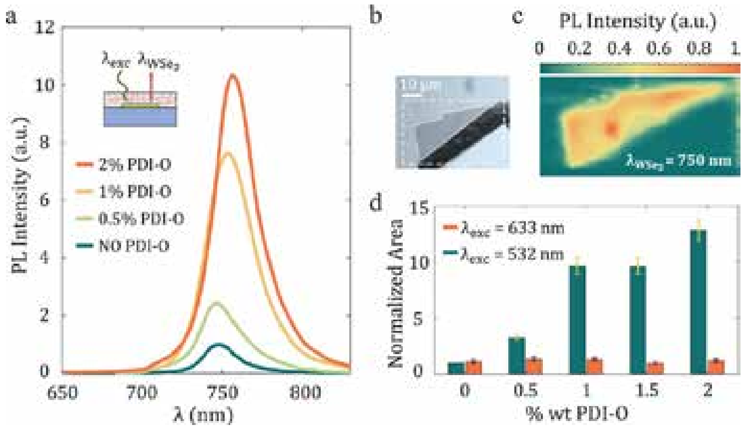


Fig 2
a) µ-PL spectra for 1L-WSe_2 flakes covered by a PS film containing different concentrations of PDI-O molecules . b) Optical microscopy image of a 1L-WSe_2 flake beneath a 1 wt% PS/PDI-O film (the single-layer area is marked with a white continuous line) c) µ-PL intensity map acquired at the area of the 1L-WSe_2 flake enclosed by the dashed line in (b). d) Integrated PL intensity for samples with varying PDI-O concentrations, using two different excitation wavelengths.

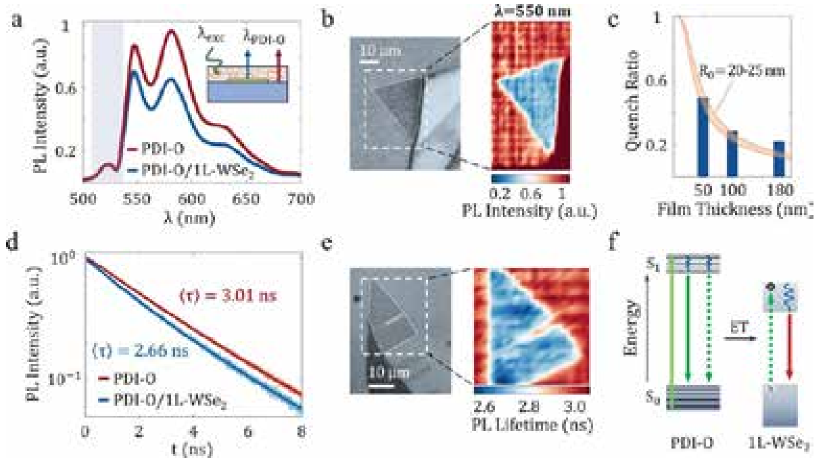


Fig 3
a) µ-PL intensity at PS/PDI-O, on and off the 1L-WSe_2 flake area. b) Optical microscopy image (left) and µ-PL map (right) for 1L-WSe_2 beneath a PS/PDI-O film. c) Quench ratio of the PDI-O µ-PL for varying thicknesses of PS/PDI-O (blue bars and orange shadow respectively represent experimental data and values estimated from energy transfer models). d) Time-resolved PL for PS/PDI-O on and off 1L-WSe_2. e) Optical microscopy (left) and PL lifetime map (right) for 1L-WSe_2 beneath PS/PDI-O. f). Illustration of optical transitions and energy transfer process for PDI-O (donor) and 1L-WSe_2 (acceptor).

Modulating Buried Interface to Achieve an Ultra-High Open Circuit Voltage in Triple Cation Perovskite Solar Cells

Junyi Huang, Zhiguo Zhang, Yanbin Zhu, Haixuan Yu, Xiongjie Li, Zhirong Liu, Samrana Kazim, Yong Hu, Wanpeng Yang, Xiaoting Ma, Letian Dai, Shahzada Ahmad, Yan Shen, and Mingkui Wang, Adv. Energy Mater. 2024, 14, 2402469

> This study enhances the perovskite solar cell performance with high open circuit voltage by tuning the buried interface with π-conjugated molecules designed with a push-pull electronic structure. By combining tin oxide nanocrystals and 2-methyl-1-aminobenzene derivatives with 4-(heptafluoropropan)-2-methylaniline, it reduces energy barriers and passivates defects, achieving a Voc of 1.241 V (95% of the Shockley–Queisser limit) and a PCE of 24.16%. Efficiency increases to 25.11% with $Cs_{0.05}MA_{0.05}FA_{0.9}PbI_3$. Integrated with a CO_2 electrolyzer, it delivers a solar-to-CO conversion efficiency of 11.76%, showcasing potential for green energy.

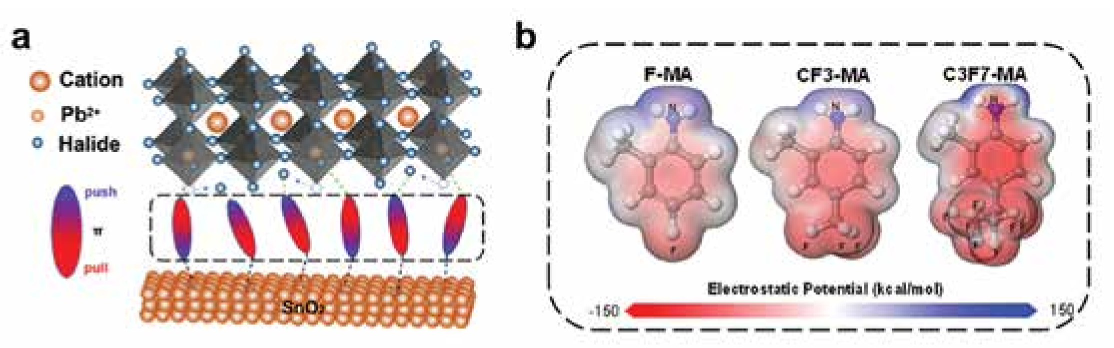


Fig 1
The buried interface structure and molecular selection a) scheme of the passivation function of π-conjugated structure molecule featuring a push-pull electronic configuration at the buried interface, and b) electrostatic potential mapping of F–MA, 3F–MA, and C3F7–MA molecules.

We adopted a novel methodology to enhance the performance of triple-cation perovskite solar cells (PSCs) by modulating the buried interface with π-conjugated molecules. These molecules, featuring a push-pull electronic structure, effectively address interfacial defects and improve energy barrier alignment at the electron transport layer (ETL)-perovskite interface. We focused on three derivatives of 2-methyl-1-aminobenzene—F–MA, CF3–MA, and C3F7–MA. The device with C3F7–MA demonstrating the best performance due to its strong defect passivation properties. The fluorine (F^-) pulled back electron density to form minimum electrostatic potential region, regarded as Lewis base and $-NH_2$ pushed away electron to form maximum electrostatic potential region, regarded as Lewis acid which has ability to form effective coordination and hydrogen bonds with undercoordinated Pb^{2+} and interstitial I^- ions respectively.

The C3F7–MA molecule lowers the work function of SnO_2(4.399 eV to 4.208 eV), reduces the interfacial energy barrier (0.5 to 0.24 eV), and enhances the alignment of energy levels between the ETL and perovskite layer. These improvements significantly reduce nonradiative recombination losses, as evidenced by steady-state and time-resolved photoluminescence measurements. Device performance metrics reveal substantial improvements with the inclusion of C3F7–MA.

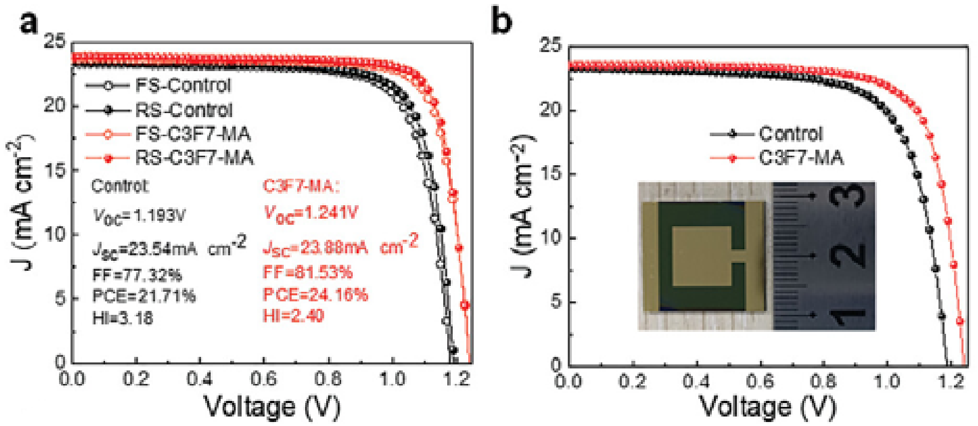


Fig 2
Photovoltaic device performance. a) J–V curves of the best-performing PSC with and without C3F7–MA modification in reverse scan and forward scan, b) J–V curves of the best performing large-area PSCs (1 cm²) with or without C3F7–MA modification. The inset shows the photograph of a large-area PSC.

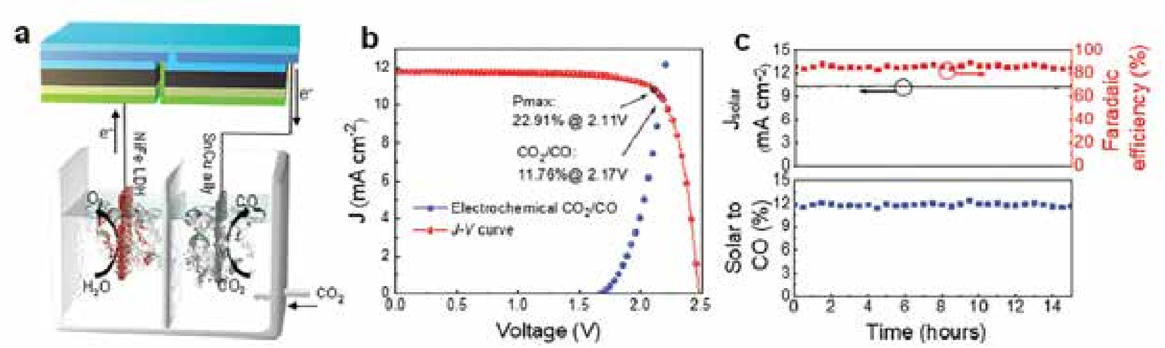
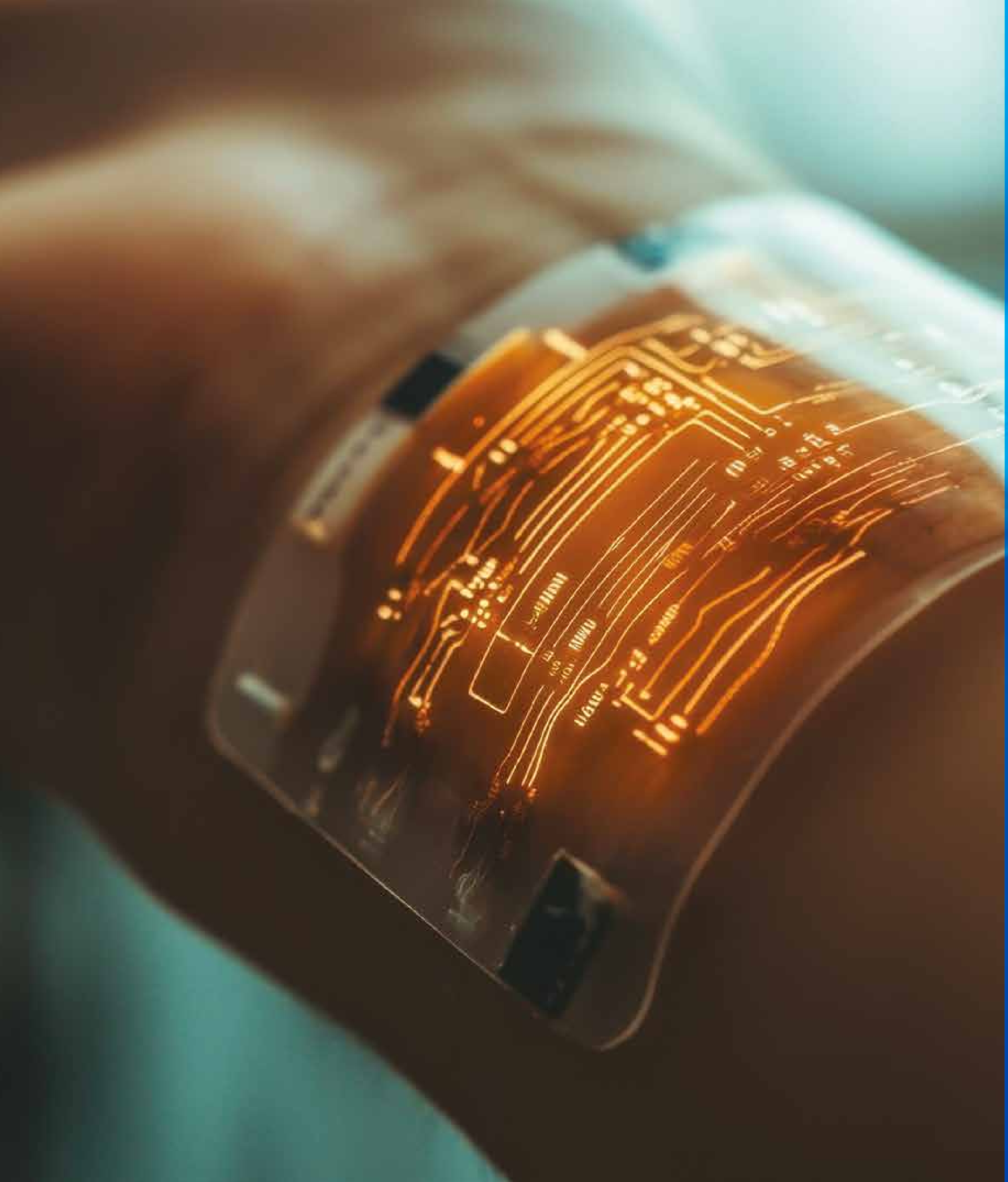


Fig 3
Performance of PV integrated CO_2 reduction system driven by a mini-module. a) Schematic of the PV-driven CO_2 reduction system consisting of a mini-module and an electrochemical cell employing Sn-Cu alloy for CO_2 reduction to CO and Ni-Fe LDH foam for oxygen evolution reaction in a CO_2 -saturated 0.1 m $KHCO_3$ aqueous electrolyte, b) J–V measurement curves of a mini-module constituted of two series PSCs under simulated AM 1.5G irradiation overlaid with the matched J–V characteristic of the CO_2 -reduction, c) Current density (black line), faradaic efficiency of CO yield (red dots), and solar-to-CO conversion efficiency (blue dots) of the device during a 15-h stability test.

The modified PSCs with lower hysteresis achieved a remarkable power conversion efficiency (PCE) of 24.16% and an open-circuit voltage (Voc) of 1.241 V, approaching 95% of the Shockley-Queisser limit. Stability tests under continuous illumination and humid conditions demonstrated that the modified devices retained over 94.5% of their initial PCE after 1000 hours of operation, highlighting the molecule's role in enhancing operational reliability.

Beyond photovoltaic performance, we explore the integration of these PSCs with a CO_2 electrolyzer. The fabricated mini-module, consisting of two series-connected PSCs, powered a CO_2 reduction system with a solar-to-CO conversion efficiency of 11.76%, sustained over 15 hours. This marks a significant achievement in solar-driven chemical fuel production, surpassing the benchmarks set by conventional photovoltaic systems. Overall, this work demonstrates the efficacy of π-conjugated molecules as interfacial modifiers for PSCs, leading to enhanced efficiency, stability, and versatility for clean energy applications. The findings pave the way for future innovations in sustainable energy technologies, particularly in the context of solar-driven fuel generation.



RESEARCH
LINE 4

MICRO & NANODEVICES

The multifunctional materials, nanostructures and surfaces being developed, allow the implementation in functional prototypes demonstrating the suitability of the materials for advanced applications. Force, deformation, magnetic, magnetostrictive and chemical sensors are being fabricated, among others. In addition, printed and flexible electronic devices are fabricated for wearables, point of care devices, interactive surfaces and structural health monitoring. Finally, microfluidic systems and organ-on-a-chip devices are being developed.

New screen-printed electrodes for Raman spectroelectrochemistry. Determination of p-aminosalicylic acid

Romay L., Nuñez-Marinero P., Perales-Rondon J.V., Heras A., del Campo F.J., Colina A. (2024) Analytica Chimica Acta, 1325, 343095

> This study introduces a novel silver-based screen-printed electrode (SPE) for time-resolved Raman spectroelectrochemistry (TR-Raman-SEC), designed to determine 4-aminosalicylic acid (PAS) in complex matrices. Using the same ink for all three electrodes reduces costs and simplifies fabrication while maintaining high sensitivity and reproducibility. Through the EC-SOERS strategy, AgCl nanocrystals are generated, amplifying the Raman signal. The SPEs achieved accurate results even in the presence of interfering compounds, demonstrating their potential for advanced chemical analysis and future applications.

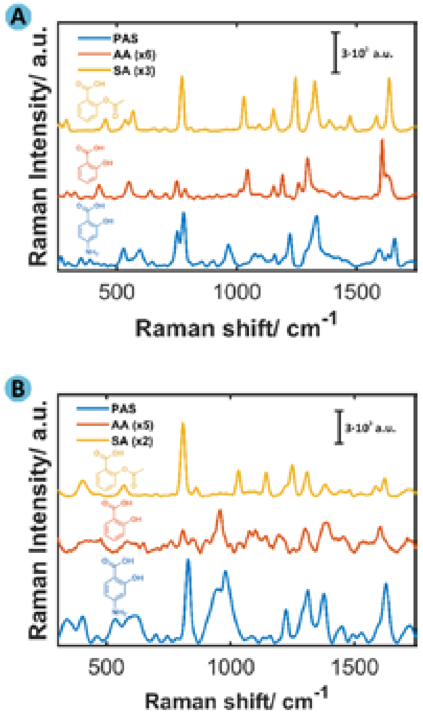


Fig 1.
Comparison of Raman and SOERS Spectra for Target and Interfering Compounds. *Raman spectra for 4-aminosalicylic acid (PAS), acetylsalicylic acid (AA), and salicylic acid (SA) in solid-state and SOERS spectra in solution during spectroelectrochemical experiments. Insets show the molecular structures of the compounds, highlighting differences in Raman enhancement.*

Detecting and quantifying molecules in complex matrices is a significant challenge in chemical analysis. This study addresses this issue by developing new silver-based screen-printed electrodes (SPEs) specifically designed for time-resolved Raman spectroelectrochemistry (TR-Raman-SEC). These SPEs employ a novel strategy called electrochemical surface oxidation-enhanced Raman scattering (EC-SOERS). In this approach, AgCl nanocrystals generated on the electrode surface significantly amplify the Raman signal, enabling precise analyte detection.

Compared to commercial SPEs, the new electrodes offer substantial advantages. Their design utilizes the same silver ink for all three electrodes (working, counter, and reference), reducing production costs and simplifying the manufacturing process. Additionally, these SPEs eliminate the need for pre-treatment, as the required amplification properties are generated during the experiments. This innovation enhances analysis efficiency and improves reproducibility, addressing a critical challenge in Raman studies.

The utility of these SPEs was demonstrated through the quantification of 4-aminosalicylic acid (PAS), an essential antibiotic for treating drug-resistant tuberculosis. The results showed high sensitivity and accuracy, even in the presence of interfering compounds such as salicylic acid and acetylsalicylic acid. The methodology achieved low detection limits and effectively distinguished close concentrations in complex matrices, including commercial drug samples.

This work highlights the potential of silver-based SPEs not only for chemical analysis but also for future applications in biomedicine and materials science. The conclusions emphasize the robustness of this methodology in tackling challenging analytical problems and pave the way for using these electrodes in complex biological samples, such as body fluids. With industrial-scale production, further improvements in reproducibility are expected, broadening their scope of analytical applications.

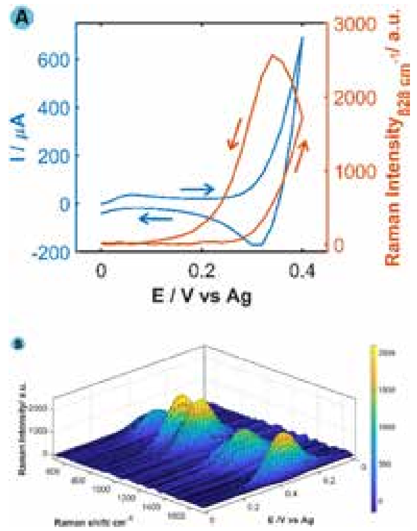


Fig. 2: VoltaRamangram and Spectral Evolution of PAS under TR-Raman-SEC
VoltaRamangram of PAS at 828 cm^{-1} showing the evolution of the Raman intensity as a function of applied potential (A), and a 3D plot of Raman intensity in the fingerprint region (450–1750 cm^{-1}) over the potential range (B). These results demonstrate the generation and optimization of the SOERS signal.

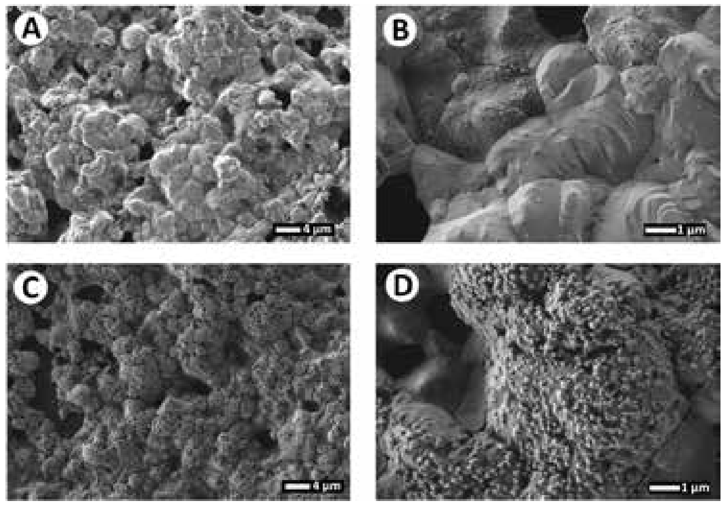
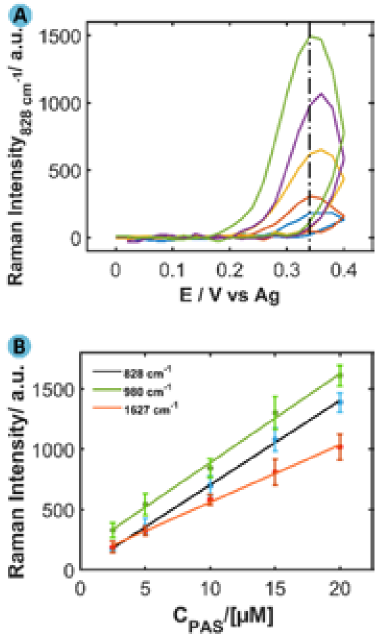


Fig. 3: Surface Morphology of Silver SPEs Before and After Raman-SEC Experiments
SEM images of silver SPE surfaces at different scales: pristine surface (A, B) and after TR-Raman-SEC experiments (C, D). The formation of AgCl nanocrystals on the working electrode surface is evident, correlating with the Raman signal amplification.

Fig 4.
Calibration Curves for PAS Detection in Complex Matrices
Calibration curves for PAS detection using TR-Raman-SEC at three selected Raman shifts (828, 980, and 1627 cm^{-1}) in the presence of interfering compounds. The strong linearity indicates the robustness of the method, even in complex sample matrices.



Screen-printed glassy carbon electrodes for electrogenerated chemiluminescence

P. Núñez-Marinero, R. K. R. Gajjala, and F. J. Del Campo. (2024) Electrochimica Acta, vol. 500, p. 144725,

This study introduces screen-printed glassy carbon (GC) electrodes for electrogenerated chemiluminescence (ECL) using the $Ru(bpy)_3^{2+}$/TPrA system as a benchmark. Various ink formulations were evaluated, with a 5:1 GC to binder ratio yielding superior performance. Compared to graphite screen-printed electrodes, GC electrodes demonstrated enhanced ECL intensity and matched the performance of conventional bulk GC electrodes. The impact of laser treatment on morphology and electrochemical properties was explored, showing limited effect. These findings support the potential of GC electrodes for scalable, low-cost analytical applications.

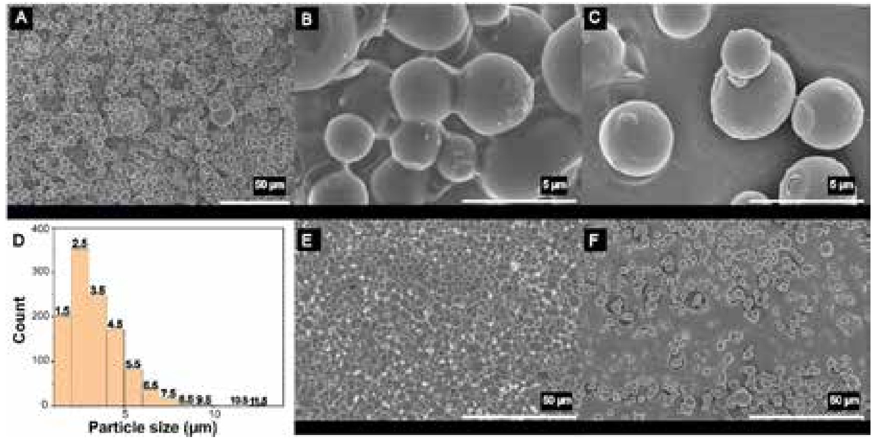


Fig. 1. Morphological Analysis of Glassy Carbon Powder and Electrodes
Scanning electron microscope (SEM) images of glassy carbon powder and screen-printed electrodes before and after laser treatment. The analysis highlights the removal of the nitrocellulose binder and the preservation of GC particles.

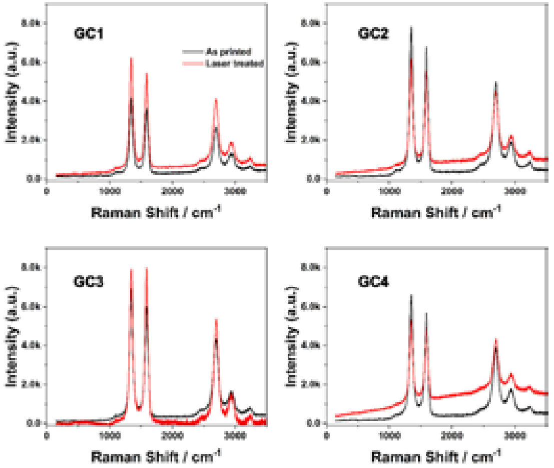


Fig 2. Raman Spectroscopy of Screen-Printed GC Electrodes.
Raman spectra of screen-printed GC electrodes before (black line) and after (red line) laser treatment, showing prominent D and G bands. The analysis confirms the structural integrity of GC particles post-laser treatment.

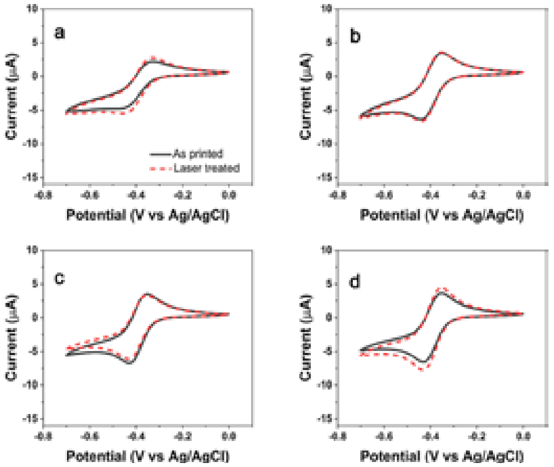


Fig. 3.Cyclic Voltammetry of $Ru(NH_3)_6^{3+}$ at GC Electrodes
Cyclic voltammograms of $Ru(NH3)6^{3}+$ at screen-printed GC electrodes of varying compositions before and after laser treatment. The results demonstrate minimal impact of laser treatment on electrochemical performance.

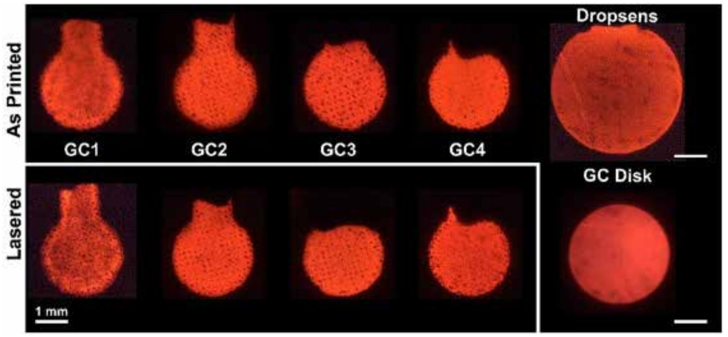


Fig. 4. ECL Response of GC Electrodes
ECL intensity of screen-printed GC electrodes recorded using a UV-Vis spectrometer and smartphone camera. The comparison highlights the enhanced ECL response of optimized GC electrodes and the minimal effect of laser treatment.

Electrogenerated chemiluminescence (ECL) combines the advantages of electrochemistry and luminescence, offering high sensitivity and selectivity. Glassy carbon (GC) is well-regarded for ECL applications due to its unique structure, thermal and chemical stability, and superior electron transfer capabilities. However, integrating GC into scalable, low-cost, and disposable systems has remained a challenge. This study addresses this gap by developing screen-printed GC electrodes and evaluating their performance for ECL applications using the $Ru(bpy)_3^{2+}$/TPrA system.

The research focused on formulating and optimizing GC inks, creating electrodes through screen-printing, and characterizing their morphology and performance. A 5:1 GC to binder ratio emerged as the optimal formulation, providing superior ECL responses compared to other formulations and commercial graphite electrodes. Notably, the performance of these GC electrodes was on par with conventional bulk GC electrodes, underscoring their potential for analytical applications.

Laser treatment was employed to modify the electrode surface, aiming to enhance electrochemical activity by removing the nitrocellulose binder. Scanning electron microscopy (SEM) and Raman spectroscopy confirmed that while the binder was effectively removed, the GC particles remained structurally intact. However, the treatment resulted in some particle loss, and its impact on electrochemical performance was minimal.

Electrochemical studies demonstrated the robustness of GC electrodes, showing high reproducibility and compatibility with ECL detection. The $Ru(bpy)_3^{2+}$/TPrA system revealed a two-step ECL mechanism involving TPrA oxidation and $Ru(bpy)_3^{2+}$ reduction, with enhanced emission on GC electrodes compared to graphite-based alternatives.

In conclusion, this study establishes screen-printed GC electrodes as a viable alternative for ECL applications, combining high sensitivity, reproducibility, and scalability. Their potential for integration into low-cost, disposable devices makes them promising for clinical diagnostics, environmental monitoring, and other analytical fields. Future work may explore advanced surface modifications to further enhance performance.

Enhanced Electrochemiluminescence at the Gas/Liquid Interface of Bubbles Propelled into Solution

Knežević, S., Totoricaguena-Gorriño, J., Gajjala, R. K. R., Hermenegildo, B., Ruiz-Rubio, L., Vilas-Vilela, J. L., Lanceros-Méndez, S., Sojic, N., & Del Campo, F. J. (2024) Journal of the American Chemical Society, 146 (32), pp. 22724 - 22735

> This study demonstrates an innovative method to enhance and extend electrochemiluminescence (ECL) using electrogenerated chlorine gas bubbles. At the gas-liquid interface, a dual mechanism involving the bubble corona effect and hypochlorite oxidation sustains luminol ECL for over 200 seconds and extends the emission range up to 5 mm from the electrode. This approach increases ECL intensity fivefold, as demonstrated in a glucose bioassay using a smartphone for detection. The findings enable new applications in dynamic bulk analysis and broaden the scope of ECL techniques in bioanalysis and interfacial chemistry

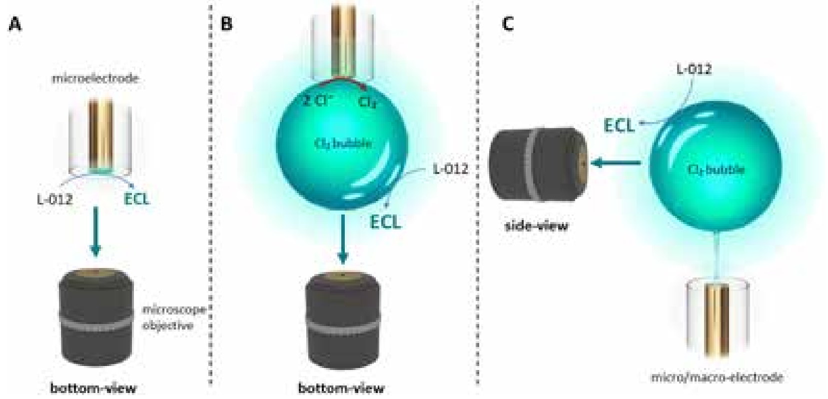


Fig 1.
Mechanism of Bubble-Enhanced ECL
Schematics illustrating luminol-based ECL at a gold electrode surface (A), gas-liquid interface of a chlorine bubble during formation (B), and after bubble detachment (C). This process extends ECL emission spatially and temporally beyond traditional boundaries.

Electrochemiluminescence (ECL), a highly sensitive analytical technique, traditionally emits light confined to a micrometric region near electrode surfaces. This study expands the spatial and temporal limits of ECL by employing electrogenerated chlorine gas bubbles to enhance luminol-based ECL. The bubbles create a gas-liquid interface where reactions occur, enabling ECL emission to extend up to 5 mm from the electrode and last over 200 seconds after bubble detachment.

The proposed mechanism relies on two parallel effects. First, the bubble corona effect generates reactive oxygen species, facilitating luminol oxidation. Second, hypochlorite, formed from chlorine dissolved at the gas-liquid interface, sustains the reaction by homogeneously oxidizing luminol. This innovative approach enhances ECL intensity up to fivefold compared to conventional methods.

To validate this method, the study employed gold microelectrodes in chloride-containing and chloride-free solutions. The emission's spatial propagation was visualized using advanced imaging techniques, revealing ECL at the electrode surface, bubble interfaces, and extended into the solution. Notably, the method achieved stable ECL in dynamic environments, which traditional ECL fails to capture. The findings were demonstrated in a glucose bioassay, leveraging the robust and prolonged ECL for sensitive detection. A smartphone camera was used for readout, highlighting the potential for accessible and scalable applications in clinical diagnostics. The robust signal enables improved quantification, even in complex matrices.

This work redefines the boundaries of ECL, showcasing its applicability for studying bulk-phase processes, interfacial phenomena, and dynamic chemical environments. By overcoming spatial and temporal limitations, it opens avenues for advanced biosensing, imaging, and analytical applications in interfacial chemistry.

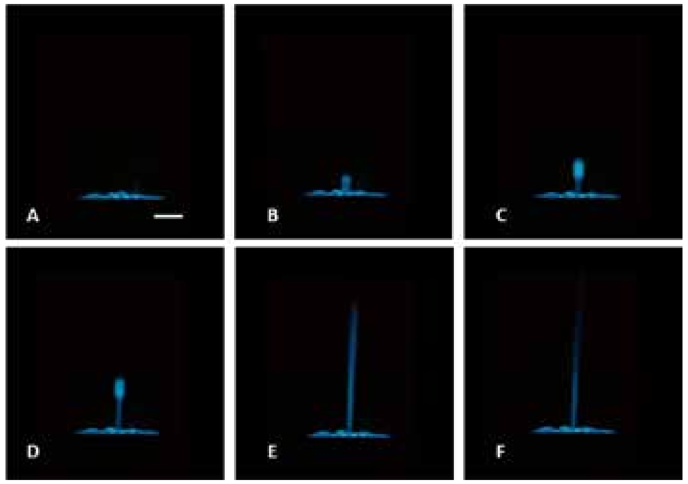


Fig 2.
Spatial Extension of ECL Emission
Side-view imaging of a chlorine bubble propagating through solution after detachment. The ECL emission is tracked up to 5 mm away from the electrode, showcasing the diffusion of reactive chlorine species into the bulk.

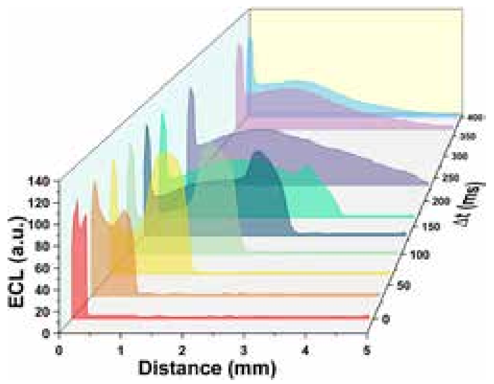


Fig 3.
Time-Resolved ECL Intensity Profiles
Temporal evolution of ECL intensity at gas-liquid interfaces of oxygen and chlorine bubbles. Chlorine bubbles sustain stronger and longer-lasting ECL due to hypochlorite formation, as shown in the time-dependent emission profiles.treatment.

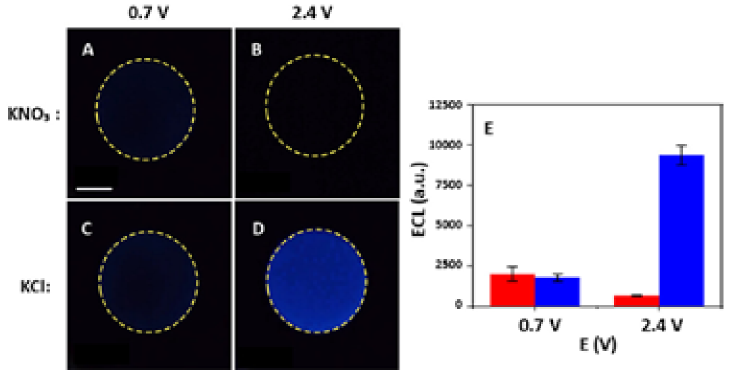
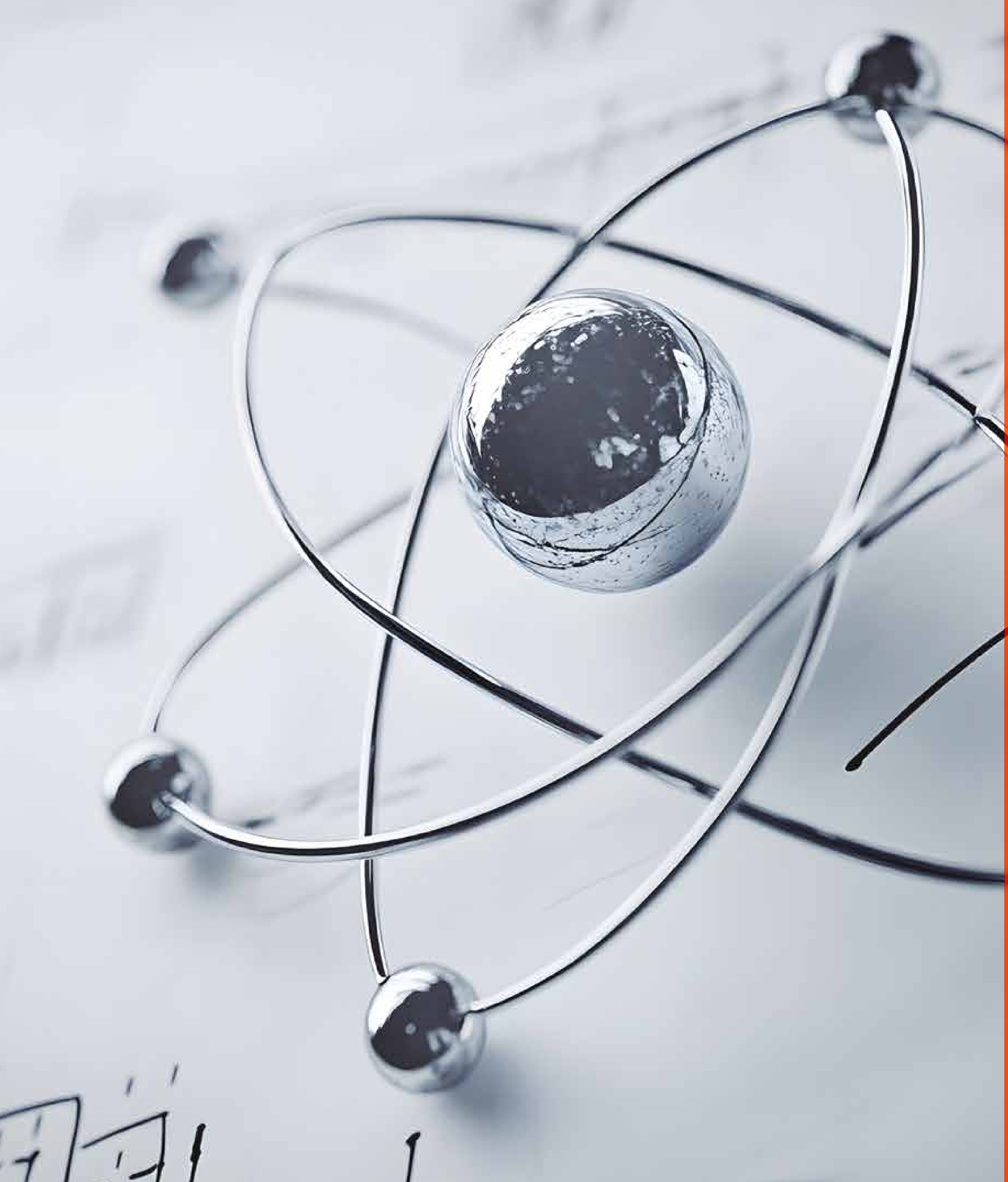


Fig 4.
Glucose Detection with Enhanced ECL
ECL emission during a glucose bioassay at low (0.7 V) and high (2.4 V) potentials. The enhanced signal at 2.4 V, especially in chloride-containing solutions, demonstrates the method's sensitivity and potential for bioanalytical applications.treatment.



TRANSVERSE RESEARCH LINE 1

NEUTRON SCIENCE

Neutron science is strongly applied in all activities of BCMaterials and it will continue to be one or the cornerstones of advanced materials characterization. SANS, diffraction, reflectometry and inelastic experiments are being performed in ANSTO (Australia) ILL (France), PSI (Switzerland) and ISIS (UK) in areas including magnetism, MOFs, energy generation and storage, soft matter and nanoparticles.

Exploring the compositional space of a metal-organic framework with ionic liquids to develop porous ionic conductors for enhanced signal and selectivity in VOC capacitive sensors

B. F. Gonçalves, E. Fernandez, A. Valverde, M. Gaboardi, H. Salazar, V. Petrenko, J. M. Porro, L. P. Cavalcanti, K. Urtiaga, José M. S. S. Esperança, D. M. Correia, F. Fernandez-Alonso, S. Lanceros-Méndez, R. Fernandez*. (2024) Journal of Materials Chemistry A, 12(24), 14595-14607.

> Monitoring non-methane volatile organic compounds (NMVOCs) is key for air quality, but current gas sensors face challenges in selective and sensitive detection. This study combines Metal–Organic Frameworks (MOFs) and Ionic Liquids (ILs) to optimize capacitive gas sensing layers. By tuning MOF:IL ratios, materials with adjustable porosity and conductivity are created. The IL's dielectric sensitivity and the MOF's porosity enhance selectivity. Tests with thirteen sensors for water, ethanol, acetone, and isopropanol vapours show that MOF/IL hybridization offers a suitable avenue to balance the porosity, magnitude of response, and partial selectivity.

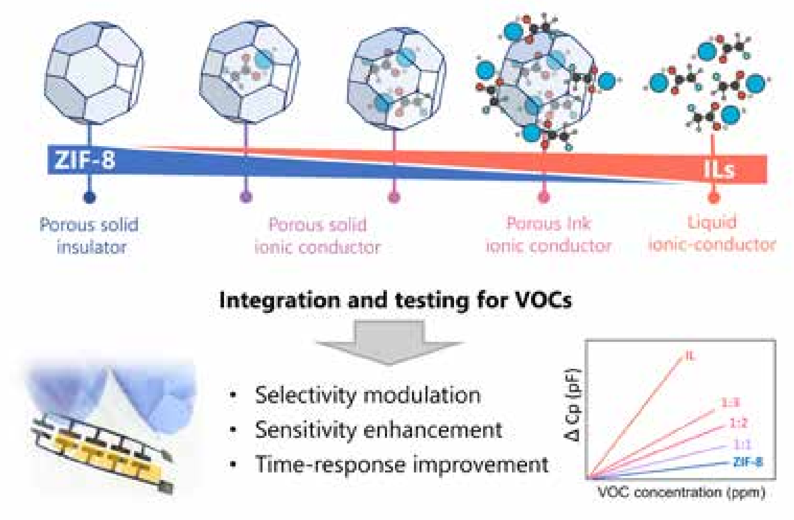


Fig 1
Illustration of the evolution of the local structure of MOF : IL composites as the molar ratio of MOF and IL components is modified, the integration of the MOF : IL into the transduction system, and the capacitive variation of the parent materials and MOF/IL systems once exposed to a VOC atmosphere.

This pioneering study has prompted further investigation into whether gas sensing sensitivity and selectivity in MOF/IL composites are primarily governed by the pore chemistry of the MOF or by the interaction between the VOC and the ILs when confined in an ordered porosity. To systematically explore these parameters, the dielectric response of the parent MOF and IL as well as the MOF/IL composites has been studied. Depending on the MOF : IL ratio, materials ranging from pure porous non-ionic conductive MOFs to MOF : IL porous ionic conductors, MOF : IL porous ion-conductive inks and slurry-like ILs can be achieved (Figure 1). X-Ray diffraction data, gas adsorption measurements, and small-angle neutron scattering (SANS), confirmed the internal and external hybridization of IL molecules inside and outside the internal structure of porous ZIF-8 nanoparticles.

SANS data fitting (Figure 2) reveals inhomogeneities with an ellipsoid shape with sizes depending on the loading of IL-TFSI (q=0.1-1 nm 1). Overall, for ZIF-8 sample, the inhomogeneities are related to the MOF interparticle space (air pores) between agglomerates of ZIF-8. The loading of IL into the ZIF-8 sample gives rise to the smothering and decrease of the scattering signal for the ZIF-8/IL (1 : 1) sample, arising from the MOF pores and interparticle space being fully filled with the excess of IL. For the samples with moderate loading of IL (1:0.1 and 1:0.4), these inhomogeneities also arise from the partially filling of MOF pores and interparticle space with IL.

When transitioning from IL to MOFs, the electric response of the system upon vapours exposure is attenuated; the MOF : IL composite exhibits a fast and recoverable reaction compared to pure IL-based sensors. In contrast, when transitioning from MOF to IL, the porosity is diminished, but the composites still maintain some selectivity in gas adsorption and, consequently, in detection (Figure 3). The dispersion and homogeneous integration of an IL into the MOF matrix offers advantages such as a fast, selective, and recoverable response of the sensors, as well as compatibility with printing processes.

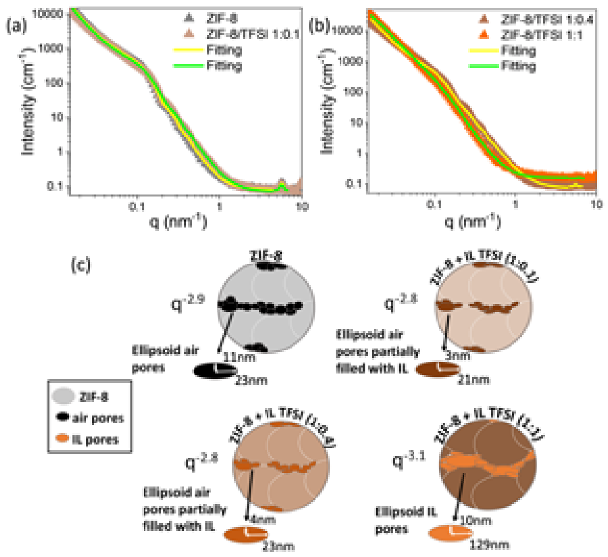


Fig 2
SANS curves of ZIF-8 and ZIF-8/IL-TFSI systems with corresponding fittings: ZIF-8 and ZIF-8/IL-TFSI 1 : 0.1 (a), and ZIF-8/IL-TFSI 1 : 0.4 and ZIF-8/IL-TFSI 1 : 1 (b); and schematic representation of a possible structure derived from SANS data analysis (c).

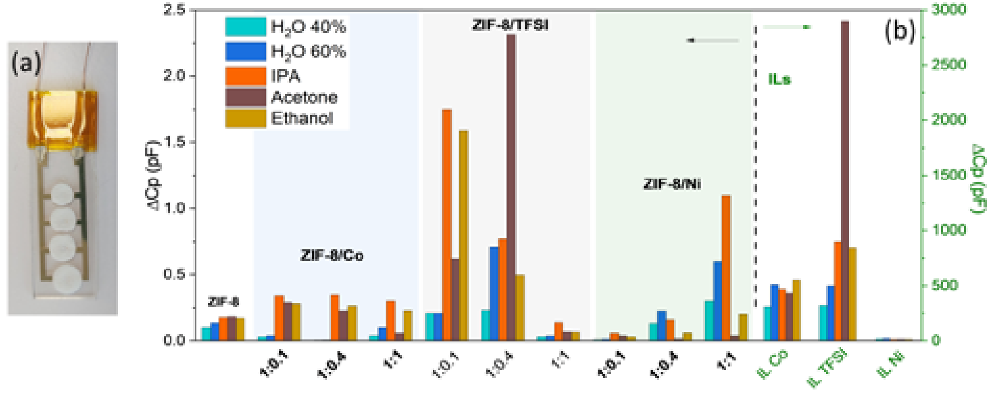


Fig 3
Photography of an assembled sensor (a); and bar chart with variation of capacitance (Cp) for all ZIF-8/IL systems at a fixed vapor concentration (b).

Finally, it is important to note that ZIF-8 not only serves as a supporting material, as the incorporation of different concentrations of the same IL produces different capacitance outputs towards the same VOC. Hence, the contribution to the selectivity of the MOF/IL composites can be further improved if the pore characteristics and inner surface chemistry of the MOF host are tuned towards the adsorption of specific molecules.

Enzyme-mimicking of copper-sites in metal-organic frameworks for oxidative degradation of phenolic compounds

Valverde A., Alkain E., Rio-López N.A., Lezama L., Fidalgo-Marijuan A., Laza J.M., Wuttke S., Porro J.M., Oyarzabal I., Jiménez-Ruiz M., García Sakai V., Arias P.L., Agirrezabal-Telleria I., Fernández de Luis R. (2024) Journal of Materials Chemistry A, 12 (8), pp. 4555 - 4571

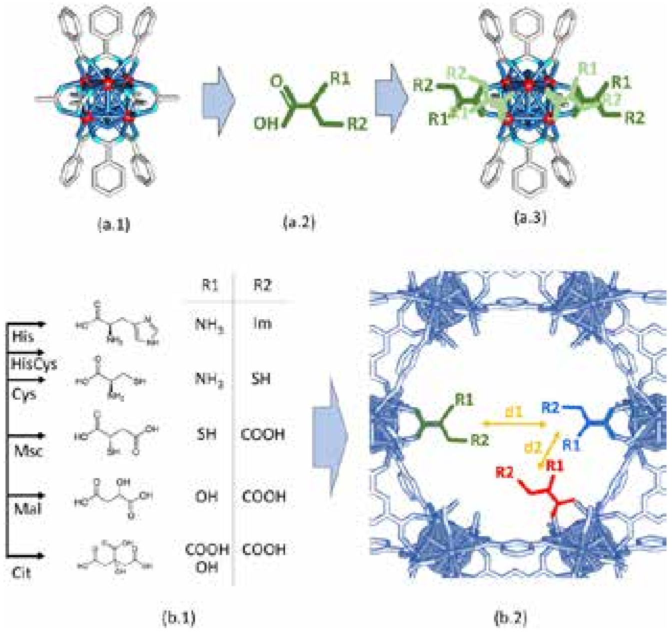


Fig 1

(a.1) Local structure of zirconium hexanuclear clusters in MOF-808. (a.2) Simplified chemical structure of (amino) acid molecules. (a.3) Tentative local structure of zirconium hexanuclear clusters after their functionalization. Colour code: red – zirconium. Light blue – oxygen. Grey – carbon. (b.1) Chemical structure and metal coordination groups of (amino) acid functions installed into MOF-808. (b.2) Simplification of the pore structure of MOF-808 once functionalized with (amino) acids.

This study explores how Metal-Organic Frameworks (MOFs) can mimic the activity of metalloenzymes, specifically laccases and copper oxidases, in the oxidative degradation of phenolic compounds. We have functionalized MOF-808 with various amino acids (Cys, His, Mal, Cit, Msc) and a combination of His and Cys (Fig.1), subsequently incorporating copper ions into these functionalized MOFs.

Using a variety of spectroscopic techniques (i.e. Raman, INS, EPR, XPS, UV-Vis) combined with Inelastic Neutron Scattering (INS) spectroscopy (Fig.2) we have characterized the copper sites within the MOFs, determining their coordination environments and degree of clustering. The analysis of the results obtained indicate that the copper ion coordination environment and clustering may be tuned by varying the type and concentration of amino acids used for the functionalization. The biomimetic MOFs were evaluated for their catalytic activity in the catalytic wet peroxide oxidation (CWPO) of various model phenolic contaminants (phenol, 2,4-dichlorophenol, catechol, hydroquinone, and dopamine). The results reveal that both the coordination environment and clustering of the copper sites significantly influence the catalytic efficiency and selectivity of the studied MOFs.

The MOF-808@His-Cu100 exhibited a specific affinity for oxidizing dopamine and was generally more efficient in oxidizing catechol and hydroquinone compared to other phenolic compounds. The robustness of MOF-808@His-Cu100 was assessed under different conditions (ionic strength, temperature, and pH). We have demonstrated that its activity increases with higher ionic strength and temperature, while pH has a minimal impact on it. However, the material's reusability was limited due to the blockage of copper sites by substrates or oxidation products.

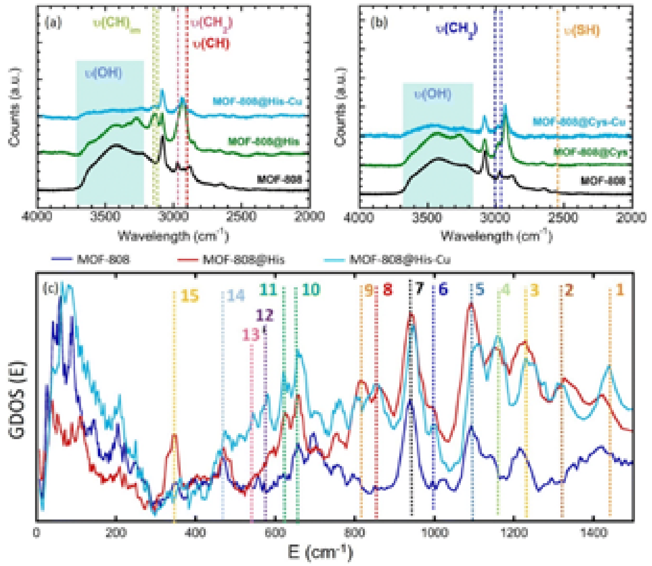


Fig 2

Raman spectra of MOF-808-His (a) and (b) MOF-808@Cys samples before and after copper metalation. (c) Inelastic

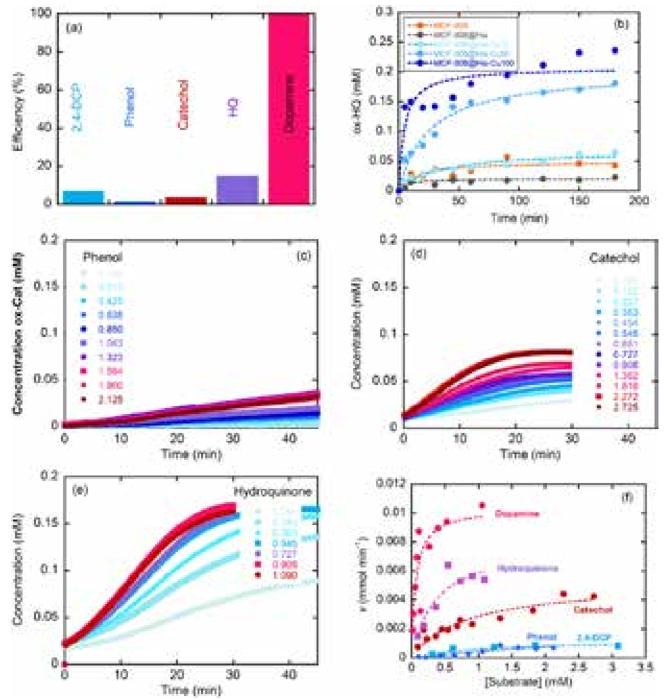


Fig 3

(a) Concentration of the oxidized products after the CWPO of different model pollutants by MOF-808@His-Cu100. (b) Evolution of the oxidation for hydroquinone by MOF-808, MOF-808@His, MOF-808@His-Cu10, MOF-808@His-Cu50 and MOF-808@His-Cu100. (c–e) Concentration dependence on the CWPO oxidation of phenol, catechol and hydroquinone. (f) Michael–Menten plot for the CWPO of catechol, phenol, 2,4-dichlorophenol, hydroquinone and dopamine with MOF-808@His-Cu100.

> “The activity and selectivity of metal sites in metalloenzymes, such as laccases and copper oxidases, are governed by their coordination environments and metal ion nuclearity. This study demonstrates that metal-organic frameworks (MOFs) can be functionalized with amino acid-copper sites, enabling partial control over these factors. The bioinspired MOF-808@(amino)acid-copper catalysts were evaluated for wet oxidation of phenolic pollutants, revealing that coordination environment and clustering significantly modulate their efficiency and selectivity. This approach paves the way for advanced enzyme active site reconstruction.

The study concludes that functionalizing MOFs with amino acids and subsequently metallizing them with copper is a promising approach for replicating the oxidative functions of metalloenzymes (Fig.3). Moreover, the activity and selectivity of these materials can be finely tuned by precisely controlling the coordination environment and clustering of copper sites. This opens up new possibilities for developing robust, highly selective biomimetic catalysts for environmental remediation applications.

TRANSVERSE RESEARCH LINE 2

COMPUTATIONAL MATERIALS SCIENCE

Computational support has been over the years used in BCMaterials research spanning from DFT to molecular dynamics, from finite element simulation to artificial intelligence and machine learning for materials design. This research line supports effors on materials design, physical-chemical interactions understanding and modulation, and device implementation.

Surface Reconstructions in II-VI Quantum Dots

Llusar J., du Fossé I., Hens Z., Houtepen A., Infante I. (2024) ACS Nano, 18 (2), pp. 1563 - 1572

> Density Functional Theory (DFT) calculations are crucial for understanding colloidal quantum dots (QDs), but simulations often use smaller models than those found experimentally. Larger QD models impact facet size, trap formation, and core–shell structure accuracy. Using DFT, we studied QDs up to 4.5 nm, finding that larger models cause band gap collapse and facet-specific HOMO/LUMO localization due to surface orbital coupling. Surface vacancies refilled with Z-type ligands reconstruct surfaces, widening the band gap and delocalizing orbitals, highlighting the critical role of facet geometry.

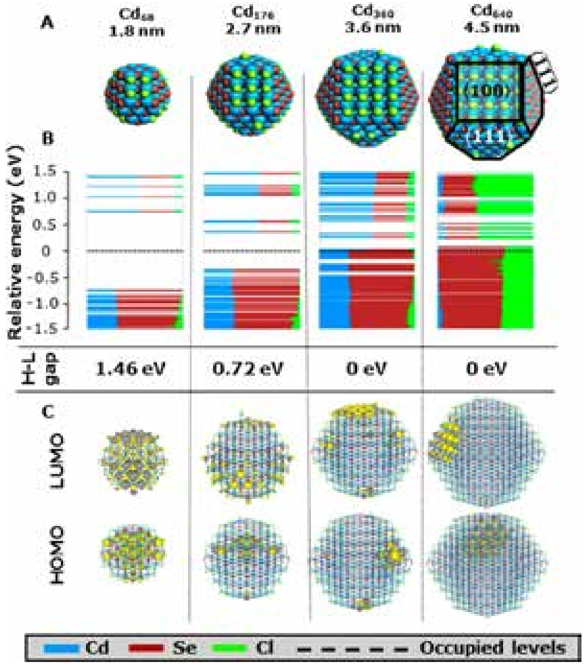


Fig 1
Effect of increasing the size of the QD model. (A) Structure of CdSe QD models with compositions of $Cd_{68}Se_{55}Cl_{26}$, $Cd_{176}Se_{147}C_{158}$, $Cd_{360}Se_{309}Cl_{102}$, and $Cd_{640}Se_{561}Cl_{158}$, respectively. (B) DOS for each QD with their respective HOMO and LUMO gap energies. Every horizontal line corresponds to an MO. The length of the colored line segments indicates the contribution of each element to an MO. Levels below the dotted line are filled with two electrons; levels above the line are empty. (C) Contour plots of the HOMO and LUMO of each system.

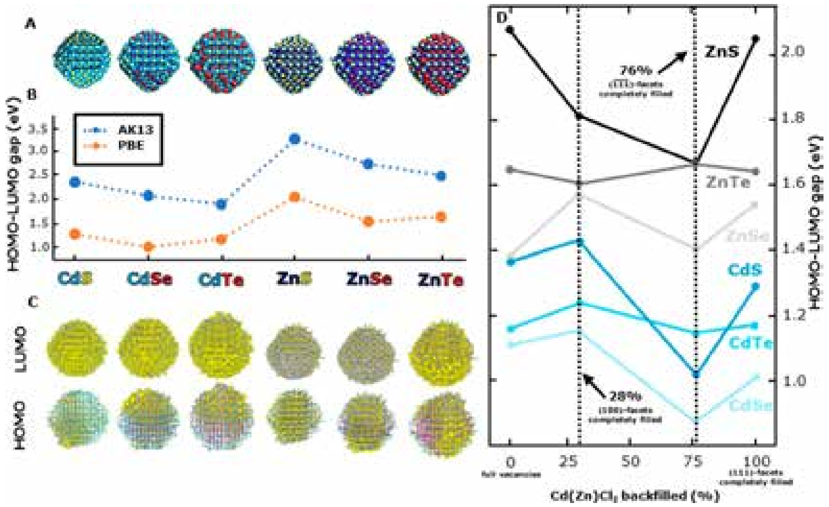


Fig 2
(A) Sketch of the different $Cd(Zn)_{360}$ models used. (B) Evolution of the HOMO–LUMO gap energy as a function of the composition of the QD. The colors displayed on the names of the materials represent the atom colors in part A. Notice the comparison between functionals PBE (orange) and AK13 (blue). (C) Contour plots of the HOMO and LUMO of each system. (D) HOMO–LUMO gap energy tuning based on the percentage of $Cd(Zn)Cl_2$ monomers backfilled in the different QDs. Blue and black-gray tonality lines represent QDs that are comprised of Cd and Zn cations, respectively.

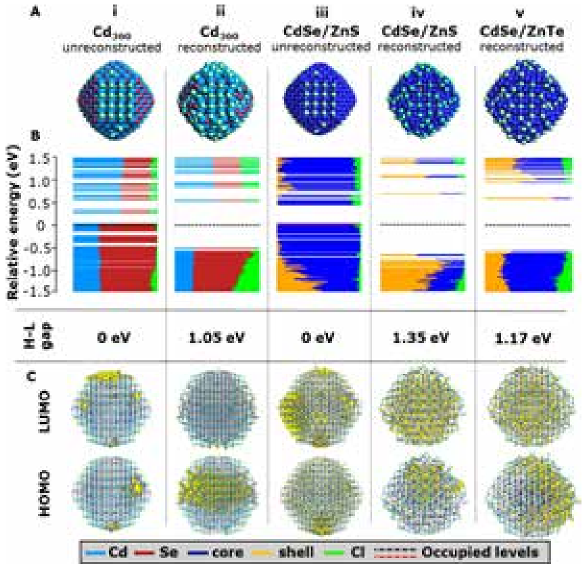


Fig 3
Comparison of the Cd360 model with the CdSe/ZnS core/shell system with and without surface reconstruction. Only the reconstructed versions of CdSe/ZnS and CdSe/ZnTe core/shell models are compared one to each other. (A) Structures of both the unreconstructed and reconstructed core-only and the CdSe/ZnS core/shell models and reconstructed CdSe/ZnTe core/shell model. (B) DOS of each system with their respective HOMO–LUMO gap energies. (C) Contour plots of the HOMO and LUMO of each system.

In this work, we explore the impact of surface reconstructions and ligand passivation on the electronic properties of II–VI quantum dots (QDs), focusing on CdSe systems, using Density Functional Theory (DFT). While DFT has been instrumental in advancing our understanding of colloidal QDs, traditional models are often significantly smaller than experimental systems. This size mismatch can lead to inaccuracies, such as surface orbital localization and the disappearance of the band gap, especially as QD models approach diameters exceeding 4 nm.

We demonstrate that increasing QD size results in the localization of HOMO and LUMO states on specific surface facets, a phenomenon attributed to surface orbital coupling and the formation of facet-specific surface bands. To mitigate these effects, we introduce surface reconstructions by creating vacancies on the 111 , -1-1-1 , and 100 facets. These reconstructions lead to the delocalization of HOMO and LUMO states and reopen the band gap, resolving the discrepancies between theoretical predictions and experimental observations.

Furthermore, we address the limitations of vacancy-based reconstructions by refilling these sites with Z-type ligands, such as CdCl . This process restores ligand densities comparable to experimental conditions, achieving uniform ligand coverage across all facets. The resulting QD models exhibit delocalized orbitals and wide band gaps, aligning with experimental findings. Importantly, this ligand passivation method ensures the stability of QD surfaces while maintaining realistic electronic properties.

We extend our approach to core–shell systems, including CdSe/ZnS and CdSe/ZnTe structures, demonstrating its general applicability to technologically relevant systems. For reconstructed CdSe/ZnS, we observe quasi-type-I band alignments, while the CdSe/ZnTe system exhibits type-II alignments. These results underscore the importance of accurate surface termination and ligand passivation in achieving realistic electronic behavior in core–shell QDs.

Our findings emphasize that surface geometry and ligand chemistry are critical factors influencing the electronic properties of QDs. By addressing the limitations of traditional QD models, our work enables the study of larger, more realistic systems and core–shell architectures using DFT. These advancements are pivotal for designing QDs with precise optoelectronic properties, bridging the gap between theoretical models and experimental systems.

UMAT4COMSOL: An Abaqus user material (UMAT) subroutine wrapper for COMSOL

Lucarini S., Martínez-Pañeda E. (2024) Advances in Engineering Software, 190, art. no. 103610

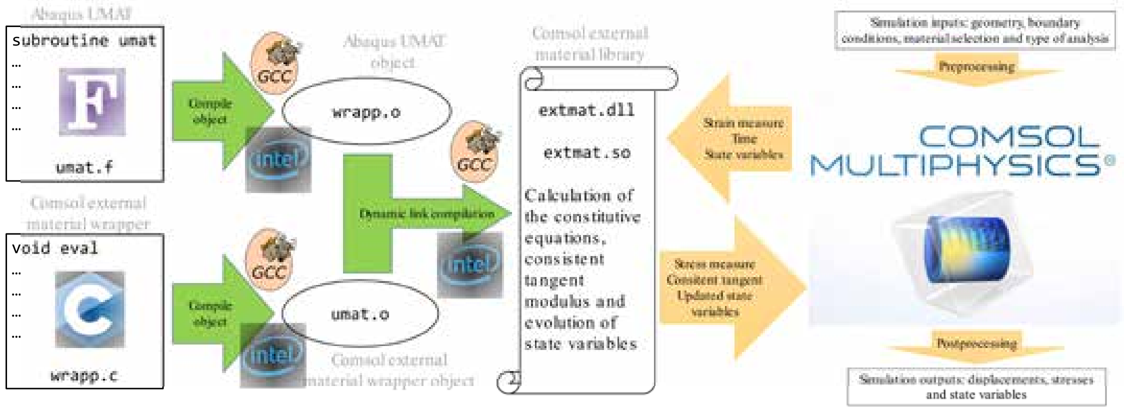


Fig 1
A schematic representation of the UMAT4COMSOL framework, detailing the input-output transformation process between COMSOL and Abaqus for material modeling.

The paper introduces UMAT4COMSOL, a versatile wrapper designed to enable the integration of Abaqus user material (UMAT) subroutines into COMSOL Multiphysics simulations. Developed in C, this wrapper transforms COMSOL's External Material subroutine variables into the format required by Abaqus UMATs. UMAT4COMSOL supports both small strain and finite strain frameworks, enabling the adoption of advanced material models like elastoplasticity, hyperelasticity, and crystal plasticity into COMSOL's environment.

Key features of UMAT4COMSOL include a transformation of inputs such as strain tensors, deformation gradients, and material properties into the formats compatible with Abaqus UMAT conventions. The outputs, including stresses and tangent matrices, are then reformatted back into the structure required by COMSOL solvers. This process enables consistent simulations in COMSOL leveraging the efforts already done in the development of UMAT materials models.

The paper validates the wrapper capabilities through three benchmarks. First, the behavior of a holed plate under small strain conditions is analyzed, demonstrating identical results in stress-strain curves and convergence rates when comparing COMSOL and Abaqus results. Secondly, a neo-Hookean material undergoing twisting is simulated, showing a less than 0.3% difference in results between the two platforms. The third benchmark consist in a polycrystalline deformation study that showcases the wrapper's ability to handle complex constitutive models, providing nearly identical stress-strain curves and stress distributions.

A fourth case study highlights UMAT4COMSOL's potential in coupled multiphysics problems, specifically modeling hydrogen diffusion and deformation in a single crystal. This analysis combines COMSOL's diffusion modules with crystal plasticity UMATs, revealing insights into stress and hydrogen concentration distributions near crack tips in hydrogen-exposed environments, a capability not achievable natively in Abaqus or COMSOL.

UMAT4COMSOL is made freely available online, offering source code, documentation, and tutorials for the broader scientific community. The tool bridges the gap between two leading finite element platforms, empowering researchers to tackle complex, multiphysics material problems, such as hydrogen embrittlement, battery degradation, and corrosion mechanisms.

> UMAT4COMSOL is a novel C-coded wrapper that allows Abaqus UMAT subroutines to work as COMSOL External Materials, bridging the gap between advanced materials models and multiphysics simulations. This wrapper transforms variable inputs and outputs between the two platforms, facilitating coupled studies in areas such as elastoplasticity, hyperelasticity and crystal plasticity. Validated and tested through several benchmarks, including coupled deformation-diffusion in hydrogen-sensitive materials, UMAT4COMSOL extends state-of-the-art material modeling capabilities, supporting multiphysics simulations by providing a freely available source code and documentation for wide community use.

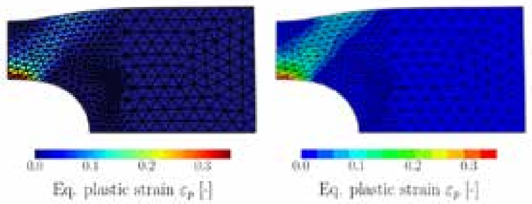


Fig 2
Equivalent plastic strain contours for a holed plate under elastoplastic deformation. Results from Abaqus (left) and COMSOL with UMAT4COMSOL (right) show perfect agreement.

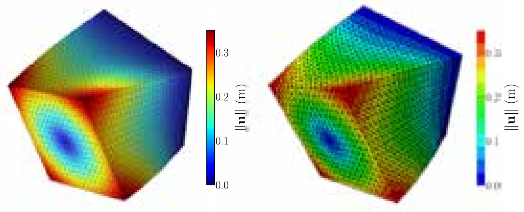


Fig 3
Displacement field magnitude for a twisted cube made of hyperelastic material, simulated using Abaqus (left) and COMSOL with UMAT4COMSOL (right).

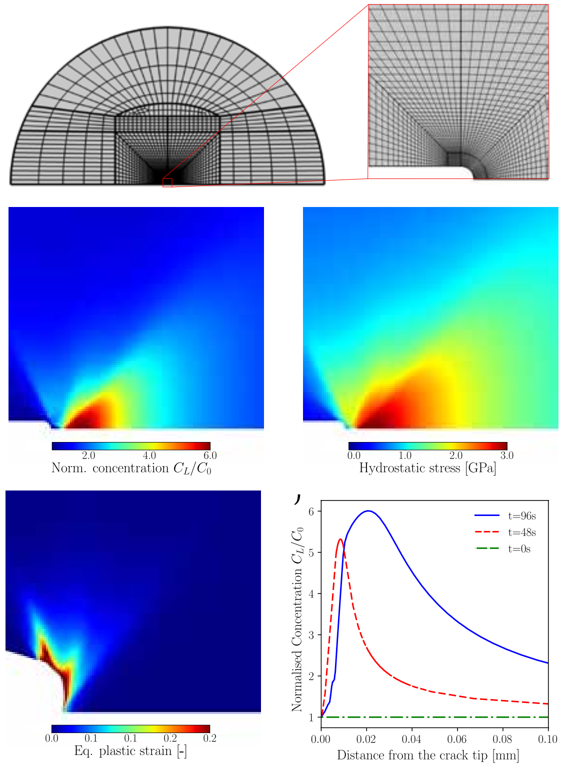


Fig 4
Hydrogen lattice concentration near a crack tip in a single crystal under mechanical load, modeled using UMAT4COMSOL with coupled diffusion and deformation physics in COMSOL.

JOURNAL COVERS
SELECTION

Eco-friendly, sustainable, and safe energy storage: a nature-inspired materials paradigm shift

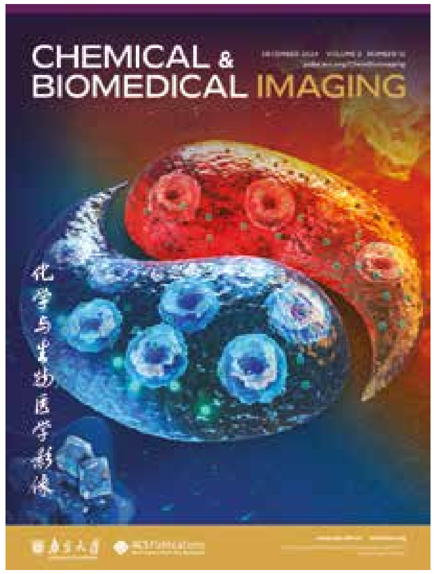
Thiago Bertaglia, Carlos M. Costa, Senentxu Lanceros-Méndez, Frank N. Crespilho

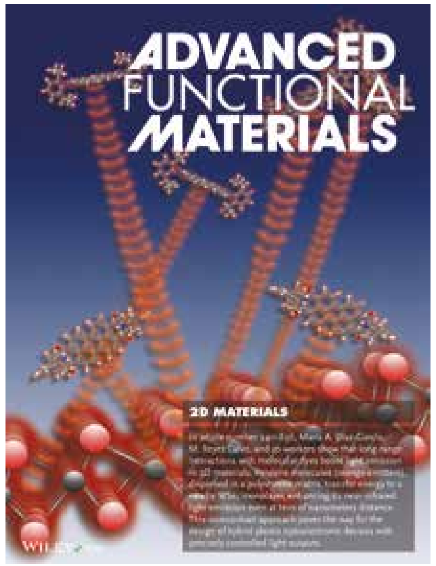
Here, we explore the paradigm shift towards eco-friendly, sustainable, and safe batteries, inspired by nature, to meet the rising demand for clean energy solutions. Current energy storage devices face challenges in performance, cost, and environmental impact. Nature-inspired strategies, drawing from billions of years of evolution, offer innovative solutions. This review focuses on how biomolecule-based electrode materials, green biobatteries, and biodegradable materials can support further developments in battery technology. Biomolecule-based electrodes mimic natural electron shuttles, enhancing capacitor performance. Nature-inspired designs applied to binders and separators allow the modulation of electrochemical performance. Green biobatteries, employing living organisms for energy generation, showcase potential applications in environmental monitoring, healthcare, and agriculture. Challenges include optimizing energy conversion efficiency and addressing scalability. This comprehensive exploration emphasizes the potential of nature-inspired materials in reshaping the landscape of energy storage.

Laser-Treated Screen-Printed Carbon Electrodes for Electrochemiluminescence imaging

Claudio Ignazio Santo, Guillermo Conejo-Cuevas, Francesco Paolucci, Francisco Javier Del Campo, Giovanni Valenti

Electrochemiluminescence (ECL) is nowadays a powerful technique widely used in biosensing and imaging, offering high sensitivity and specificity for detecting and mapping biomolecules. Screen-printed electrodes (SPEs) offer a versatile and cost-effective platform for ECL applications due to their ease of fabrication, disposability, and suitability for large-scale production. This research introduces a novel method for improving the ECL characteristics of screen-printed carbon electrodes (SPCEs) through the application of CO2 laser treatment following fabrication. Using advanced ECL microscopy, we analyze three distinct carbon paste-based electrodes and show that low-energy laser exposure (ranging from 7 to 12 mJ·cm–2) enhances the electrochemical performance of the electrodes. This enhancement results from the selective removal of surface binders and contaminants achieved by the laser treatment. We employed ECL microscopy to characterize the ECL emission using a bead-based system incorporating magnetic microbeads, like those used in commercial platforms. This approach enabled high-resolution spatial mapping of the electrode surface, offering valuable insights into its electrochemical performance.





Enhancing Single-Layer WSe$_2$ Light Emission in Perylene-Doped Polymer Films through Efficient Energy Transfer

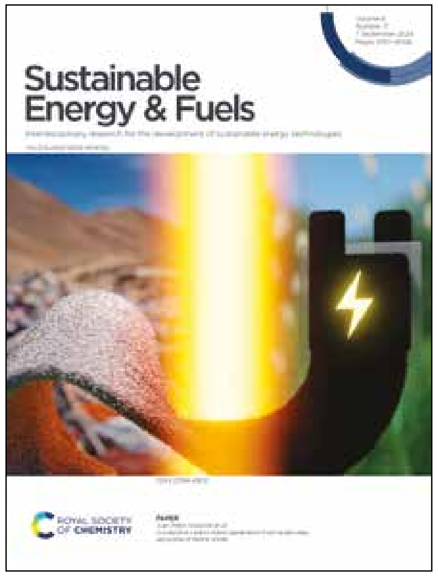
Marcos Gadea, Aswin Asaithambi, Raúl Bernabeu-Cabañero, Alex Farrando-Pérez, María Ramos, Juan C. Sancho-García, Ilka Kriegel, María A. Díaz-García, M. Reyes Calvo

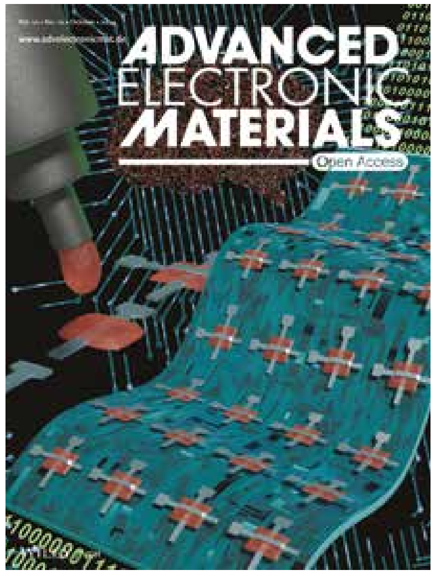
The optical and mechanical properties of 2D semiconductors make them excellent candidates for the active components of plastic optoelectronic devices. Here, the integration of single-layer WSe2 (1L-WSe2) into a polystyrene (PS) film containing dispersed perylene orange (PDI-O) molecules is investigated. The findings reveal a notable enhancement in the light emission of 1L-WSe2, which occurs exclusively upon PDI-O excitation and scales with the concentration of molecules in the PS film. Moreover, the increase in 1L-WSe2 photoluminescence coincides with a quenching of the PDI-O light emission intensity and a decrease in its lifetime. These results point to efficient long-range interactions, such as Förster energy transfer, between PDI-O (acting as the donor) and 1L-WSe2 (acting as the acceptor), as the mechanism responsible for the enhanced light emission in the latter. These findings are of great interest for the development of flexible optoelectronic devices integrating active 2D materials; the polymeric matrix plays a dual role, serving as both physical support and host for organic dopants that can optimize the light emission properties of the active 2D material.

Conductive carbon fabric generation from single-step upcycling of textile waste

Carles Tortosa, Marina Navarro-Segarra, Pedro Guerrero, Koro de la Caba, Juan Pablo Esquivel

Environmental impacts from the fashion industry are at the top of global pollution. Fiber production, fabric preparation and distribution, and disposal of textiles combined with the excessive consumerism of clothing result in the wastage of thousands of million cubic meters of fresh water, the release of gigatons of CO2 equivalent, and tens of millions of metric tons of textile waste generation every year. This situation shows that there is an urgent and mandatory need to change the fashion paradigm, but, even if accomplished, the current textile waste spread worldwide still needs to be managed in an environmentally conscious way. Upcycling textile waste by pyrolysis is gaining interest as an alternative management option. The goal is to endow waste with new functionalities for its repurposing into new applications. This study focuses on applying pyrolysis to convert discarded clothing into a conductive carbon textile while avoiding treatments with hazardous chemicals. Envisioned to be applied for current collection in all-organic primary power sources, the ultimate goal is to replace synthetic polymers in commercial carbon current collectors.



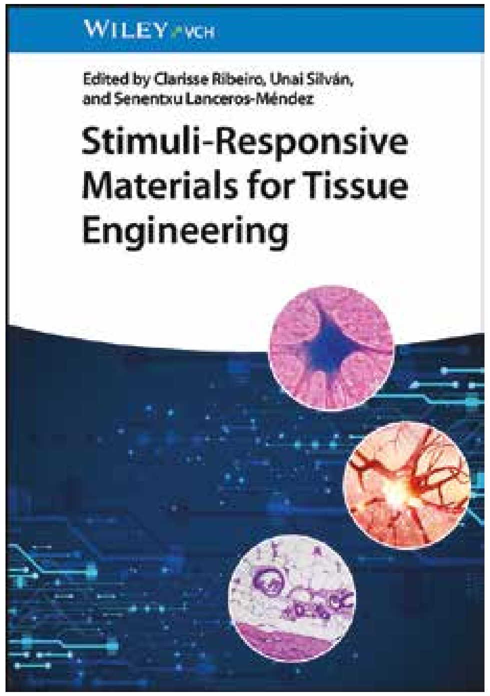


Printed Memristors: An Overview of Ink, Materials, Deposition Techniques, and Applications

Miguel Franco, Asal Kiazadeh, Rodrigo Martins, Senentxu Lanceros-Méndez, Emanuel Carlos

As the world shifts towards Industry 4.0, the growth of connected devices is accelerating, resulting in increased data generation. Miniaturization and power consumption challenges require efficient computation, with memristor being the next technological leap. Printed electronics have opened new avenues for low-temperature, low-cost processes for material processing and manufacturing. The review by Asal Kiazadeh, Senentxu Lanceros-Méndez, Emanuel Carlos, and co-workers (see article number 2400212) offers an insight into printed electronics' potential for the creation of sustainable memristive devices, a significant new field that has seen impressive advancements in novel neuromorphic paradigms.

PUBLISHED BOOKS



WILEY-VCH

Edited by Clarisse Ribeiro, Unai Silván, and Senentxu Lanceros-Méndez

Stimuli-Responsive Materials for Tissue Engineering

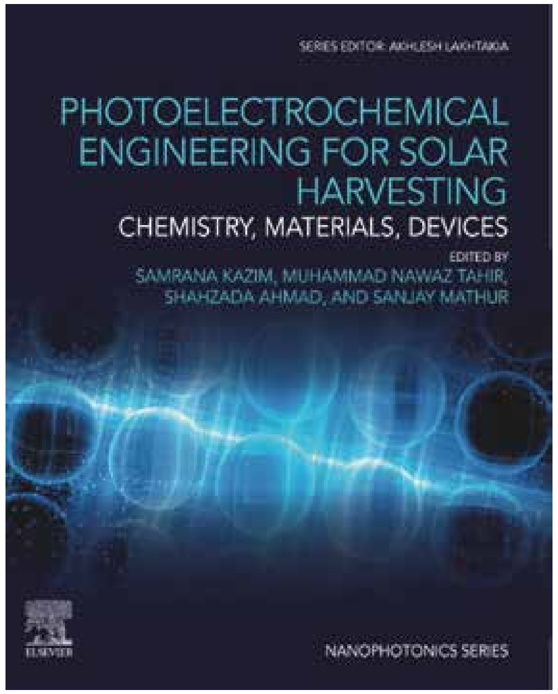
Stimuli-Responsive Materials for Tissue Engineering

Editors:Clarisse Ribeiro, Unai Silván, Senentxu Lanceros-Méndez

'Stimuli-Responsive Materials for Tissue Engineering'comprehensively reviews the use of stimuli-responsive materials in the context of advanced tissue engineering approaches, highlighting applications, challenges, and solutions and reporting on the current state of the art of smart and multifunctional materials being used for tissue engineering, focusing on material types and their properties.

The progress that has already been achieved in the field is put into perspective by covering the remaining challenges in the research field of tissue engineering, and solutions are outlined to overcome those. By addressing challenges and ways to overcome them, Stimuli-Responsive Materials for Tissue Engineering is a highly practical resource on advanced tissue regeneration.

With comprehensive coverage of the subject, Stimuli-Responsive Materials for Tissue Engineering is an essential resource for materials scientists, bioengineers, engineering scientists, and biotechnologists seeking to understand advanced tissue regeneration approaches, current challenges, and potential solutions to advance progress in the field.



SERIES EDITOR: AKHLESH LAKHTAKIA

PHOTOELECTROCHEMICAL ENGINEERING FOR SOLAR HARVESTING

CHEMISTRY, MATERIALS, DEVICES

EDITED BY

SAMRANA KAZIM, MUHAMMAD NAWAZ TAHIR, SHAHZADA AHMAD, AND SANJAY MATHUR

ELSEVIER

NANOPHOTONICS SERIES

Photoelectrochemical Engineering for Solar Harvesting

Editors:Samrana Kazim, Muhammad Nawaz Tahir, Shahzada Ahmad, Sanjay Mathur

'Photoelectrochemical Engineering for Solar Harvesting: Chemistry, Materials, Devices' provides an up-to-date appraisal of the photon engineering of innovative catalysts for solar energy harvesting. This book analyzes the overall progress, potential challenges, and the industrialization of new catalysts in the near future. The primary emphasis is on experimental approaches from materials synthesis to device applications, however, there is also an introduction to relevant photochemistry concepts. This book is suitable for materials scientists and chemists who, through the use of photonics, are in continuous pursuit of improving the efficiencies of different devices used to capture solar energy for the generation of sustainable fuel.

Sunlight-driven fuel synthesis is the most sustainable and potentially economical option for producing energy vectors through water splitting. Thus, this book focuses on the design of photocatalysts and water oxidation catalysts, as artificial photosynthesis and hydrogen fuel production via water oxidation (in place of fossil fuels) are two promising approaches towards renewable energy.

SELECTED REVIEW PAPERS

MXene-Based Energy Devices: From Progressive to Prospective

Kazim S., Huang C., Hemasiri N.H., Kulkarni A., Mathur S., Ahmad S.

(2023) Advanced Functional Materials, 33 (16), art. no. 2213744

Nanoscience and nanotechnology for water remediation: an earnest hope toward sustainability

Dutta S., Sinelshchikova A., Andreo J., Wuttke S.

(2024) Nanoscale Horizons, 9 (6), pp. 885 - 899

Materials and Strategies to Enhance Melt Electrowriting Potential

Saiz P.G., Reizabal A., Vilas-Vilela J.L., Dalton P.D., Lanceros-Mendez S.

(2024) Advanced Materials, 36 (24), art. no. 2312084

Magnetoelectrics for biomedical applications: 130 years later, bridging materials, energy and life

Martins P., Brito-Pereira R., Ribeiro S., Lanceros-Mendez S., Ribeiro C.

(2024) Nano Energy, 126, art. no. 109569

PRICES & AKNOWLEDGMENTS

Ikerbasque Outstanding Scientists

Itziar Oyarzabal, Ikerbasque Research Associate at BCMaterials, received an special mention at the Basque Foundation for Science annual awards for outstanding scientists.

World’s top 2% most influential scientists


Senentxu
Lanceros-Méndez


Koro
de la Caba


Shahzada
Ahmad


Javier
del Campo


Volodymyr
Chernenko


Qi
Zhang


Pedro
Guerrero


Ivan
Infante

11 BCMaterials researchers in this annual list published by the Standford University (USA).


José Luis
Vilas


Joel
Villatoro


Erlantz
Lizundia


ISMIT 2024

Advanced Technology Award

Senentxu Lanceros-Mendez

Advanced Technology Award - ISMIT2024

Senentxu Lanceros-Méndez, Scientific Director of BCMaterials, received the Advanced Technology Award at the 35th Annual International Society for Medical Innovation and Technology Conference, held in Cáceres (Spain) in September 2024. Lanceros-Méndez received this acknowledgement for his invited talk “Electroactive Materials in te scope of biomedical applications: from biomedical monitoring and actuation to advanced tissue regeneration strategies”.

UPV/EHU PhD Extraordinary Prize

Mikel Rincón Iglesias received the one of the UPV/EHU PhD extraordinary prizes in 2024 for his thesis titled “Sustainable multifunctional materials with tailored magnetic and electrical properties for electronics applications”.

Best posters at IMOH2024

Paula Rodríguez Lejarraga and Mariana Ríos Naranjo won the prize for the best poster presentations at the 2nd International Meeting on Challenges and Opportunities for HiCANS - IMOH 2024 held in Leioa in October.

TRAINING ACTIVITIES

As a research center of excellence, BCMaterials is committed, mostly together with the UPV/EHU but also with other regional, national and international institutions, with the training of the next generation of scientist. This is our duty, but mostly our conviction and pleasure. We offer our expertise, laboratories and human resources to motivate, guide and advise the next generation of scientist in all our areas of expertise. Thus, BCMaterials offers a complete PhD program to graduate students from all around the world who wish to start a research career in a materials science-related field at a top international research institution. BCMaterials collaborate with various official master and graduate programs, and we offer different internship possibilities.

14

PHD
Thesis Defended

1. Eduarda Barbosa Fernandes
Biomimicry profiling supporting drug discovery for topical applications

2. Liliana Sofia Correia Fernandes
Magnetic ionic liquid/polymer composites for printable sensors and actuators

3. Ainhoa Barroso Garcia
Tratamiento de perforaciones de la membrana timpánica e incontinencia urinaria de esfuerzo mediante ingeniería tisular

4. Miguel Alexandre Martins Franco
Microfabricated Development of conductive inks and memristive active material for printed electronic applications

5. Nekane Nieto
Advanced Materials for energy storage: From negative electrodes to sustainable batteries

6. Estela Marisa Oliveira Carvalho
Electroactive materials-based strategies for improving orthopedic implant interfaces through antibacterial and cell stimulation effects

7. Luís Amaro Ribeiro Martins
Microfluidic Processing of Smart Polymers for Tissue Engineering

8. Natalia Ahiova Río López
Relation between microstructure and properties in magnetic shape memory alloys studied by neutron diffraction

9. João Luís Rodrigues
Multifunctional air filters based on emerging natural polymers for VOCs removal

10. Tiago André Rodrigues Marinho
Printable energy harvester systems for wearable sensor devices

11. Bosco Rodríguez Crespo
Development of Heusler – Alloy – Based Magnetocaloric Inks For 2D – 3D Printing

12. Julia Sánchez Bodón
Click Reactions: An Efficient Tool Towards Biofunctional Materials

13. Luis Henrique Santolin Reichembach
Development of biodegradable films for packaging based on pectins from agricultural waste from coffee processing

14. Yifeng Wang
Green recycling of lithium-ion batteries using deep eutectic solvents and alginate hydrogels

15

Master
Thesis Defended

13

Final Degree
Projects Defended

MASTER SCHOLARSHIPS

BCMaterials offers Master Scholarships to perform research in areas as diverse and challenging as materials for sensors and actuators, which are critical for the Internet of Things and Industry 4.0; materials for advanced biological and biomedical applications; materials for energy (both generation and storage) or materials for environmental monitoring and remediation.

Master in
New Materials

Its objective is to provide a solid training in the most current methodologies for the synthesis, characterization, properties and applications of new materials, in fields as diverse as biomaterials, nanomaterials, intelligent materials, materials for energy, electronics, catalysis, etc.

Master in Environmental Contamination and Toxicology

The master will train the students as a professionals in the biological assessment of the health of ecosystem, both marine and fresh water, and terrestrial.

Master in
Biomedical Research

The master offers updated training on the molecular, cellular and physiological mechanisms involved in the development of the disease, necessary to carry out research that leads to the achievement of valid results and conclusions on topics of biosanitary interest.

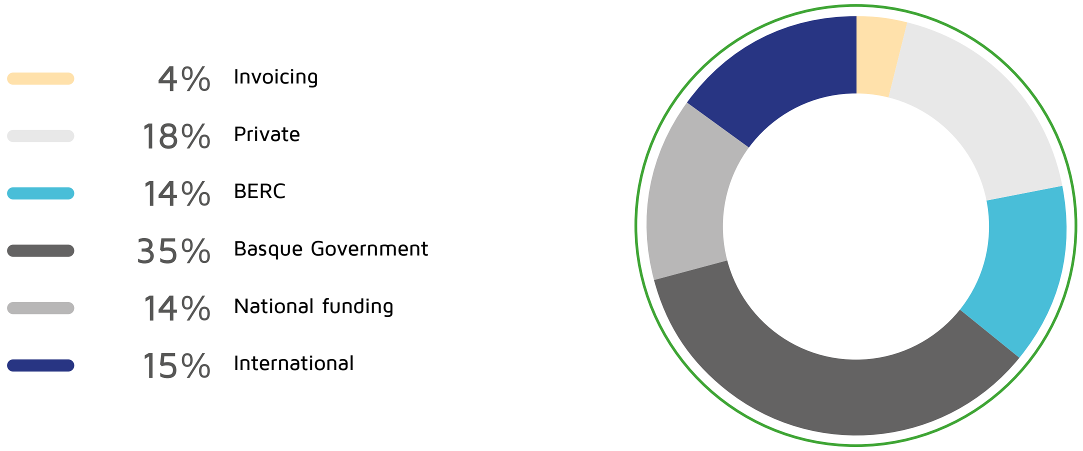
03

PROJECTS & TECH-TRANSFER

Research projects represent the core of our activities as, most often in collaborative endeavours, set as specific framework for scientific or technological advances. Research projects represent also timely innovations for the generation of knowledge and technology transfer for the benefit of society.

FOUNDING SOURCES & RESEARCH PROJECTS

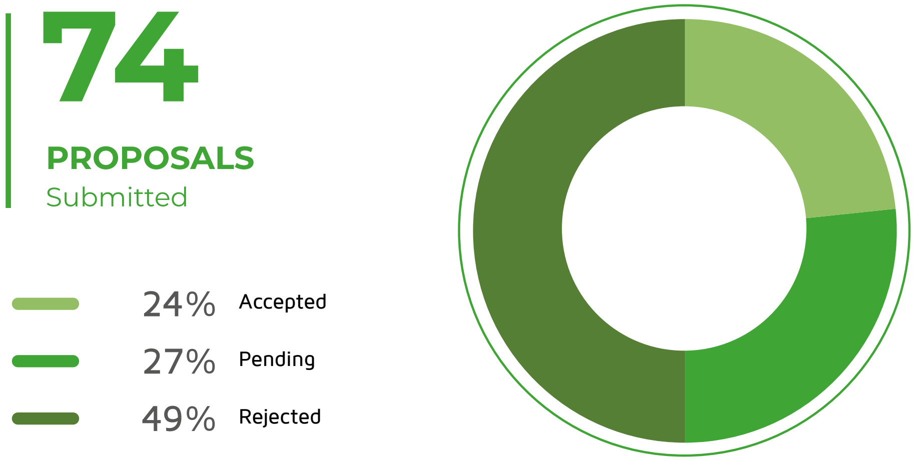
FOUNDING **SOURCES**



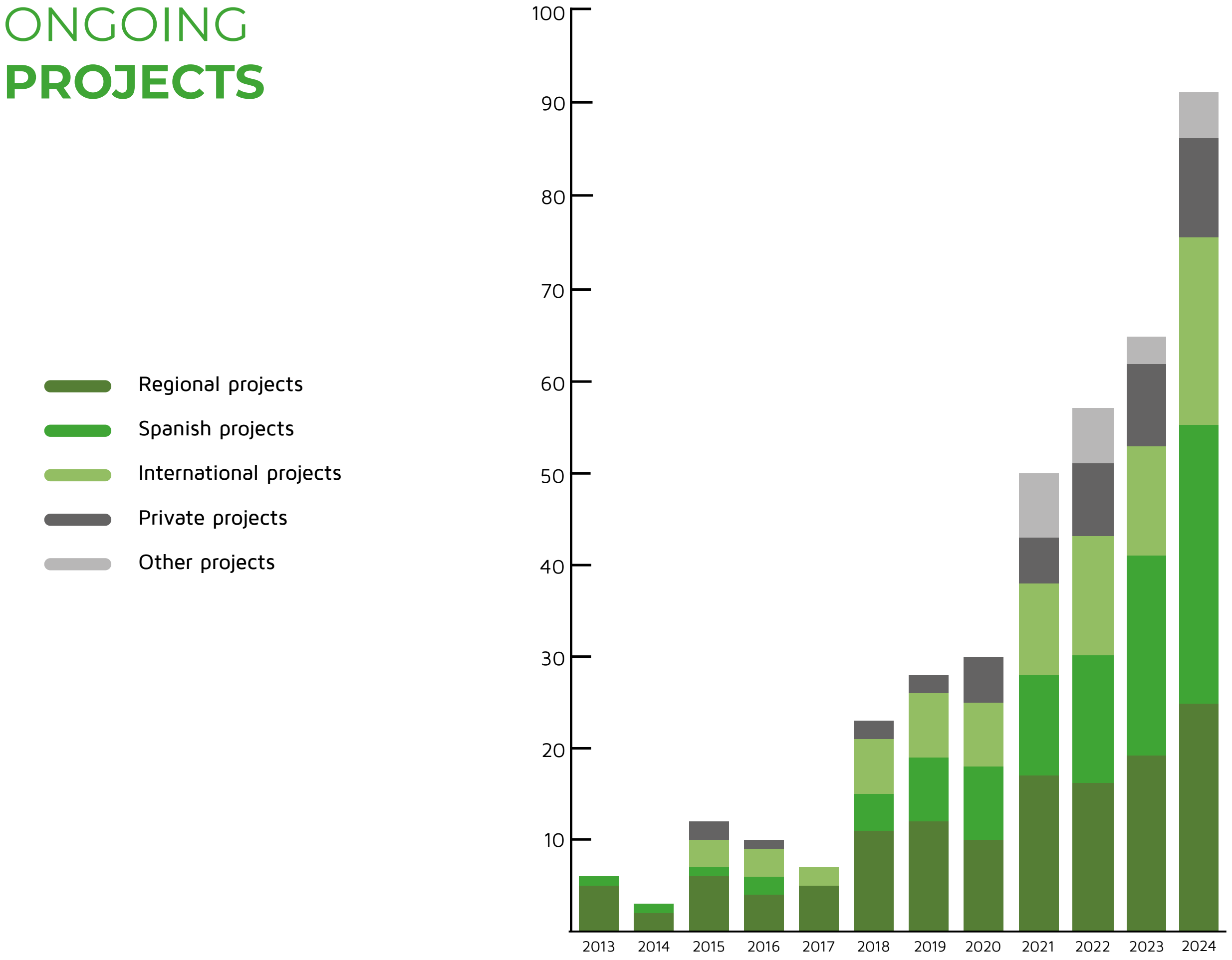
PROJECT **PROPOSALS**

74

PROPOSALS
Submitted



ONGOING **PROJECTS**



FINANCIAL **BODIES**

erc
European Research Council
Established by the European Commission

European Commission

HFSP
International Human Frontier Science Program Organization

GOBIERNO DE ESPAÑA
MINISTERIO DE CIENCIA E INNOVACIÓN

GOBIERNO DE ESPAÑA
MINISTERIO DE EDUCACIÓN, FORMACIÓN PROFESIONAL Y DEPORTES

Plan de Recuperación, Transformación y Resiliencia

AGENCIA ESTATAL DE INVESTIGACIÓN

Fundación BBVA

EUSKO JAURLARITZA
GOBIERNO VASCO

ikerbasque
Basque Foundation for Science

BFA DFB
Bizkaiko Foru Aldundia
Diputación Foral de Bizkaia

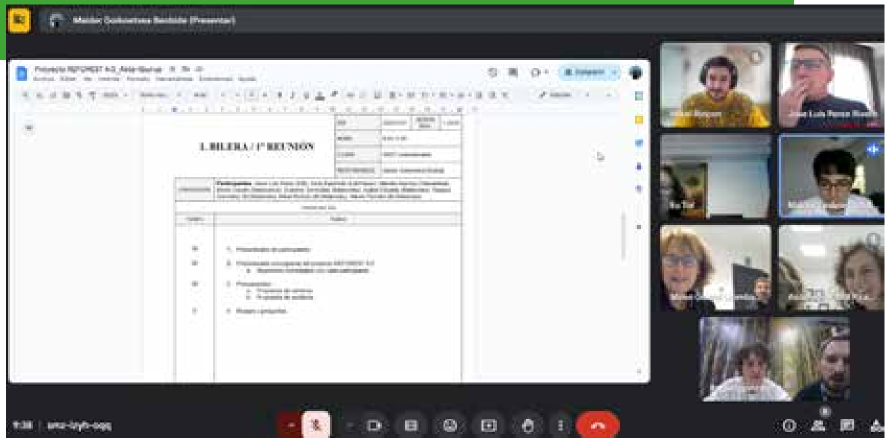
euskampus
Fundazioa

PROJECT MEETINGS
& EVENTS

BIOTIER HOTIZON EUROPE PROJECT'S KICK OFF MEETING
Heraklion (Greece), October 2023

GIANCE HORIZON EUROPE PROJECT'S WORKSHOP
at the Graphene 2024 Industrial forum in Madrid. Carmen Rial presented on behalf of BCMaterials the talk called "Development of graphene-based membranes for environmental and energy applications: design rules and framework for sustainable development"
Madrid, July 2024

***"SOST-CDTI CONFERENCE FOR EUROPEAN PROJECTS MANAGERS" AND "BEYOND THE HORIZON"** evets organized by CDTI, with the presence or our Project and Technology Transfer Manager, Raquel González.*
Brussels (Belgium), November 2024



KICK-OFF MEETING OF THE REFOREST NATIONAL PROJECT
December 2024

HIGH RISK-HIGH GAIN SEED PROJECTS

The BCMaterials 'High Risk – High Gain' seed project contest aims to promote disruptive research in materials science among the center's researchers, especially the postdoctoral ones. Each of the winning proposals receives 5,000 euros to launch the research.

These were the four winning proposals of 2024:

- **Manuel Salado (MSCA Post-Doctoral Fellow and Ikerbasque Research Fellow) and Vera Macedo (pre-doctoral researcher):** "Next-Generation Solid-State Batteries: Leveraging Glassy MOFs and 3D Printing - NEXBAT ".
- **Andrey Shibaev (Post-Doctoral Researcher):** "Biodegradable polymer/MOF hydrogels for real-time monitoring of tissue regeneration - BioHydroMOF".
- **Maibelín Rosales. (MSCA Post-Doctoral Fellow):** 'Bioinspired dual photoreactor for sustainable hydrogen and clean water production - BIP-H2'

BASQUE REGIONAL PROJECTS

ADMAG Additive Manufacturing of Molecule-based Magnets
EJ/GV, PIBA_2023_1_0027 2023-2025

AIMOFGIF Artificial Intelligence Guided Platform for Experimental Synthesis and Preclinical Assay of Metal-Organic Frameworks Drug Release Systems for Gastrointestinal (GI) Cancer Treatment and Prevention
EJ/GV, ELKARTEK Tipo 1 KK-2022/00032 2022-2023

ALOPRP V "Creación de apósitos con plasma rico en plaquetas alogénicos para la curación de heridas crónicas"
EJ/GV, Ayudas a Proyectos de Investigación y Desarrollo en Salud 2024

BISUMII Bio-Inspired Surfaces for Machine Elements II
EJ/GV, ELKARTEK Tipo 1 KK-2024/00048 2024-2025

DCEE Descifrando la respuesta celular a la estimulación electroactiva (DCEE)
EJ/GV, PIBA_2022_1_0023 2022-2024

ECLICARE2 Bioensayos Electroquemiluminiscentes para Diagnóstico Personalizado
EJ/GV, EUREG_2021 2024-2026

ENHARPE Nuevos sistemas de energy harvesting para dispositivos de baja potencia autoalimentados mediante soluciones impresas y materiales sostenibles
EJ/GV, ELKARTEK Tipo 1 KK-2024/00104 2024-2025

FRONTIERS 2024- Superficies multifuncionales en la frontera del conocimiento
EJ/GV, ELKARTEK Tipo 1 KK-2024/00099 2024-2025

FOTOPOL Tecnologías circulares y eficientes de fabricación de composites basadas en fotopolimerización
EJ/GV, ELKARTEK Tipo 1 KK-2023/00054 2023-2024

IDEA III Investigación en nuevos materiales y procesos para una electrónica impresa integrada y sostenible
EJ/GV, ELKARTEK Tipo 1 KK-2023/00056 2023-2024

INFRAESTRUCTURA Infraestructura para caracterización optoelectrónica a temperatura variable de micro-dispositivos basados en materiales avanzados con alto rendimiento y bajo consumo energético esenciales en el contexto de la digitalización sostenible de la sociedad y la enconomía.
DFB, Transferencia tecnologica Linea 2 INFRAS_DFB_2024 2024

INNOSENSE Desarrollo de soluciones innovadoras para su aplicación a biosensórica de sustancias químicas
EJ/GV, ELKARTEK Tipo 1 KK-2024/00059 2024-2025

MIME2 Mejorando la Interfaz de los Materiales para su uso Médico
EJ/GV Ayudas a Proyectos de Investigación y Desarrollo en Salud 2023333036 2023

MMASINT Materiales magnetoactivos avanzados para nuevos sistemas inteligentes
EJ/GV, ELKARTEK Tipo 1 KK-2023/00041 2023-2024

MOSINCO Monitorización sin contacto de composites, desde su fabricación hasta su fin de vida
EJ/GV, ELKARTEK Tipo 1 KK-2024/00037 2024-2025

μ4Smart Microsistemas Avanzados y Sostenibles Integrados en la Fábrica Inteligente y Digital
EJ/GV, ELKARTEK Tipo 1 "KK-2023/00016 2023-2024

NeutroMOF Desentrañando la estructura en la nanoescala de compuestos de polímero / MOF a través de la dispersión de neutrones: hacia membranas mejoradas para separadores de baterías y remediación ambiental.
EJ/GV PIBA PIBA_2022_1_0032 2022-2024

ONBODY Materiales magnetoactivos avanzados para nuevos sistemas inteligentes
EJ/GV, ELKARTEK Tipo 1 KK-2023/00070 2023-2024

ONCOKLINEFERTI III Programa experimental nacional de preservacion de fertilidad en varones prepuberes con cancer o sindromes
EJ/GV, Promoción de la actividad investigadora sanitaria 22111067 2023-2026

PoliSosBat Desarrollo de electrolitos en forma de gel basados en polímeros de origen renovable para una nueva generación de baterías de iones de sodio y de iones de zinc ambientalmente sostenibles
EJ/GV PIBA_2022_1_0047 2022-2024

SMARTEYE Nuevas técnicas fotónicas multisensor en línea para la caracterización físico-química y control para un uso sostenible de recursos
EJ/GV, ELKARTEK Tipo 1 KK-2023/00021 2023-2024

SMYRNA Nuevos Materiales y Procesos para Tratamientos Fisicoquímicos de Aguas
EJ/GV, ELKARTEK Tipo 1 KK-2023/00028 2023-2024

SPANISH NATIONAL PROJECTS

BIDEKO Biodegradable and compostable batteries for precision agriculture and decentralized energy systems
LINEAS ESTRATÉGICAS PLEC2021-007801 2021-2024

BIOELECTROSURF Bioimitación de superficies electroactivas a través de la ingeniería de patterning de parches
RETOS I+D PID2022-139467OB-I00 2023-2026

CARNK_OTS "CAR-NK "off the shelf":nuevas mejoras y perspectivas de inmunoterapia contra cánceres hematológicos en recaída o refractarios. Ensayo clínico fase I para evaluar la viabilidad y seguridad de la terapia
ACADEMIC CLINICAL TRIALS CALL PICI21/00095 2022-2024

DAMIS Dynamically adaptive microenvironment for spinal cord regeneration
RETOS I+D PID2022-138572OB-C42 2023-2026

ELECTROBIONETS-Red de Sensores y Biosensores Electroquímicos
RED2022-134120-T 2023-2024

EC-SERS2SOERS Desarrollo de dispositivos para EC-SERS/EC-SOERS
PROYECTOS I+D+I PID2020-113154RB-C22 2021-2024

ENZYMOF Imitando las funciones de transformación enzimáticas de CO2 y CH4 en materiales metal-orgánicos
Transicion Ecologica y digital TED2021-130621B-C42 2022-2024

EVOLMOF Mimicking directed evolution of metalloenzymes into Metal-Organic Frameworks
RETOS I+D PID2021-122940OB-C31 2022-2025

GHGAPTURE Evaluating the potentials of Metal-Organic Frameworks as direct harvesters of hydrophobic greenhouse gases from air
MCIN-ILL 2023-2025

HERALD Halide perovskites as Low Switching Power Neuromorphic Devices
BBVA 2023-2024

HERMES Harnessing Energy thRough new Materials, procEsses, and architectureS in Self-powered Biosensing
GENERACION DE CONOCIMIENTO 2024-2027

HIERACHMOFS Adsorbentes metal organicos jerarquicos para acondicionamiento de combustibles renovables en pilas de óxido sólido
PROYECTOS I+D+I PID2020-115935RB-C42 2021-2024

INTERACTION Interface tuning of perovskite solar cells through MXenes
RETOS I+D PID2021-129085OB-I00 2022-2025

JUAN DE LA CIERVA FORMACIÓN Jacopo Andreo
FJC2021-048154-I 2022-2024

JUAN DE LA CIERVA FORMACIÓN Subhajit Dutta
JDC2022-049611-I 2023-2025

JUAN DE LA CIERVA FORMACIÓN Hugo Salazar
JDC2022-050319-I 2023-2025

JUAN DE LA CIERVA FORMACIÓN Ricardo Pereira
JDC2023-052829-I 2024-2026

LIT A SPIN Corrientes de spin inducidas por luz en materiales antiferromagnéticos bidimensionales
CNS2023-145151 2024-2026

MAGCALORICH Búsqueda de materiales magnetocalóricos mejorados para la licuefacción de hidrógeno aprovechando la anisotropía magnética
RETOS I+D PID2022-138256NA-C22 2023-2026

MTBOTS Guiado y control de bacterias magnetotácticas para terapias del cancer
PROYECTOS I+D+I PID2020-115704RB-C32 2021-2024

NABICO Baterías secundarias basadas en ion de sodio biodegradables y compostables
RETOS I+D PID2022-139250OB-C31 2023-2026

PROPEL-E Baterías secundarias basadas en ion de sodio biodegradables y compostables
RETOS I+D PID2022-139250OB-C31 2023-2026

SPANISH NATIONAL PROJECTS

RAMÓN Y CAJAL Jorge Saiz
RYC2022-037186-I 2024-2027

RAMÓN Y CAJAL Jose María Porro
RYC2023-044841-I 2024-2028

RAMÓN Y CAJAL Davide Spirito
RYC2022-037186-I 2024-2028

REFOREST 4.0 revalorización de residuos forestales para la agricultura 4.0.
PROYECTOS DE INNOVACIÓN E INVESTIGACIÓN APLICADAS Y TRANSFERENCIA DEL CONOCIMIENTO EN LA FORMACIÓN PROFESIONAL AINN23/00030
2024-2025

RETROFIT Fuentes de energía portátiles hechas a medida para dispositivos electrónicos sostenibles
PROYECTOS DE COLABORACIÓN PÚBLICO-PRIVADA CPP2023-010864 2024-2026

SOLBIO Soluciones de detección y remediación para la eliminación de antibióticos en cursos de agua potables o residuales
Next generation EU MFA/2022/011 2022-2025

SpinRed2-Exploring spintronic potential for low-power consumption devices
RED2022-134649-T 2023-2025

STEMIN2D-OS-Enhancing Structural, Electric, Magnetic, and Optoelectronic properties in 2D materials by Strain-Engineering
GENERACION DE CONOCIMIENTO 2024-2027

TAILINGR32GREEN Mine tailings reprocessing, revalorization and risk reduction through sequential innovations in metal recovery, geopolymerization, ceramics and sealing processes
ERAMIN 2021- PROYECTOS COLABORACION INTERNACIONAL PCI2022-132969 2022-2025

EUROPEAN & OTHER INTERNATIONAL PROJECTS

4AIRCRAFT Air Carbon Recycling for Aviation Fuel Technology
H2020-LC-SC3-2020 2021-2025

BIONTIER Breaking Frontiers in sustainable and circular biocomposites with high performance for multi-sector applications
HORIZON-JU-CBE-2023-IA-07 101155925 2024-2027

ECLECTIC ElectroChemiLuminescence doctoral network for early sepsis diagnosis
MSCA-DN 101119951 2023-2027

EPROT Engineered Conductive Proteins for Bioelectronics
PATHFINDER OPEN 964593 2024-2025

EU4MOFS European metal-organic framework network: combining research and development to promote technological solutions
COST ACTION CA22147 2023-2027

FLUFET FLow detection of virUses by graphene Field Effect Transistor microarrays
Pathfinder 101130125 2024-2027

GIANCE Graphene Alliance for Sustainable Multifunctional Materials to Tackle Environmental Challenges
HORIZON-CL4-2022-DIGITAL-EMERGING-02-20 101119286 2023-2026

HFSP Modeling electric fields at the heart of enzyme catalysis and function
HFSP GRANT RGP0047/2022 2022-2025

HFSP-S4S Science 4 Scientist Special program. Orysia Zaremba
SCIENCE4SCIENTIST HFSP RGP047/2022 2022-2026

HFSP-S4S Science 4 Scientist Special program. Anna Sinelschchikova
SCIENCE4SCIENTIST HFSP RGP047/2022 2022-2026

MERLIN PlasMonic photo-thErmo-catalyzed composite membranes for Remediation of persistent poLlutants IN water
HE-MSCA-PF HFSP 101026163 2024-2026

MOFSORMET IMetal-organic frameworks for recovery and separation of critical metals
The research council of Norway 2021-2024

EUROPEAN & OTHER INTERNATIONAL PROJECTS

MOLEMAT Molecularly Engineered Materials and process for Perovskite solar cell technology
ERC-COG 2017-2024

NETSKINMODELS European Network for Skin Engineering and Modeling
COST ACTION CA21108 2022-2026

PASS Photocurable Solid-State batteries with self-healing property and smart-functionalities
HE-MSCA-PF 101153574 2025-2027

PIEZO 2D Piezoelectricity in 2D-materials: materials, modeling, and applications
HORIZON-MSCA-2022-SE 101131229 2023-2027

ROCHE Multilayer approach for solid-state batteries
H2020-MSCA-GF-2020 2022-2025

RETROTRAFO Development of knowledge and technology to implement retrofilling in power transformers using biodegradable or recycled fluids and fostering circular economy
MSCA-DN 101182948 2024-2028

SELFAQUASENS Advanced manufacturing of self-sensing bio-based membranes for environmental detoxification and revalorization
HORIZON-MSCA-2022-SE-01-01 101131379 2023-2027

TRACK THE TWIN Tracking Nanomaterial Performance, Towards Digital Twins of Quantum Dots Under Loading
MSCA-DN 101168820 2024-2028

UNICORN Hybrid Nanocomposite Scintillators for Transformational Breakthroughs in Radiation Detection and Neutrino Research
EIC PATHFINDER OPEN 101098649 2023-2027

HIGHLIGHTS: NEW EUROPEAN PROJECTS

BIONTIER

BIOntier is a project aimed at developing a new generation of multifunctional, lightweight, recyclable, and sustainable bio-based composites with advanced properties (thermal, mechanical, chemical resistance, etc.) for high-level industrial applications (TRL≥6). This project aligns with European strategic priorities (Green Deal, bioeconomy strategy) and Sustainable Development Goals (SDGs).

BIOntier focuses on innovation in the design and manufacturing of biocomposites, improving synthesis processes, recyclability, and sustainability, while creating a European innovation ecosystem. The project relies on a comprehensive industrial consortium (including Stellantis), with measurable objectives to strengthen European competitiveness, reduce environmental impact, and generate jobs and economic growth.

SELFAQUASENS

The SELFAQUASENS project proposes a technology able to eliminate heavy metals from water, recovering in parallel the valuable elements as lithium, cobalt or rare-earth elements. To this end, the project will assemble by additive manufacturing self-sensing membranes able to monitor the process during and after operation. SELFAQUASENS pursues processing bio-based and bioinspired porous materials by additive manufacturing to shape them as versatile and modular self-sensing filters and membranes able to prevent and monitor the water pollution coming from mining activities, and in parallel, to selective recover and separate CREs

TRACK THE TWIN

Track The Twin is a MSCA Doctoral Network that will train researchers at PhD level around the creation of a digital twin of colloidal quantum dots (QDs). Awarded the 2023 Noble Prize in Chemistry, QDs exemplify the successful transfer of a new nanomaterial from a lab-scale invention to a technology that offers better and more power-efficient electronic devices, or makes buildings generate renewable energy. Through the development of a QD digital twin, Track The Twin aims at creating a new generation of QDs that are resilient against loading-induced ageing and loss of performance.

PRIVATE PROJECTS

BIOSPIN Bioinspired spin-selective electrocatalysis for CO2 conversion
TOYOTA 2023-2024

DEMOSENSE Oferta de desarrollo de escalado y demostración de nuevo sistema de monitorización de husillos a bolas online en entorno real
KORTA 2024-2025

E-POLYMER Nuevos grados de abs sus copolímeros y blends termoplasticos con funcionalidades avanzadas para automocion e-mobility
ELIX POLYMERS 2020-2023

E-ONTECH Development towards to next generation lithium batteries
E-ONTECH 2022-2024

FUELIUM Ecodiseño, integración y caracterización de celdas electroquímicas
FUELIUM 2022-2024

MELEXIS Magnetic Sensor for Battery Production
MELEXIS 2024-2025

MELEXIS Verifying the feasibility of GMI sensor based on Melexis IMC soft magnetic materials
MELEXIS 2022-2024

OSASUNKO Nuevos productos de inyección con superficies con capacidad sensorial táctil
BIOLAN 2023-2025

Prótesis mamarias inteligentes.
ALLOY MEDICAL IMPLANTS SL 2023-2024

UNIKARE
UNIKARE 2024

IKUR ESTRATEGY IMPACT

IKUR is the Basque strategy promoted by the Education Department of the Basque Government to boost the Scientific Research in specific strategical areas and to position them at international level. BCMaterials is strongly aligned with and committed to contribute to the success of this importat strategic endeavour, which in turn has been also very positive for our development. Further, the IKUR strategy has been not just a platform for scientific and technological excellence, but also for fruitful collaborations and the formation of new generation of excellent scientists.

BCMaterials contributions

1. Neurobioscience

Within this area, BCMaterials has been focussing on the development of biomimetic active microenviroments based on multifunctional materials. In particular, electroactive materials and stimuli responsive nanoparticles for neural tissue engineering have been developed, together with novel concepts for organ-on-a-chip systems.

2. Quantum Technologies

In this area, BCMaterials has worked in the development of molecular materials as relevant players in quantum technologies, as well as in exploring the potential of artificial spin-ice systems.

3. Neutrionics

The strong committment of BCMaterials in the use of neutron sciences for the development of next generation materials has been reflected in the extensive use of neutron science in all our areas of activities, ranging from the study of advanced materials for energy storage systems to improving the understanding of protein-electroactive scaffolds interactions, or from the design, development and characterization of a large variety of multifunctional materials to the evaluation of their implementation into applications. Neutron experiments have been carried out in leading facilities around the world in excellent national and international collaborations.

4. High performance computing and artificial intelligence

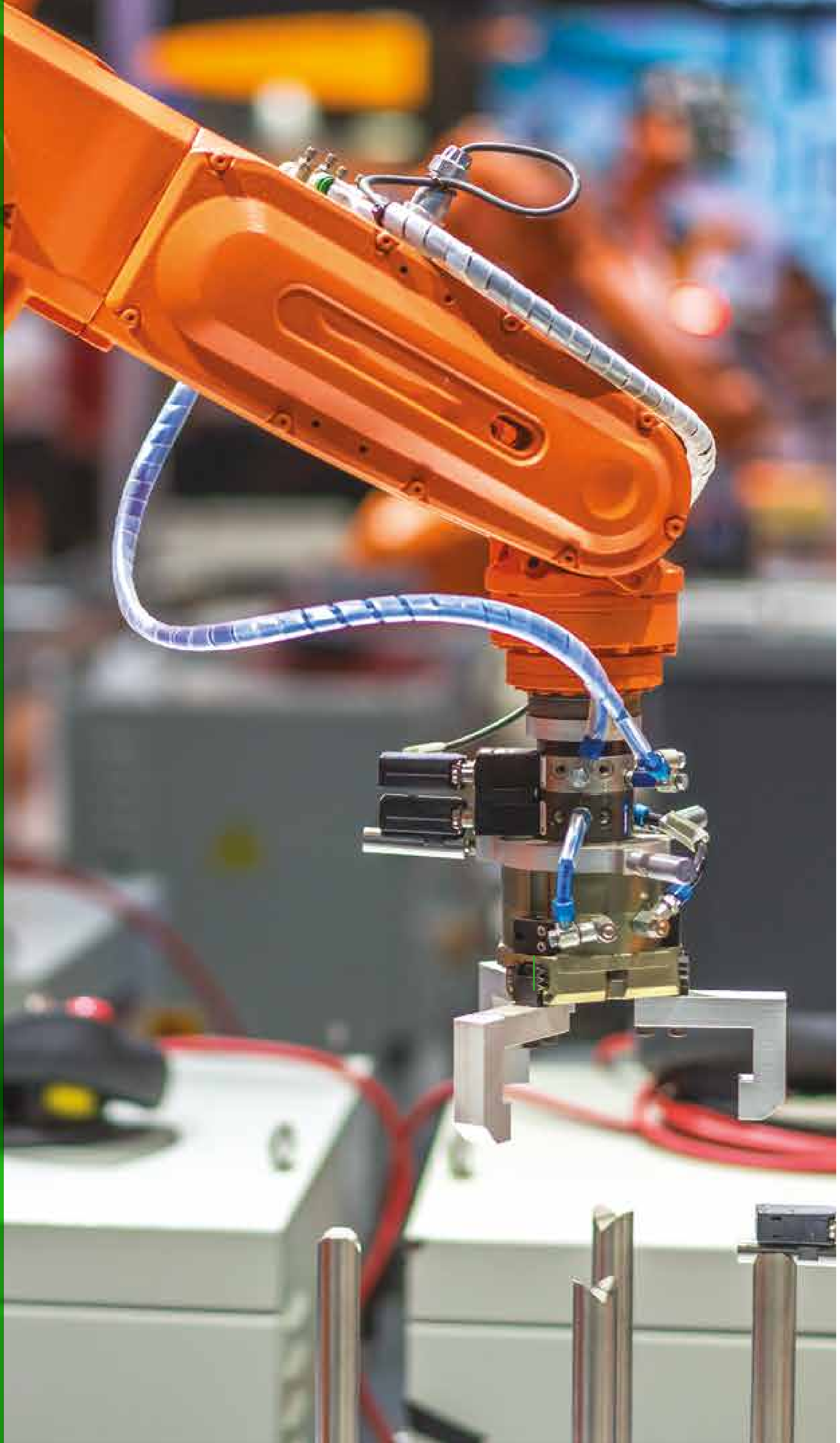
High performance computational materials science and artificial intelligence/machine learning approaches has been extensively implemented for the design of functional and stimuli-responsive materials and for their implementation into specific applications, including energy, sensing, environmental and biomedical areas.

PATENT

TACTILE ACTUATOR FOR ROBOT ARMS

BCMaterials obtained in 2024, together with Gaiker technology center, a patent for a tactile actuator for robot arms, comprising: a deformable gripper adapted for its attachment to a robot arm, wherein the gripper is configured to adopt a contracted position for holding an object and an extended position for releasing the object, and at least one force and/or deformation sensor made of a piezoresistive material.

Name of the Patent:
Tactile Actuator for Robot Arms
Reference:
EP 4 393 659 A1
Authors:
José Ramón Dios
Juan Carlos Manchado
Senentxu Lanceros-Méndez
Carmen Rial
Nikola Perinka
Nelson Castro



BCMATERIALS CONTRIBUTION

We have developed the piezoresistive material for the high-sensitivity touch sensor. For its part, Gaiker has integrated the material into the gripper of the robotic arm.

HOW DOES IT WORK?

The force and/or deformation sensor is attached to a part of the gripper, such that the force and/or deformation sensor is deformable by deformation of that part of the gripper when it adopts the contracted configuration or when it transitions to that configuration.

APPLICATIONS

The tactile actuator is capable of grasping an object in any position, and having manipulation capability with high precision in controlling the gripping force of the object.

04

FACILITIES & SERVICES

As a research center of excellence, BCMaterials runs advanced infrastructures for materials synthesis, processing, characterization and integration into proof-of-concepts devices. Those facilities are open to all our collaborators and services are also provided whenever we can be useful to the scientific, technological or industrial sectors.

OUR LABS

LABS SERVING RESEARCH AREAS

- BIOMATERIALS & BIOMEDICINE
- ENVIRONMENTAL MATERIALS & PROCESSES
- ADVANCED MATERIALS & THIN FILMS
- MATERIALS FOR ENERGY
- ADDITIVE MANUFACTURING

LABS SERVING RESEARCH TECHNIQUES

- MULTIFUNCTIONAL NANOCHEMISTRY
- MULTIFUNCTIONAL MATERIALS SYNTHESIS
- ELECTRICITY & ELECTRONICS
- METALLURGY & CERAMICS
- OPTICS & OPTOELECTRONICS

MATERIALS **SYNTHESIS**

Synthesis of advanced and multifunctional materials is one of the cornerstones of materials innovations. State of the art facilities for chemical and physical synthesis of materials are available at different laboratories of BCMaterials. We design, synthesize and modify organic and inorganic, crystalline and amorphous materials. Mesoporous materials, nanoparticles, metallic, ceramic and polymer materials are synthesized with tailormade properties and functionalities.

Methods available

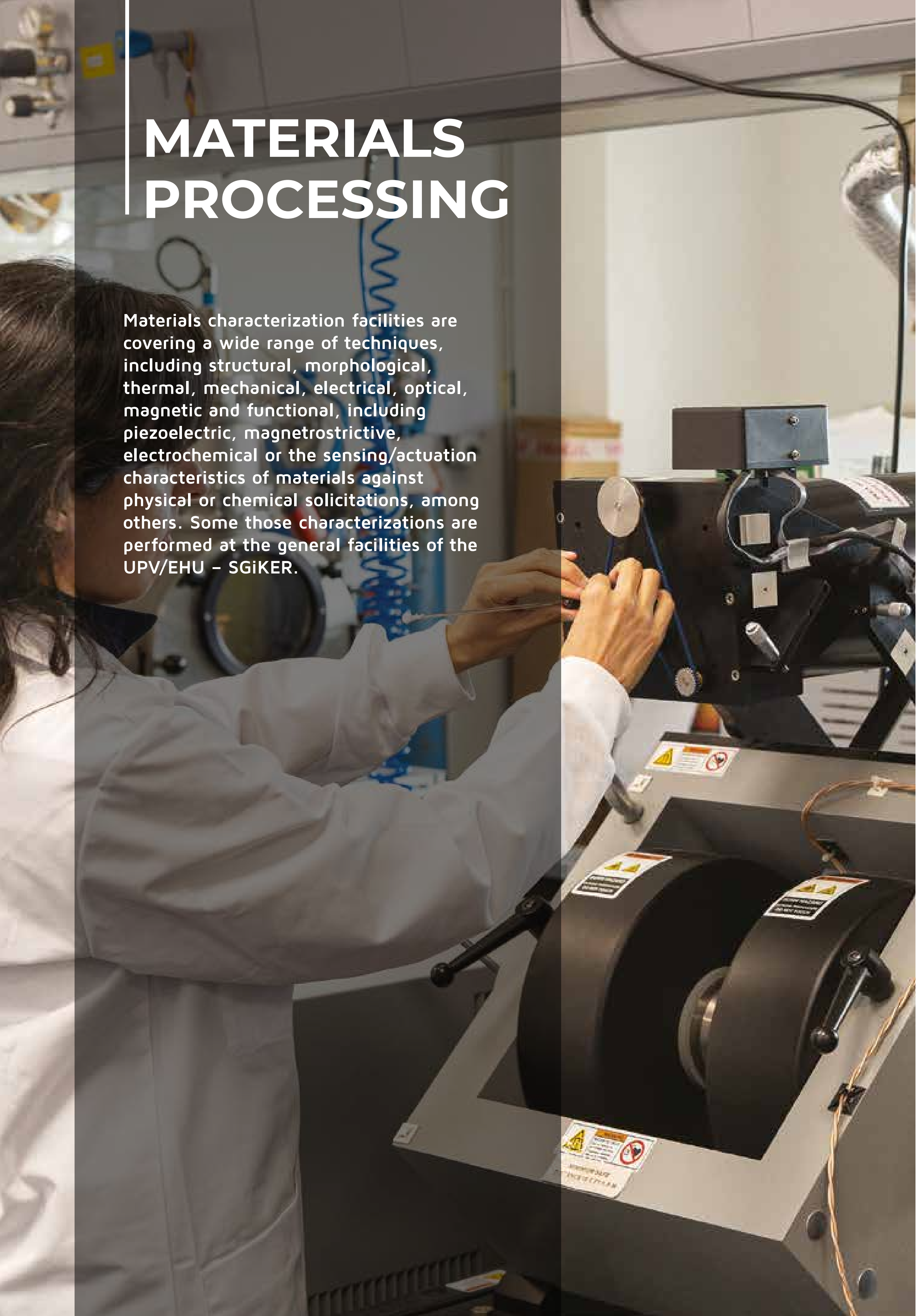
Among many others, our labs offer the possibility to use:

- Hydrothermal synthesis of wide scope of inorganic and hybrid materials and nanoparticles.
- Synthesis of mesoporous materials.
- Synthesis of monocrystalline and amorphous metals, and ceramics. It includes both Synthesis and thermal treatments.
- Synthesis of polymers and hydrogels.
- Floating Zone Optical Furnace.
- Crystal System Corp./ FZ-T-P1200-H-I-S 2013.
- Anton Parr Monowave 400 equipped with autosampler MAS24: High throughput synthesis of nanoparticles.
- Sigma 3-30KS: Centrifuge for isolation of nanoparticles.
- Büchi C-850 FlashPrep: Purification of small molecules.
- Büchi Rotavapor R-300: Distillation of solvents.

Some of our **services**

We provide advice and support for the design and synthesis of materials with tailor made properties for specific applications including:

- Tailored physical properties: magnetic, electrical, mechanical or thermal, among others.
- Functional properties: photocatalytic, piezoelectric, magnetostrictive, magnetocaloric, among others.
- Advanced properties: self-healing, electrochromic, thermochromic, among others.



MATERIALS PROCESSING

Materials characterization facilities are covering a wide range of techniques, including structural, morphological, thermal, mechanical, electrical, optical, magnetic and functional, including piezoelectric, magnetrostrictive, electrochemical or the sensing/actuation characteristics of materials against physical or chemical solicitations, among others. Some those characterizations are performed at the general facilities of the UPV/EHU – SGiKER.

Methods available

Among many others, our labs offer the possibility to use:

- Design and processing of composite polymer-filler materials.
- Design and processing of inks for screen, ink-jet and direct write printing.
- Processing of thin films by physical and chemical deposition techniques.
- Processing of materials in the form of filament, wires and films.
- Processing of materials in the form of nano- and micro particles.
- Mill Mini Rotary Tube Furnace.
- Melt Spinner.
- Plasma portable system for processing substrates and thin films.
- Turbomolecular pumped coater.
- A variety of printing and coating techniques.
- Thermal evaporator.

Some of our **services**

We provide advice and support for the design and processing of materials with tailor made properties for specific applications including:

- Tailored physical properties: magnetic, electrical, mechanical or thermal, among others.
- Functional properties: photocatalytic, piezoelectric, magnetostrictive, magnetocaloric, among others.
- Advanced properties: self-healing, electrochromic, thermochormic, among others.
- Plasma cleaning processes and activation (functionalization) of surfaces.

MATERIALS CHARACTERIZATION

Materials are processed in a variety of shapes and forms either to explore their intrinsic properties, to tune them and/or to make them compatible with a variety of applications.
From bulk materials to thin-films, from single phase to hybrid materials and composites, materials are processed in our laboratories.

Methods available

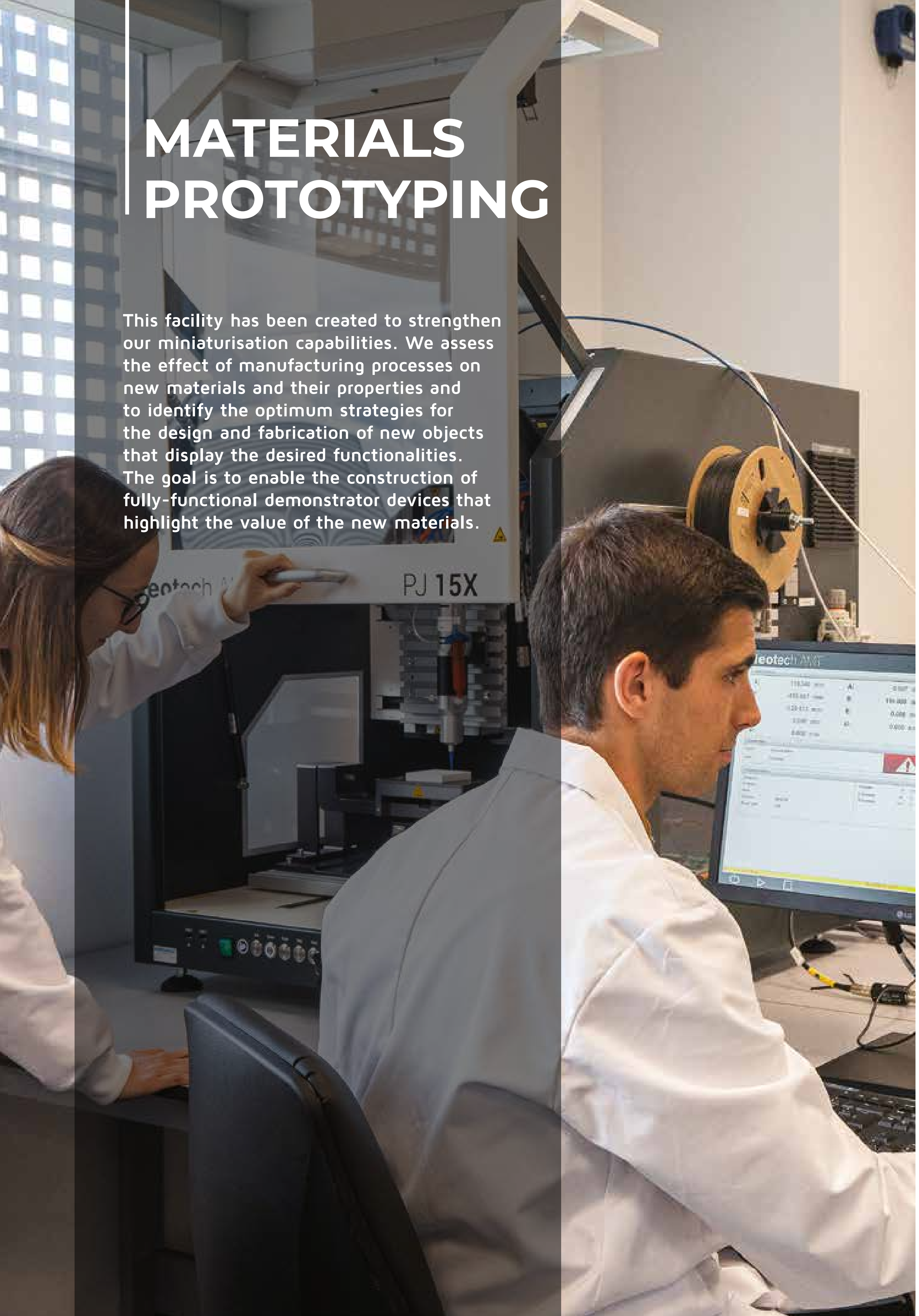
Among many other, our labs offer the possibility to use:

- AttoDRY800 optical cryostat. Temperature control of samples in vacuum between 4 and 300 K (-270 and 27°C).
- Spectrograph + CCD Camera
  High resolution optical spectroscopy in the visible range.
- Gas and vapor adsorption analyser: 3P vapor 100C station is adapted to acquire vapor and gas adsorption isotherms in the micro to mesopore range. Measuring and analysis of the adsorption and porous properties of porous materials as zeolites, activated carbons, MOF and COFs, or porous polymeric or composite systems.
- Fluorescence microscope. Live imaging of cells on flat materials.
- X-Ray Diffractometer. Empyrean 810-02997231. Measuring of different kinds of samples: powders, thin films, nanomaterials, solid objects at different temperatures, inert atmosphere...
- Atomic Force Microscope (AFM). NX10 ES10005-291122. Nanoscale imaging for a wide range of applications: cell biology, analytical chemistry, electrophysiology, neuroscience...
- VSM-Vibrating Sample Magnetometer. Microsense, LLC EZ7-20150305 MicroSense. To measure magnetic moment and coercivity of thin films or studying the magnetic properties of liquids, powders, or bulk samples.
- Perkin Elmer- Diamond DSC N536-0021 (P/N) Melting, Crystallization, Glass Transition, Polymorphism, Purity, Specific Heat, Kinetic Study and Curing Reaction.
- The Ossila Contact Angle Goniometer provides a fast, reliable, and easy method to measure contact angles and surface tensions of liquid droplets.
- Tensile strength tester Shimadzu Instruments AGS-J 500N. High precision and high reliability in material testing Forces are measured with a precision better than ±1% of indicated values, within the range from 1/1 to 1/250 of the rated force.
- Complex impedance equipment Agilent-Keysight E4980. Offering fast measurement speed and outstanding performance at both low and high impedance ranges.
- Custom made photothermal instrument equipped with high power red and near-IR lasers (LUMICS, 672, 784 and 808 nm of 4W of optical power), optical coupling lenses, thermometer based on phototherrmal IR camera (FLIR), thermal based power sensor, and control software.
- The VMP3 is a research-grade multi-channel potentiostat. With its modular chassis design, up to 16 independent potentiostat channels can be installed. The VMP3 can be equipped with additional capabilities, including low current measurement, impedance and high current via plug-in modules.
- Custom made Magnetoelastic measurement system: Automated experimental system for measuring magnetoelastic resonance from 10Hz up to 150 MHz and a field resolution of 8 A/m and maximum magnetic field of 11 kA/m.

Some of our **services**

We provide advice and support for the characterization of a wide variety of materials properties, including the interpretation of the results and the possible ways to tune/modify those properties. Those characterizations include:

- Structural, morphological, thermal, mechanical, electrical, optical, magnetic, among others.
- Functional, including piezoelectric, magnetrostrictive, electrochemical, among others.



MATERIALS PROTOTYPING

This facility has been created to strengthen our miniaturisation capabilities. We assess the effect of manufacturing processes on new materials and their properties and to identify the optimum strategies for the design and fabrication of new objects that display the desired functionalities. The goal is to enable the construction of fully-functional demonstrator devices that highlight the value of the new materials.

Methods available

Among many others the methods available are:

3D printing (DLP and FDM), CNC milling (Roland MODELA MDX-50), CO2 laser cutting and engraving (Epilog Mini 18 CO2 laser engraver), blade cutting (Roland GS-24 CAMM-1) and thermoforming with suitable CAD/CAM software.

TECAPRIT-TPE100 with open inking system, semi-automatic pad printer for prototyping and manufacturing of microstructures.

Any combination of processes is possible, including with printing methods such as screen-printing and inkjet-printing.

Some of our **services**

Among the services that we can offer we have:

- 3D printing of thermoplastic polymers and functional polymer thermoplastic composites by FDM/FFF.
- 3D printing of functional water- and solvent-based inks by direct ink writing.
- 3D printing of functional UV curable resins by selective laser sintering (SLS).
- 2D printing of functional inks by screen printing and inkjet printing.

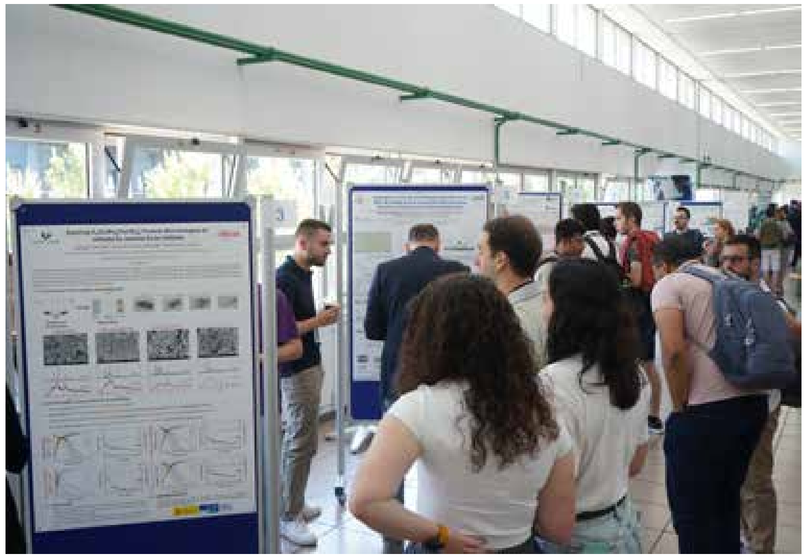
OUTREACH ACTIVITIES

Outreach activities are divided between the dissemination events we do for scientists to show them our progress (or events in which we receive knowledge from them) and the outreach activities in which we take part to make society part of our research. Regardless the public target we address, outreach and dissemination are key in the activities and working philosophy of BCMaterials.

GERSEQ44 + 5 E3MS

ELECTROCHEMISTRY CONFERENCE

> This conference has been the biggest event organized by BCMaterials to date



210 ATTENDEES

115 ORAL PRESENTATIONS

5 PARALLEL SESSIONS

83 POSTERS PRESENTED

8 THEMATIC AREAS

From July 3 to 5, more than 200 international specialists in electrochemistry gathered at the 44th Meeting of the Specialized Group in Electrochemistry of the Royal Spanish Society of Chemistry (RSEQ). BCMaterials and the Faculty of Science and Technology of the University of the Basque Country (UPV/EHU) co-organized the conference under the acronym GERSEQ44.

The event, the biggest organized by BCMaterials to date, hosted more than 100 oral presentations (in up to 5 parallel sessions) and more than 80 posters.

The program was an update on the latest advances in areas such as materials electrochemistry, electroanalysis, molecular and fundamental electrochemistry, bioelectrochemistry, and electrochemical process technology and engineering.

Two of the main topics of the contributions were energy generation and storage and environmental electrochemistry, areas included in the 5th E3 Mediterranean Symposium (5 E3MS), a biennial event that this year was held within GERSEQ44.

The Symposium, which attracted a good number of scientists from Italy, brought extra internationality to the congress.

Besides the very positive reception from the attendees, the event brought BCMaterials the opportunity to showcase our important work in Electrochemistry. For example, in fields such as the miniaturization of electrochemical sensors for healthcare uses, environmental monitoring, etc.

Thanks to GERSEQ44, the center has established new and important collaborations in the field of Electrochemistry.

> The Faculty of Science and Technology of the UPV/EHU offered an invaluable collaboration and a magnificent venue for the event

The Faculty of Science and Technology of the UPV/EHU was the main venue of the GERSEQ44+ 5 E3MS conference, with 4 rooms for parallel sessions. BCMaterials facilities also served as a conference spaces, as it happend with the Electrobionets Excellence Network symposium’s presentations.

In addition to the extensive scientific program, the conference also offered contact with scientific industry companies willing to showcase their lab equipment to the conference attendees.
Up to 6 companies took part sharing spaces with the posters and lunch area at the Faculty’s Grande Salle.

GERSEQ44 + 5 E3MS

PHOTO GALLERY

The Specialized Group in Electrochemistry of the Royal Spanish Society of Chemistry awarded young sciesntists through the ‘Jóvenes Talentos (‘Young Talents’) prize, as well as with the ‘Antonio Aldaz’ award. There were also three awards for the best poster presentations at the conference.

ORGANISERS

SPONSORS

GERSEQ 44

44th Annual Meeting of
the RSEQ Specialized Group
in Electrochemistry +
5th E3 Mediterranean Symposium

JULY, 3-5 2024
LEIOA (BILBAO-BIZKAIA)
UPV/EHU CAMPUS

CONFERENCE PROGRAM

44gerseq2024.com

IMOH 2024

2ND INTERNATIONAL MEETING

From 15 to 17 October, the BCMaterials headquarters hosted the second edition of the 'IMOH 2024, 2nd International Meeting on Challenges and Opportunities for HiCANS' congress, dedicated to neutron science and industry. More than 80 scientists from Europe, America and Asia examined the evolution of projects and ideas for the construction of HiCANS (High Current Accelerator-driven Neutron Sources).

These medium-sized facilities could be a complement to classic neutron sources, such as spallation sources or nuclear reactors, offering a more economical and accessible option for scientific experiments.

BCMaterials, ESS Bilbao, CFM/MPC and Ineustar were the organisers of this second edition. The success of the first event, held in 2022, made it necessary to monitor the evolution of this technology, which includes projects such as 'Argitu', from ESS Bilbao, to build a HiCANS in the Basque Country.

The program was divided in three parts, one for each day of the conference. The first day was devoted to the state of the art of the HiCANs projects around the world. The second one focused on neutron science techniques and developments, and the final day explored the industrial opportunities of these facilities.

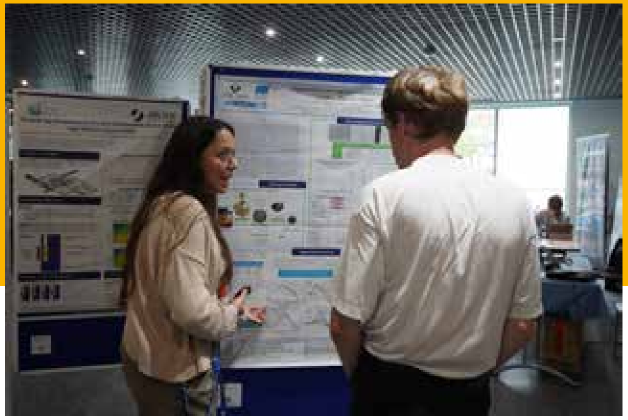
81
ATTENDEES

10
COUNTRIES

11
PLENARY & INVIT. SPEAKERS

22
ORAL PRESENTATIONS

22
POSTERS



IMOH24

2nd INTERNATIONAL MEETING ON CHALLENGES AND OPPORTUNITIES FOR HICANS

A look into the revolution of new compact accelerator-based neutron sources

NM4BL 2024

ANNUAL WORKSHOP

NM4BL.ORG

NEW MATERIALS FOR A BETTER LIFE! WORKSHOP

2024

Materializing the future:
Fostering social and economic impact of basic science on advanced materials

LEIOA. NOV, 27 2024
MARTINA CASIANO AUDITORIUM

TOPICS

- GENERAL FRAMEWORK FOR INNOVATION ON MATERIALS SCIENCE AND TECHNOLOGY
- TOOLS FOR TECH TRANSFER
- SUCCESS STORIES

To close a year plenty of scientific meetings organized by BCMaterials, the center held its annual workshop, New Materials for a Better Life! in November, 27. Around 100 attendees met at a new edition of workshop, this time focused on technological transfer and innovation applied to advanced materials. The program brought together leading experts in the field, from institutions responsible for developing policies (at European, national and Basque level), to companies, research centers and entrepreneurs who presented their success stories. All of this without forgetting, of course, the agents and entities responsible for providing the tools to facilitate said technological transfer.

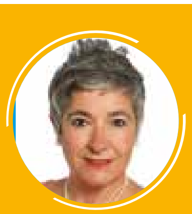
The 2024 workshop was a magnificent opportunity for researchers of all career stages to notice about how important are innovation and technology transfer for basic science to keep being significant and to contribute to the revolution of the digital era and its challenges.

SPEAKERS PANEL

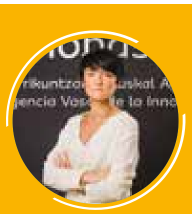
Senentzu Lanceros-Méndez
BCMaterials

Amaia Esquisabel
Basque Government

María José Tomás
CDTI



Amaya Igartua
Tekniker



Alaitz Landaluze
Innobasque

Naogre Tellado
UPV/EHU

Amaia Martínez
SPRI

Susana Barasoain
Functional Print Cluster

Rikardo Bueno
BRTA

Raquel Ubarrechena
Basque Country Tech. Park

Beatriz Alonso
Graphenea

Juan Pablo Esquivel
BCMaterials

Larraitz Añorga
Biolan

Óscar Castillo
UPV/EHU

Jesús Marcos
Lanzo Batteries

SEMINARS & INVITED TALKS

BCMaterials continued its work of organizing seminars and invited talks. The aim is to enrich the vision of its researchers about different disciplines of study of materials science and also to provide them with non-strictly scientific tools for the best development of their research career.

The fortnightly seminars continue to be important events for BCMaterials scientists to present their progress to their colleagues at the centre. And in the case of pre-doctoral researchers, they are also a powerful tool to strengthen their public presentation skills.

Invited talks wiith Marco Sangermano, from Politecnico Torino (Italy), and Sang Young Lee, from Yonsei University (South Korea)

Fortnightly seminar with BCMaterials post-doctoral researcher Anna Sinelshchikova

ISIS- BCMaterials Workshop

On February 7 and 8, we organized the workshop 'Opportunities to build collaborations and impactful science' in collaboration with ISIS Neutron and Muon Source from the United Kingdom. The event aimed to present the different research areas, capabilities and facilities of both centers in order to strengthen cooperation between them. The workshop consisted of 12 talks presented by scientists from ISIS and BCMaterials, a poster session, a visit to the BCMaterials facilities and a session of conclusions and future opportunities.

Presentation of the "2024 Innobasque Foresight Report. Innovation Trends", by the Basque Agency for Innovation - Innobasque.

31
EVENTS

12
FORTNIGHTLY SMINARS

16
INVITED TALKS

3
OTHER EVENTS

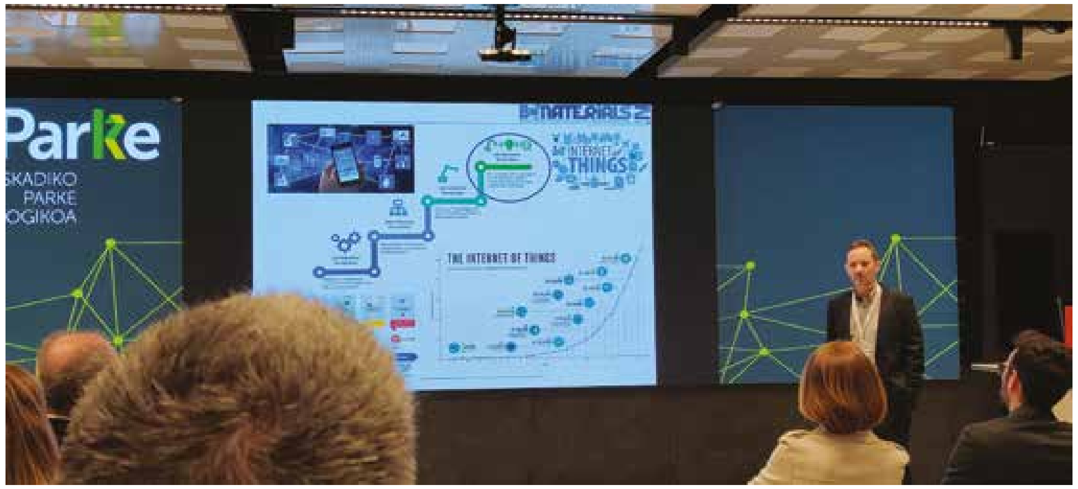
OUT
BCMATERIALS

EXTERNAL
DISSEMINATION

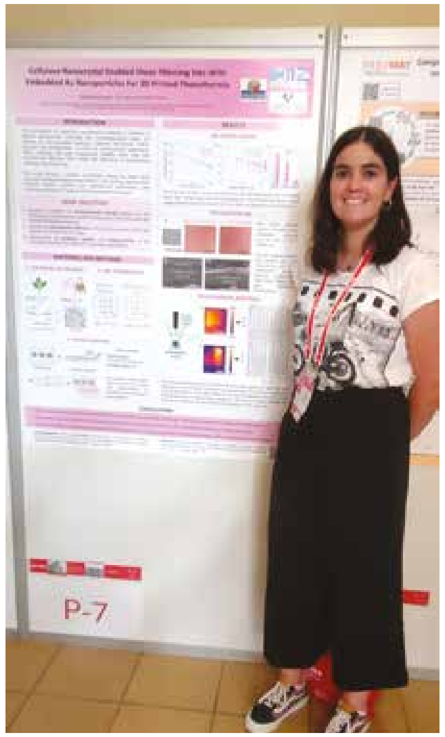
51
INVITED TALKS

104
ORAL PRESENTATIONS

44
POSTER CONTRIBUTIONS

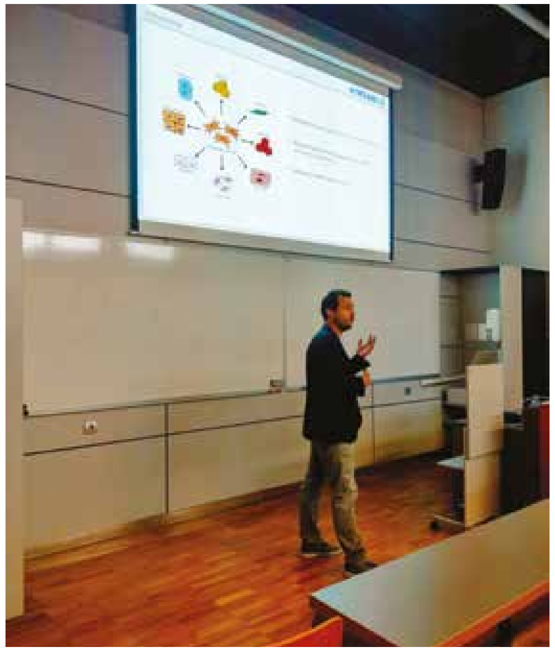


Senentxu Lanceros-Méndez, presentation on the 'Opportunities for Science and Industry' event organized by Ineustar.(Bilbao. February 2024)



José María Porro's invited talk at the University of Boise (Idaho, USA. March, 2024) and porter presentation by Marta García at GEP SLAP Conference (Madrid, Spain. September 2024)

Maibelín Rosales oral presentation at the XXIX Congreso Iberoamericano de Catálisis ç (Bilbao September, 2024)



Invited talk by Unai Silván at the Faculty of Chemistry and Chemical Technology of University of Ljubljana, Slovenia (May, 2024)

Manuel Salado at the Forum on Materials Design and Structural Analysis of Advanced Functional Materials. Wuhan University of Technology (Wuhan, China. November, 2024)

Vera Macedo at the 'Batteries Event International. Energy & power supply Conference and Exhibition (Lyon, Fance. October 2024)

SCIENCE FOR SOCIETY

In addition to the dissemination work focused in the science sphere, there is a huge work we do to address the general public through different outreach initatives carried out by BCMaterials or organized by third parties in which we take part. This is our resposibility to make our research understandable by society. We need that people see that the work we do has a possitive impact in their daily lives. At the same time, we want to encourage the younger generations to devote to science and technology, because everyone's efforts will be necessary to address the challenges our planet is facing for the present and the near future.

SCIENCE
FOR SOCIETY

M4S
MATERIALS FOR SOCIETY
A SCIENTIFIC, CULTURAL & SOCIAL INITIATIVE BY BCMATERIALS

In October 2024, BCMaterials laid the first stone of the 'Materials for Society' initiative. This scientific, cultural and social project aims to explore the involvement of science with the most diverse aspects of society.

The first event, the first stone of 'Materials for Society', took place with the talk/colloquium ''La Física y las palabras, las dos pasiones de José María San Juan', held in the auditorium of the Martina Casiano building, headquarters of BCMaterials.

In this meeting we discovered how the Professor of Physics at the UPV/EHU José María San Juan took a leap of faith by turning his love of reading into the dream of writing and publishing his first novel: 'El Círculo Milenario' (2020). This title has already become a historical fiction saga set in medieval Europe that will see its third volume published in 2026.

The talk outlined the steps and challenges that José María San Juan has gone through in the last 20 years to shape the saga 'El Circulo Milenario', from the first sketches of the story, through his writing methods and habits to the process of editing and publishing his work.

Materials for Society will continue developing in the coming years with new events and talks with scientists, philosophers, artists to keep exploring the thin frontiers between science, culture and society.

M4S
MATERIALS FOR SOCIETY
A SCIENTIFIC, CULTURAL & SOCIAL INITIATIVE BY BCMATERIALS

BCMATERIALS

CHARLA/COLOQUIO

La Física y las palabras, las dos pasiones de José María San Juan

8 OCTUBRE
(MARTES)

11:00

AUDITORIO
EDIF. MARTINA CASIANO
CAMPUS UPV/EHU LEIOA

Watch M4S online!

You can watch the first event of 'Materials for Society' with José María San Juan at BCMaterials Youtube Channel.

SCIENCE
FOR SOCIETY

BCMaterials did not miss its traditional appointment with the **UPV/EHU SCIENCE WEEK**, which takes place annually in November. For five days at the Bizkaia Aretoa in Bilbao, it showed the public of all ages the work carried out at the centre. Hundreds of people experimented with us and interacted with demonstrators for water cleaning with MOFs, the elimination of contaminants through photocatalysis, the creation of materials that help bone regeneration… More than 20 scientists of BCMaterials volunteered at this activity as a demonstration of our commitment with outreach events.

Another event marked in red on our agenda for scientific dissemination is the **EUROPEAN RESEARCHERS' NIGHT**, organized by the UPV/EHU. This event takes place on the last Friday of September. From our stand located in Bilbao downtown, we demonstrated how the science of new materials can help decontaminate the aquatic environment, create increasingly precise sensors and actuators and improve the treatment of certain diseases such as bone cancer.

SCIENCE
FOR SOCIETY

The **ZIENTZIA AZOKA** (Science Fair), organised annually by Elhuyar Fundazioa, is one of the major STEAM education events held in the Basque Country. BCMaterials collaborates with the event by evaluating the scientific and technological projects presented by secondary school students, which are exhibited in June in the centre of Bilbao. At the end of the Zientzia Azoka, our centre welcomed some of the award-winning groups in the competition, showing them part of the work we do in materials science. In 2024, we welcome students from the Bihotz Gaztea ikastola and the Etxebarri Institute.

Daniel Bacigalupe,
Carmen Rial y Javier Vicente
BC Materials

Técnicas de impresión 3D

In January we participated for the first time in the **FIRST LEGO LEAGUE EUSKADI**. This event, organised by the Basque Innovation Agency - Innobasque, brings together hundreds of Basque students who compete to present the best scientific and technological projects. At BCMaterials we collaborated with this initiative by offering a training session for these students based on the possibilities of 3D printing to create functional materials. In addition, we were present with a scientific outreach stand at the final of the First Lego League Euskadi, which took place in Vitoria-Gasteiz.

SCIENCE
FOR SOCIETY

MEET THE **BCMATERIALS**

WOMEN IN SCIENCE

ON OUR YOUTUBE CHANNEL

BCMaterials entered the organizing commitee of the Emakumeak Zientzian (Women in Sience) initiative and organized school visits during the Women and Girls in Science Week.

2024 was a particularly busy year in terms of outreach activities to promote women in science, organised by BCMaterials and/or with the participation of our centre. Special mention should be made of the participation within the framework of the Emakumeak Zientzian initiative, in which around thirty Basque academic and research institutions programme activities on the occasion of the Week of Women and Girls in Science, around 11 February. BCMaterials had already joined the Emakumeak Zientzian organising committee in 2023 and made a very important contribution to the programme of activities. Firstly, it organised visits by secondary education centres to its facilities on 14 and 15 February, which included workshops and a tour of the laboratories. A dozen BCMaterials researchers participated in them. These visits were supplemented by the participation of BCMaterials researchers Itziar Oyarzabal and Mariana Ríos in the series of talks ‘Emakume Zientzilariak Atzo eta Gaur’, in Vitoria-Gasteiz and Bilbao on 15 and 16 March, and by Mariana Ríos herself in the programme ‘Eskolara Itzulera’, in which she visited students at the Lea Artibai institute in Markina in March.

Itziar Oyarzabal and Mariana Ríos were speakers at the ‘Emakume Zientzilariak. Atzo eta Gaur.(Women in Science. Now and then)’ talks program. Ríos also took part in the school visits program ‘Eskolara Itzulera (Back to School)

SCIENCE **FOR SOCIETY**

For the second consecutive year, BCMaterials was part of the coordination team for the series of scientific outreach talks **PINT OF SCIENCE BILBAO.** The Pint of Science festival takes place simultaneously in hundreds of cities in more than 500 cities in 27 countries. From May 13 to 15, 2024, 4 bars in Bilbao hosted 24 talks on topics as varied as neuroscience, artificial intelligence, the relationship between mathematics and literature and, of course, materials science. On behalf of BCMaterials, Sergio Lucarini, Ikerbasque Research Fellow, and Aritz Villar, postdoctoral researcher, participated as speakers in the talks.

SCHOOL **VISITS**

As a center open to scientific dissemination, BCMaterials regularly receives **VISITS FROM SCHOOLS AND HIGH SCHOOLS**. During these visits, students, mainly from Secondary and High School, learn first-hand about the work carried out on a daily basis by our scientists. To do so, in addition to attending a brief presentation on what BCMaterials is and what it does, they participate in simple experiments and visit our laboratories. In 2024, more than 100 students participated in these visits.

FAMILY **OPEN DAY**

In 2024, we carried out a very successful activity for the first time: we opened the doors of BCMaterials to the families of our researchers. The goal osf this activity, called **FAMILY OPEN DAY**, was very simple: to show in a close-up way the work they do every day in new materials science. The activity, essentially aimed at children,was so much fun, so we will definitely repeat it in the future.

SCIENCE FOR SOCIETY

MEDIA IMPACT

NEWS

Tecnología

BCMaterials, a por nuevas generaciones de grafeno

Empresa XXI
GIANCE Project
April 2024

Etorkizuneko baterien bila

Berria
44GERSEQ Conference
July 2024

WWW

Proyecto PReBIO2: Innovación para el desarrollo de bioplásticos sostenibles

Estrategia Empresarial
PReBIO2 Project
April 2024

mapping ignorance

Fit-to-purpose power sources: portable batteries ecodesigned within the planetary boundaries

Mapping Ignorance
February 2024

Daniel Bacigalupe
Onda Cero Gipuzkoa
Feb 2024

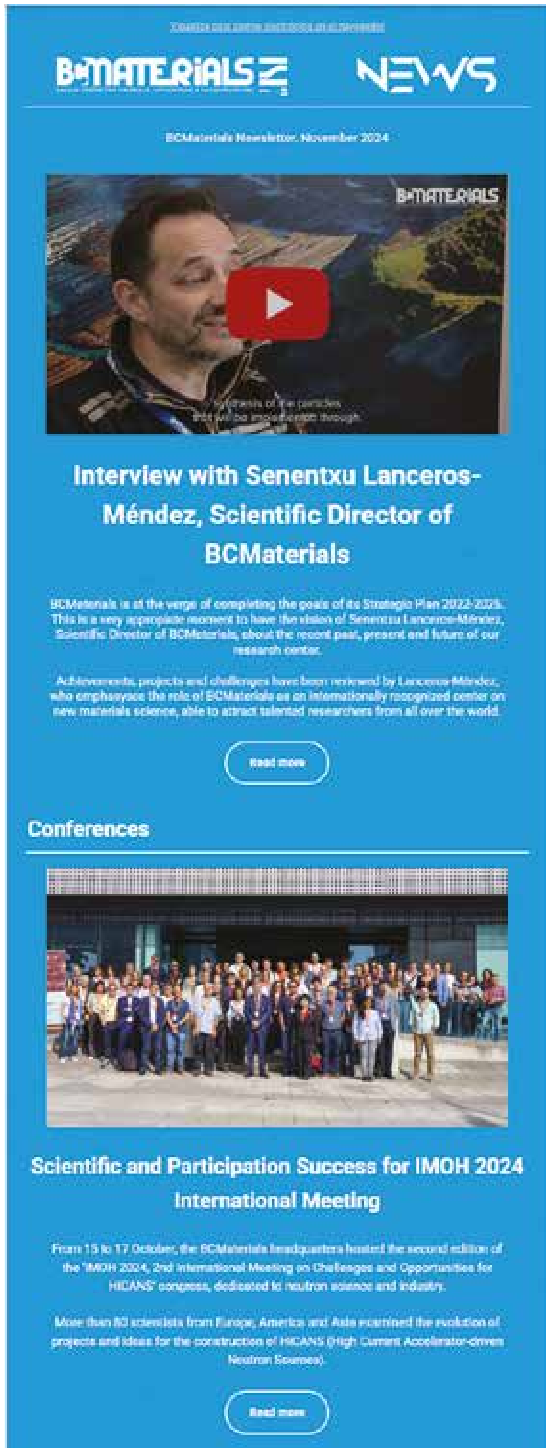
Daniel Bacigalupe
Radio Popular Bilbao
Mayo 2024

Javier del Campo
Radio Euskadi
Julio 2024

Unai Silván
Radio Euskadi
Julio 2024

Maibelín Rosales
Radio Exterior de España (RNE)
September 2024

OUR MEDIA



BCMaterials Newsletter. November 2024

Interview with Senentxu Lanceros-Méndez, Scientific Director of BCMaterials

BCMaterials is at the verge of completing the goals of its Strategic Plan 2022-2025. This is a very appropriate moment to have the vision of Senentxu Lanceros-Méndez, Scientific Director of BCMaterials, about the recent past, present and future of our research center.

Achievements, projects and challenges have been reviewed by Lanceros-Méndez, who emphasizes the role of BCMaterials as an internationally recognized center on new materials science, able to attract talented researchers from all over the world.

Read more

Conferences

Scientific and Participation Success for IMOH 2024 International Meeting

From 15 to 17 October, the BCMaterials headquarters hosted the second edition of the "IMOH 2024, 2nd International Meeting on Challenges and Opportunities for HiCANS" congress, dedicated to neutron science and industry.

More than 80 scientists from Europe, America and Asia examined the evolution of projects and ideas for the construction of HiCANS (High Current Accelerator-driven Neutron Sources).

Read more

In November we launched our ***NEW MONTHLY NEWSLETTER****. The bulletin is aimed at all those involved and interested in the activity of BCMaterials, from the scientists who work at the centre, to the entities with which we work on research projects, and also to the institutions of the Basque science and technology network. Some of the usual sections of the newsletter are interviews, research projects, dissemination, events...*

We work on new materials for a better life!

BASQUE CENTER ON MATERIALS, APPLICATIONS AND NANOSTRUCTURES

223

116

4.860.000

www.bcmaterials.net

Metrics	Monthly average	Total 2024
Sessions	2615	31381
Users	1558	18706
Pages per session	2.7	2.7

Country	Visits	Pages/ Session
Spain	14916	2.1
India	1937	2.8
United States	864	4.6
Portugal	682	2.2
Pakistan	643	2.1
Germany	582	3.0
France	472	3.1

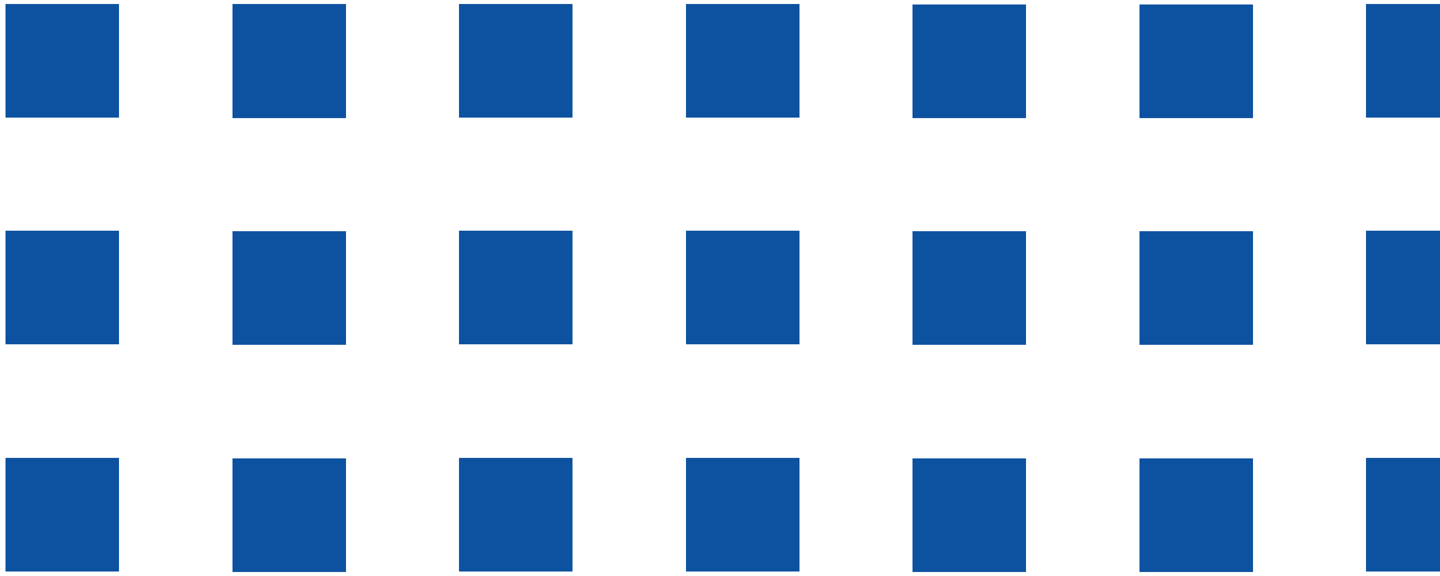
83229
PAGE VIEWS

1292
FILES DOWNLOADED

SOCIAL
MEDIA

X	1,260 followers
Facebook	227 followers
Instagram	278 followers
LinkedIn	2,319 followers
YouTube	4,000 views

NOTES



2024

BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES

www.bcmaterials.net
info@bcmaterials.net

Bld. Martina Casiano,
3rd. Floor
UPV/EHU Science Park
Barrio Sarriena s/n
48940 Leioa, Spain