BC MATERIALS

BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES

ehu group

Universidad del País Vasco
Euskal Herriko Unibertsitatea

ikerbasque
Basque Foundation for Science

EUSKO JAURLARITZA
GOBIERNO VASCO

ANNUAL REPORT

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ANNUAL REPORT

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BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES

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CONTENTS

2018-2023
THE YEARS IN WHICH **EVERYTHING CHANGED**
see final pages

WORKING TOGETHER FOR A BETTER LIFE

Senentxu Lanceros-Méndez
Scientific Director

In the following pages you will find the **scientific report** with the activities of BCMaterials in **2023**. A scientific report demonstrating the **commitment** with scientific excellence of our research center, but also compromise with technology transfer, with the formation of young scientist and with society.

Over the pages, the structure of an already **consolidated research center**, its growing laboratories and infrastructure, the research outcomes in the form of scientific highlights and technological contributions, together with the number of students that completed their formation with us and the increasing interaction with society, highlights the dynamic of a research center in which each day counts as an opportunity to develop materials and solutions "for a better life".

Particularly relevant this year has been the commitment with **international collaborations** and the large number of **international projects.** In a difficult historical moment with dramatic and unjustifiable conflicts and wars in different parts of the world, which echo directly into BCMaterials in the form of hard personal histories and experiences, the best message a research center can provide is this international sharing: living and working together to tackle the main relevant challenges of present society and world. Working together for what really matters: a "better life" everywhere, every time.

> **Things could have happened any other way, nevertheless, they happened like this.**
>
> **"The path"**
> **Miguel Delibes (1920–2010)**

This year we shared our knowhow and expertise through the first autumn course on printable functional materials and technologies (**PrintFun!**). In the year in which society strongly experienced the potential impact of the Artificial Intelligence in all aspects of our lives, the event **New Materials for a Better Life** gathered extraordinary specialists to discuss with us on the challenges and opportunities of advanced computing, artificial intelligence, and quantum technologies as essential tools to improve materials and materials related technologies. Materials aimed to provide a more sustainable, interconnected and efficient world. To contribute to novel biomedical solutions and overall life quality in our planet.

The scientific report you are about to enjoy has been possible **thanks to all BCMaterials members, colleagues and friends** contributing to each of the events and discoveries, each action, and each interaction. People that represent the true soul of BCMaterials through commitment, dedication, collaboration, and vision.

Never in history science and technology **has offered so much** to improve our daily experience and life in a better way. Astonishing, the ghost of the past still haunts us with a terrible and avoidable present in too many parts of the world.

In this context, **our best contribution** remains to continue being the unselfish and committed center working together to tackle those challenges that open the possibility of a more interconnected, sustainable, healthier and efficient world. Let´s continue working to further improve our daily activity and results, with the conviction that both, what we do and how we do it, are contributing, though advanced materials and advanced materials technologies, to a "better life".

> **Remember upon the conduct of each depends the fate of all.**
>
> **Alexander the Great**
> **(356 BC –323 BC)**

01

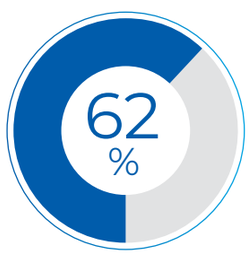
THE CENTER

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.

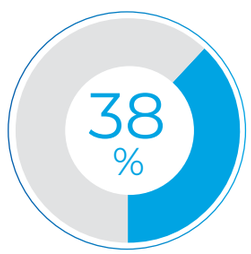
BCMATERIALS **IN NUMBERS**

RESEARCH **COMMUNITY**

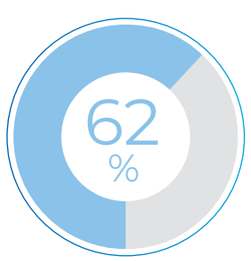
199
RESEARCHERS
Visitors included



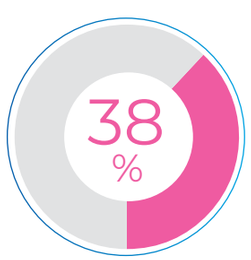
National= 124



International=75



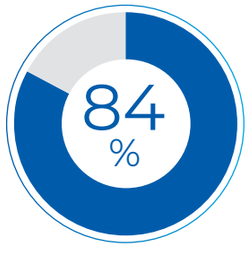
Men= 123



Women=76

RESEARCH **OUTPUT**

223
SCOPUS
Indexed Items



Q1 Publications

78
H INDEX

8299
CITATIONS

2
BOOKS

8
BOOK CHAPTERS

PROJECTS & FUNDING

65
ONGOING PROJECTS

= 4.860.000 €
FUNDING

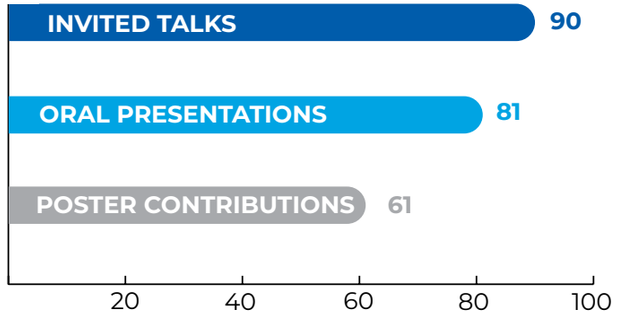
TRAINING

20
PHD
Thesis Defended

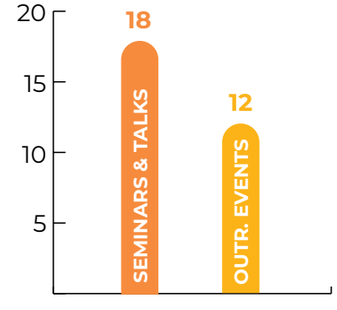
16
Master
Thesis Defended

20
Final Degree
Projects Defended

OUTREACH

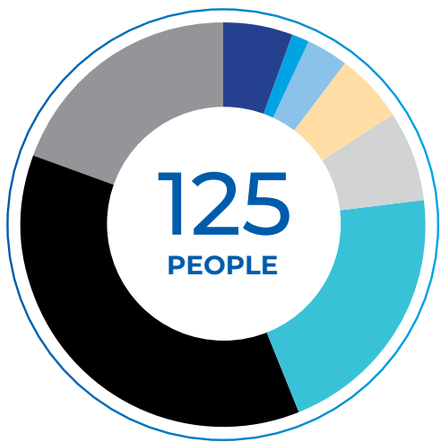


OUTSIDE BCMATERIALS

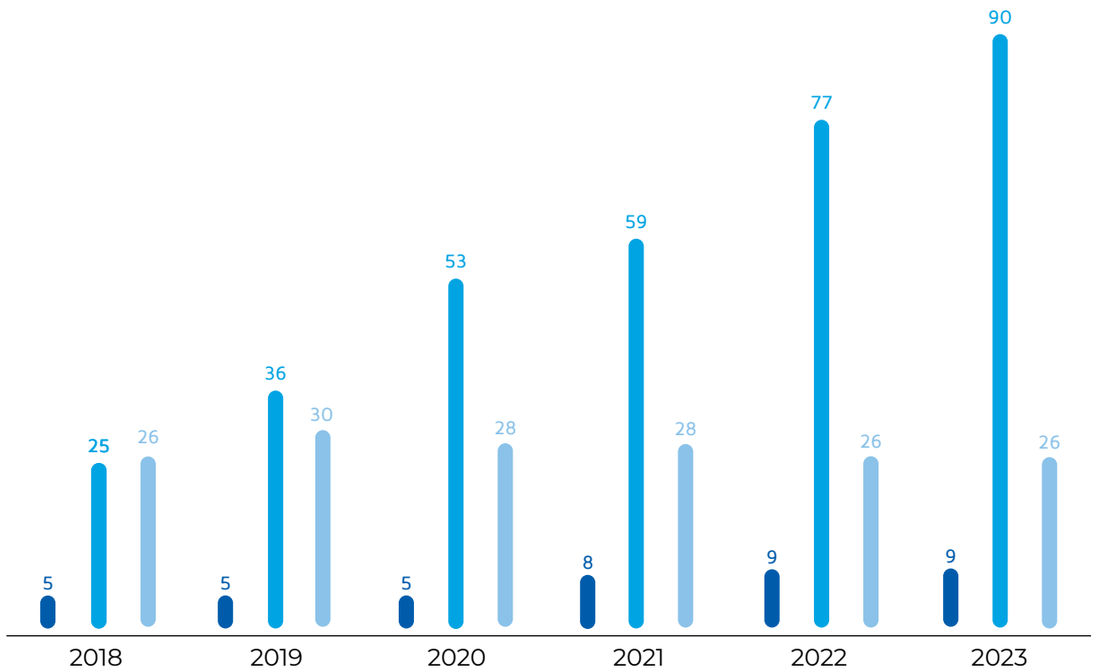


ORGANIZED BY OR WITH PARTICIPATION OF BCMATERIALS

BCMATERIALS
COMMUNITY



5.6%	Ikerbasque Research Professors
1.6%	Ikerbasque Research Associates
3.2%	Ikerbasque Research Fellows
5.6%	Research Fellows
7.2%	Administration / Services
20.8%	UPV/EHU Research Associates
36.8%	Pre-doctoral Researchers
19.2%	Post-doctoral Researchers



INTERNATIONAL REPRESENTATION

116 BCMATERIALS RESEARCHERS

83 VISITING RESEARCHERS

Argentina		4
China	2	3
Colombia	4	1
Czech Republic	1	
Egypt	1	1
France		1
Germany	2	1
Greece		1
India	5	2
Iran	1	
Italy	3	5
Morocco	1	
Pakistan	1	
Portugal	4	13
Poland		1
Russia	3	
Slovenia		1
Spain	82	42
Tunisia	1	6
Ukraine	2	1
United Kingdom	2	
United States of America	1	

RESEARCH **NETWORK**

395
COLLABORATORS

284
INTERNATIONAL

55
COLLABORATIONS
IN SPAIN

46
REGIONAL
COLLABORATIONS

32 RCVT | **7** CLUSTER | **17** 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, meant to be granted during 2023. 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.

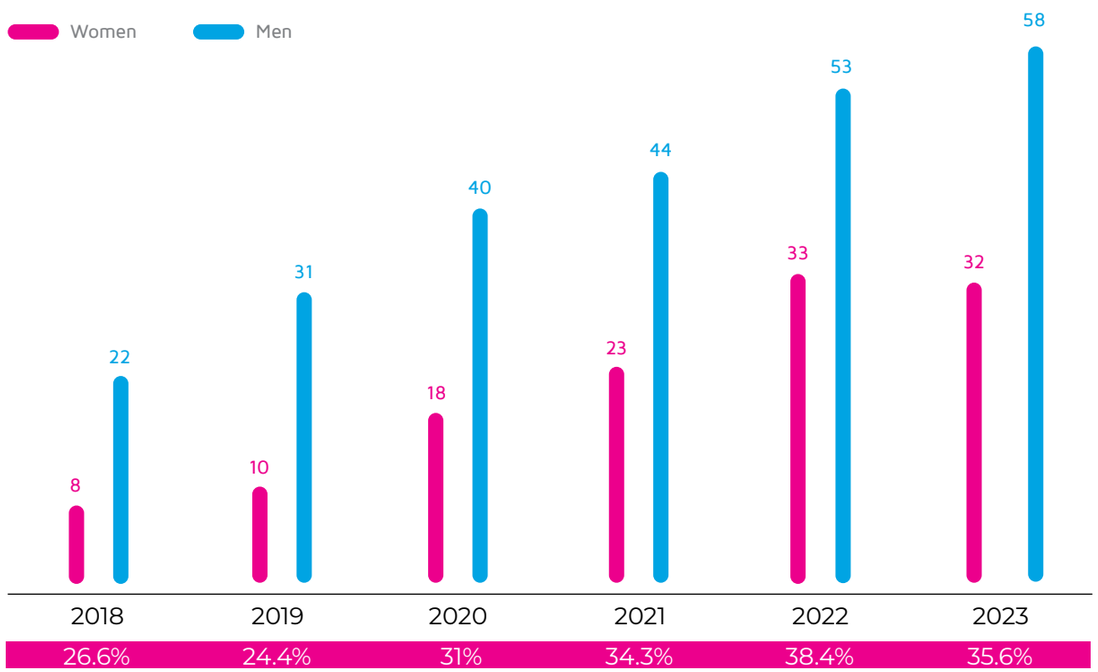
To contribute to the development of the European Research Area (ERA), The European Charter for Researchers and The European Code of Conduct for the Recruitment of Researchers (Charter and Code) were established by the European Commission in 2005. Charter and Code ensures open, **transparent and merit-based 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.



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

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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

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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

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

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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).

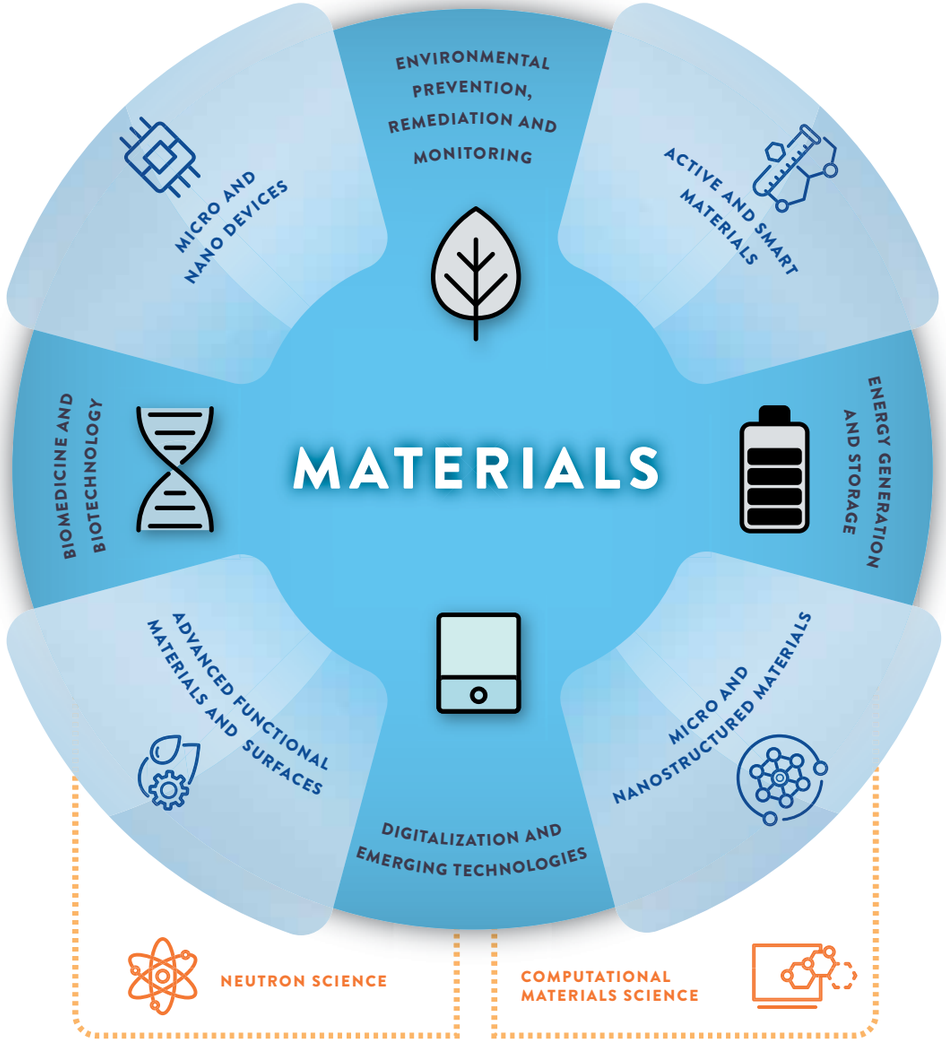
02

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 essentiao to determined 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.

Electroactive Materials Surface Charge Impacts Neuron Viability and Maturation in 2D Cultures

Marques-Almeida, T., Ribeiro, C., Irastorza, I., Miranda-Azpiazu, P., Torres-Alemán, I., Silvan, U., Lanceros-Méndez, S. ACS Applied Materials and Interfaces, 15 (26), pp. 31206-31213.

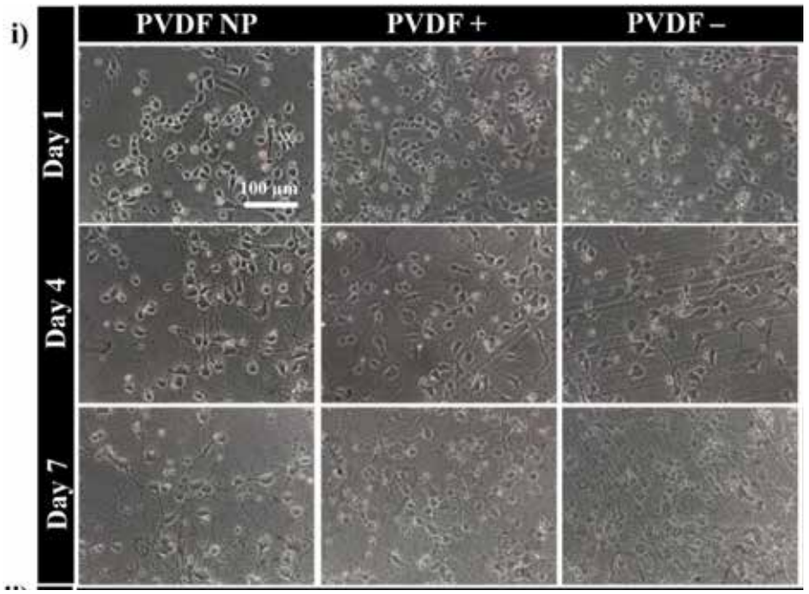


Fig 1
Optical microscopy images of neurons cultured for 1, 4, and 7 days on different surfaces (Scale bar represents 100 µm).

A number of experimental techniques for the in vitro maintenance of neurons have been developed over the last decades. These methods have been further adapted and refined to study specific neurobiological processes under controlled experimental conditions. Nevertheless, the impact of the net surface charge of the substrates to which neurons adhere when cultured in vitro has not been sufficiently considered. In the present work, we have analyzed the response of primary neurons when cultured on polyvinylidene fluoride (PVDF) surfaces with different surface electric charges. Since PVDF has otherwise identical surface properties and topographies, the response of neuronal cells to the various materials can be directly related to the net electric charge of those surfaces. Our results reveal that non-transformed neural cells display increased viability at early timepoints when seeded on PVDF substrates with a net charge, either positive or negative. Furthermore, the expression of maturation markers such as Neuronal Cell Adhesion Molecule (NrCAM), N-Cadherin (N-Cad), and Neuronal Nuclear protein (NeuN) appear also upregulated in neurons

Since neurons were first cultured, a number of experimental techniques for their in vitro maintenance have been developed. However, the impact of the net surface charge of the substrate to which cells adhere when cultured has not been sufficiently considered. We used an electroactive polymer with different electric poling states to evaluate the impact of the net electric surface charge on the behavior of primary neurons. Our results show that average negative and positive surface charges promote increased metabolic activity and enhance the maturation of primary neurons, demonstrating the relevance of considering the electric charge of the culture surfaces.

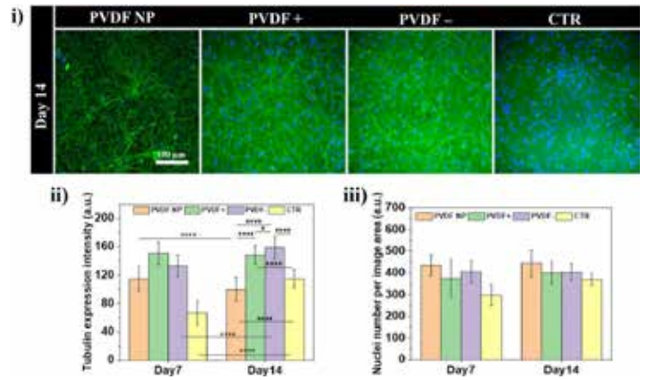


Fig 2
Fluorescence images of β-III tubulin (green) and nucleus (DAPI blue) in neurons cultured for 14 days (Scale bar represents 100 µm).

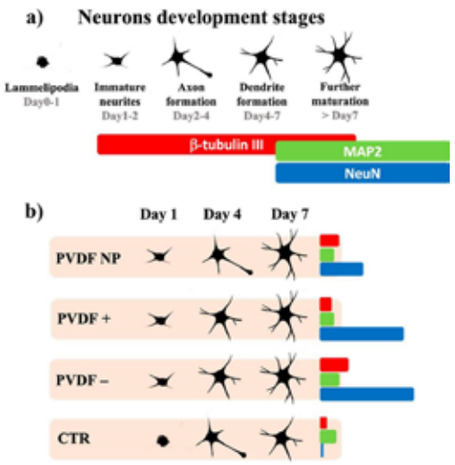


Fig 3
Differentially expressed proteins in C2C12 cells cultured on polarized PVDF samples relative to control: a) "poled -" and b) "poled +", as depicted in their networks by STRING and visualized through Cytoscape. Each dot represents a protein of interest and the lines represent the protein interactions predicted by STRING. The color varies between red for the upregulated and blue for the downregulated proteins.

cultured on surfaces with net negative charge. These results highlight the importance of considering the electric charge of the culture surface when working with cells of the nervous system, demonstrating the suitability of 2D substrates based on surface-charged materials and, in particular, of PVDF due to its outstanding electroactive characteristics. These findings further pave the way for the development of novel therapeutic strategies for the regeneration of neural tissues, particularly based on dynamic surface charge variation that can be induced in the electroactive films through mechanical solicitation.

Analysis of the impact of handling and culture on the expansion and functionality of NK cells

Martin-Iglesias, S., Herrera, L., Santos, S., Vesga, M.Á., Eguizabal, C., Lanceros-Mendez, S., Silvan, U. (2023) Frontiers in Immunology, 14, art. no. 1225549.

Natural killer (NK) cells are lymphocytes of the innate immune system that play a key role in the elimination of tumor and virus-infected cells. The simplicity of its activation mechanism has allowed the development of immunotherapies based on the transduction of NK cells with CAR (chimeric antigen receptor) constructs for the treatment of cancer. Nevertheless, the production of such cell treatments still encounters a number of limitations that need to be addressed before their widespread use in clinical practice. With that in mind, in the present work we critically examined the steps required for NK cell isolation, expansion and storage, and analyzed the response of the NK cells to these manipulations.

Natural killer (NK) cells represent a promising approach for allogenic CAR immunotherapy thanks to their ability to kill cancer cells and their low tendency to provoke graft-versus-host disease. Nevertheless, their low count in blood, representing around 10% of all lymphocytes, and limited expandability are significant challenges for developing off-the-shelf CAR-NK therapies. In this context, we have critically examined a number of elements of the initial steps of NK cell handling that are required for their clinical application. Specifically, our results show that immunomagnetic NK separation leads to activation of NK cells, which is characterized by increased expression of CD16+. Although the complete elimination of antibodies from the isolation procedure might not be possible, it is important to note that such activation occurs and could affect downstream NK functions. Furthermore, based on the importance of surface potential on cellular responses, the influence of polyvinylidene fluoride (PVDF) substrates with different net surface charge on NK cells was evaluated, and revealed that NK cells displayed higher proliferation rates on charged surfaces than on non-charged ones. Further experiments should decipher the mechanism by which surface potential enhances expansion of NK cells in RPMI-based custom culture medium to exploit this and further enhance the already superior expansion obtained with the commercial medium specific for NK cells. This may also help to understand the molecular mechanism by which NK cell clustering occurs, and thereby promote it and increase the rate of NK expansion. Taken together, the present work highlights the relevance of NK cells manipulation for improving the applicability and effectiveness of NK cell-based therapies.

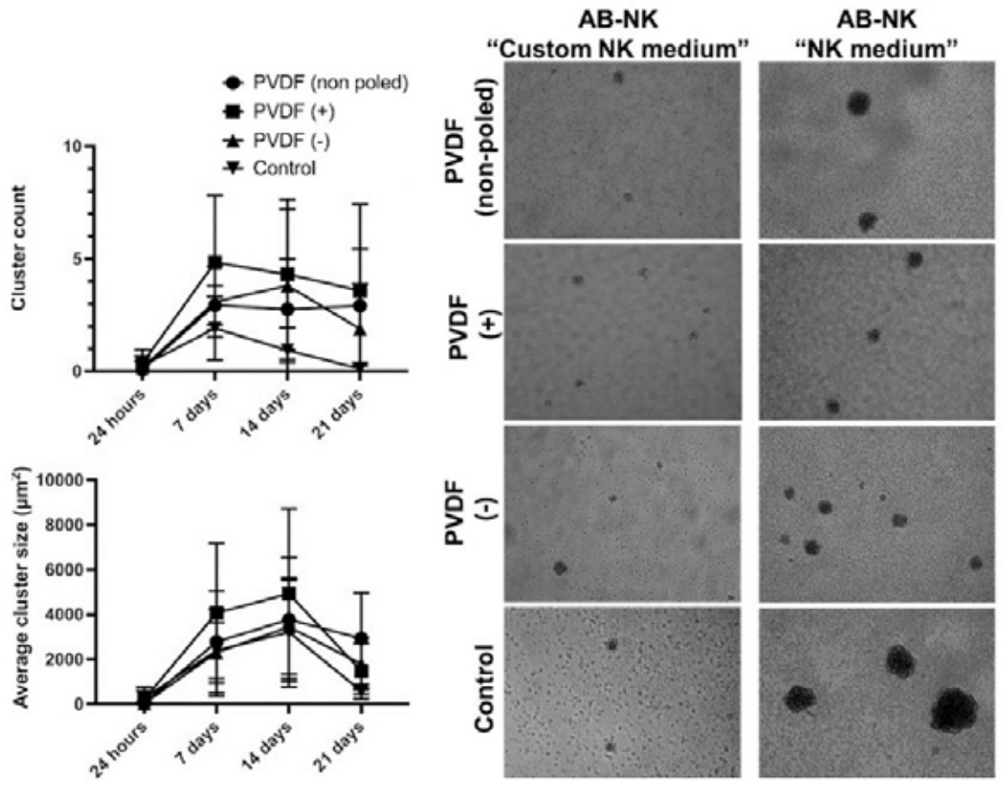


Fig 1
NK clustering in presence of poled and non-poled PVDF. Cluster number and average size of NK cells cultured on surfaces with a net positive, negative or neutral charge (left panels) and representative images of the cultures 14 days after seeding (right panels).

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.

Au-sensitised TiO_2 and ZnO nanoparticles for broadband pharmaceuticals photocatalytic degradation in water remediation

Zheng, F., Queirós, J.M., Martins, P.M., de Luis, R.F., Fidalgo-Marijuan, A., Vilas-Vilela, J.L., Lanceros-Méndez, S., Reguera, J. (2023) Colloids and Surfaces A: Physicochemical and Engineering Aspects, 671, art. no. 131594.

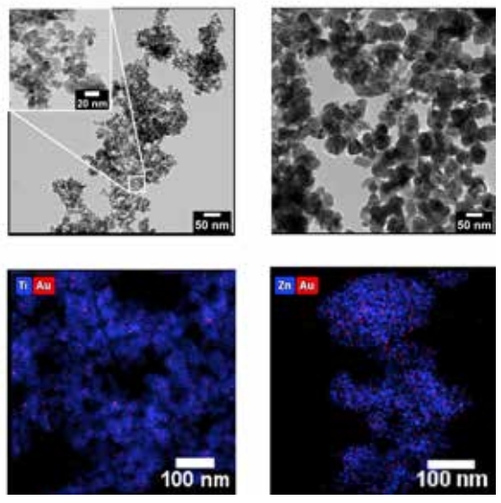


Fig 1
TEM images (a, b) of pristine TiO_2 (a) with different magnification (inset) and ZnO (b) nanoparticles. EDX mapping (c, d) of TiO_2:Au (c): Au (red) and Ti (blue) and ZnO:Au (d): Au (red) and Zn (blue).

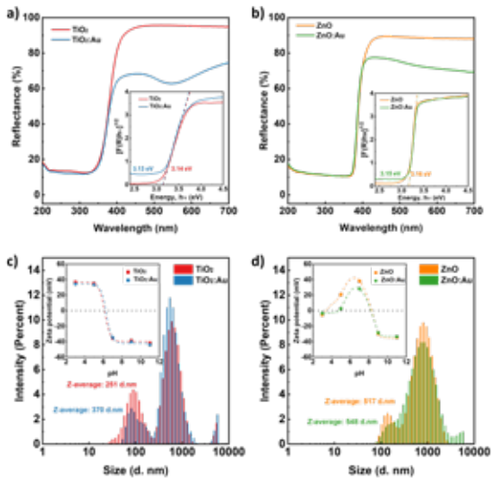


Fig 2
UV-Vis reflectance spectra (a, b) with the estimation of the bandgap (inset) at [F(R)hν]1/2 → 0, and the intensity size distribution and respective Z-average hydrodynamic size with zeta potential measurements (inset) performed at different pHs (3, 5, 7, 9, and 11) (c, d) for pristine TiO_2 and TiO_2:Au nanoparticles (a, c) and pristine ZnO and ZnO:Au nanoparticles (b, d).

Herein, semiconductors TiO_2 and ZnO nanoparticles were synthesized by co-precipitation and then functionalized by Au nanoparticles (0.05 wt.%) to obtain TiO_2:Au and ZnO:Au hybrid nanoparticles through deposition-precipitation (Figure 1). The surface properties of semiconductors were maintained after Au functionalisation, while the optical properties were enhanced by the appearance of a plasmonic band in the visible region, which makes them suitable for photocatalysis under sunlight illumination (Figure 2). Regarding the ROS generation, despite the difference in their surface area, ZnO(:Au) generated nearly 2.3 times more ROS than TiO_2(:Au) (Figure 3).

Afterwards, their photocatalytic efficiency was tested on the degradation of four highly abundant and chemically different pharmaceuticals, identified as CECs in water reservoirs: chloroquine phosphate (CLQ), paracetamol (PAR), diclofenac sodium (DCF), and ciprofloxacin (CIP). A correlation was observed between the affinity of pollutants and nanoparticles' surface and the photocatalytic degradation kinetics (Figure 4).

Under UV and at neutral pH, zwitterionic molecules such as CIP were highly degraded by all photocatalysts with efficiencies of 83% and 94% for TiO_2 and ZnO. On the other hand, cationic molecules such as CLQ

> Contaminants of emerging concern (CECs) such as pharmaceuticals cause severe aquatic environmental issues. To address this, semiconductor-based and semiconductor-plasmonic photocatalysis have emerged as a promising solution. However, it remains challenging to select an adequate photocatalyst for efficient and broadband pollutant removal under solar radiation. In this work, we present a systematic study that correlates photocatalytic efficiency with the amount of reactive oxygen species (ROS) produced by plasmonic photocatalysts and their interaction with different pharmaceuticals.

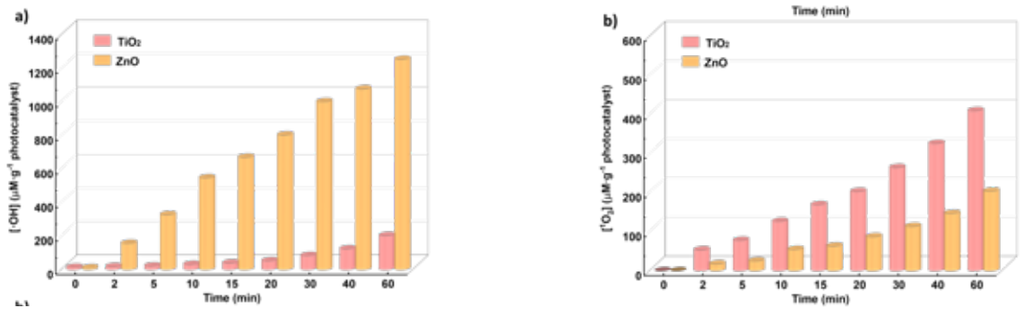


Fig 3
Quantification of photogenerated hydroxyl radical ('OH) (a) and singlet oxygen ('O2) (b) by TiO_2 and ZnO under 60 min of UV radiation.

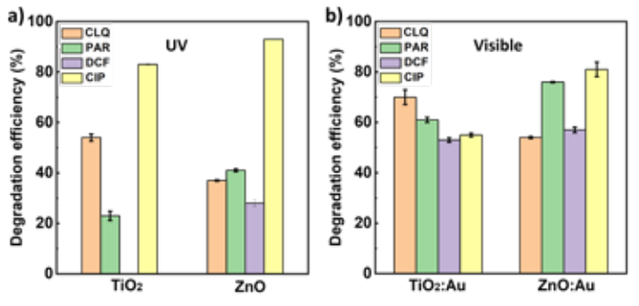


Fig 4
Photocatalytic degradation for CLQ (30 mg/L), PAR (15 mg/L), DCF (30 mg/L) and CIP (5 mg/L) removal under 60 min of UV radiation (a) and under 240 min of visible radiation (b) in presence of TiO_2 and ZnO (a), and TiO_2:Au and ZnO:Au (b).

were superiorly degraded under TiO_2 showing a degradation efficiency of 54%. Moreover, anionic molecules such as DCF were more efficiently degraded by ZnO, with an efficiency of 28%, but with low or negligible degradation by TiO_2. For the case of neutral molecules such as PAR, all nanocatalysts show degradation, although better for the ZnO nanoparticles, attributed in this case to the higher amount of generated ROS.

The sensitisation of semiconductors with Au made photocatalysis possible under visible light (figure 4b); the nanoparticles could absorb a higher amount of light (reflectance decreased from 94% to 74% for TiO_2:Au, and from 88% to 68% for ZnO:Au) and use it as the driving energy source to degrade the different pharmaceutical pollutants. The trend of efficiencies was very similar to the case observed under UV light. In short, this work presents a systematic evaluation of the photocatalytic process for emerging contaminants removal using advanced plasmonic photocatalysts and makes a broad classification possible for selecting the best photocatalyst, or combinations of photocatalysts, for more efficient degradation of pharmaceuticals in polluted water bodies under sunlight.

On The Multiscale Structure and Morphology of PVDF-HFP@MOF Membranes in The Scope of Water Remediation Applications

Valverde, A., de Fernandez-de Luis, R., Salazar, H., Gonçalves, B.F., King, S., Almásy, L., Kriechbaum, M., Laza, J.M., Vilas-Vilela, J.L., Martins, P.M., Lanceros-Mendez, S., Porro, J.M., Petrenko, V.I. (2023) Advanced Materials Interfaces, 10 (31), art. no. 2300424

Incorporation of MOFs into polymers based membranes is used to enhance metal-adsorption properties. In this study, it is examined how the micro to nanoscale structure of PVDF-HFP@MOF membranes influences their adsorption performance for Cr^{VI}. Small-angle X-ray and neutron scattering allowed to describe the nanostructure of the complex nanocomposites systems. By correlating nanoscale structural features with the adsorption capacity of the MOF nanoparticles, different degrees of full encapsulation-based on the polymer processing and structuration from the macro to nanometer scale are observed.

Metal-Organic Frameworks (MOFs) are becoming an interesting family of porous materials to face problems of low adsorption capacity and selectivity of existing materials. The immobilization of MOFs with mechanically robust polymeric matrixes stands out as one of the most appealing strategies for environmental science.

PVDFHFP@MOF membranes were prepared through two different phase inversion methods: thermal-induced phase separation (TIPS) and nonsolvent-induced phase separation (NIPS) and thus membranes with a well-interconnected porosity network suitable for water remediation were obtain.

The templating effect of MOF nanoparticles (MOF-808, UiO-66-NH2, and MIL-125) into the porous structure of PVDF-HFP@MOF composites processed by TIPS and NIPS has been investigated by means of X-ray diffraction, infrared spectroscopy, thermogravimetric analysis and scanning electron microscopy. The macro, meso, and microporous structure of the composites have been characterized by a combination of specific experimental techniques, including mercury porosimetry, SEM, SAXS, and SANS. Altogether, a complete landscape from the macro to the nanometer scale of the structure of the composites has been obtained and correlated with the encapsulation degree of the MOF nanoparticles into the polymeric matrix, and hence to their capacity to capture chromate oxyanions ($CrO4^{2-}$).

In general, four SANS and SAXS features can be observed in the experimental data plotted in Figure 1: i) the scattering arising from the nano-inhomogeneities generated within the membranes due to the phase/domain structuration of the polymer itself (characteristic size ≈2–3 nm); ii) the interparticle space created due to the MOF particles agglomeration within the polymer (characteristic size ≈10–20 nm); iii) the power law decay of the scattering data that is related to the aggregates with mass or surface fractal structures in the composites; and iv) the diffraction peak in the large q region due to the crystal structure of the MOF.

Considering the information from the SEM images and the one obtained by SANS and SAXS, the shape of the branched fractal structuration of the pores in PVDF-HFP membranes are summarized as schematized in Figure 2. In this simplified model, it can be found MOF nanoparticles finely decorating the pore space of the PVDF-HFP, as in the case of MOF-808 TIPS membrane, agglomerated MOF nanoparticles, and even single nanoparticles encapsulated within the PVDF-HFP matrix.

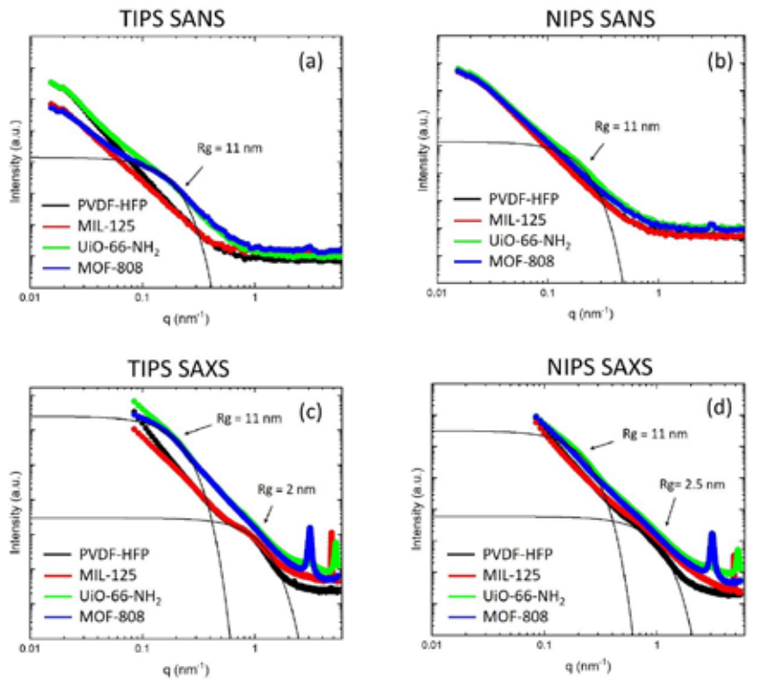


Fig 1
NK clustering in presence of poled and non-poled PVDF. Cluster number and average size of NK cells cultured on surfaces with a net positive, negative or neutral charge (left panels) and representative images of the cultures 14 days after seeding (right panels).

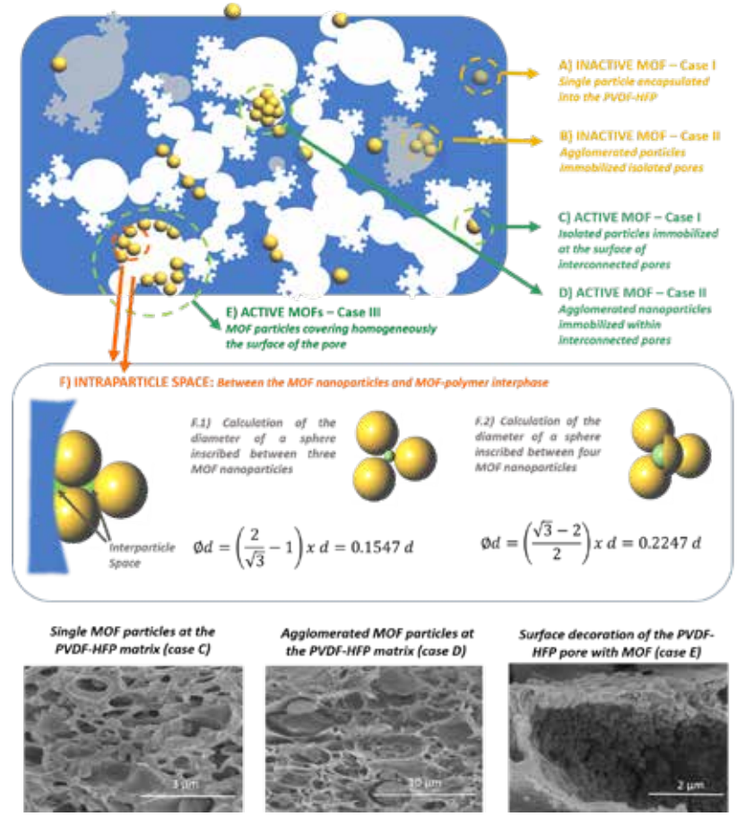


Fig 2
Schematic representation of the overall structuration of PVDF-HFP@MOF composites. (a-e) Schematic illustration of the fractal pores interconnected structure of the PVDF-HFP matrix, the MOF immobilization possibilities within the membrane, and (f) the mathematic description of the interparticle space between MOF particles and at the polymer-MOF interphase. Bottom of the figure: SEM images of the different cases.

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.

Unveiling challenges and opportunities in silicon-based all-solid-state batteries: thin-film bonding with mismatch strain

Zhao, M., Zhang, J., Zhang, X., Duan, K., Dong, H., Lanceros-Méndez, S., Wang, W., Zhang, Q. (2023)
Energy Storage Materials, 61, art. no. 102857

> For Li-metal anodes, Li-ions stripping/depositing on the surface leads to gaps and Li dendrite formation, which is an electrochemical behavior and unavoidable. For Si-based anodes, Li-ions inserting/extracting within the Si-based electrode causes volume changes and a local separation from the SE, which is a mechanical behavior and avoidable by mitigating the strain mismatch of thin-film bonding between anode and SE

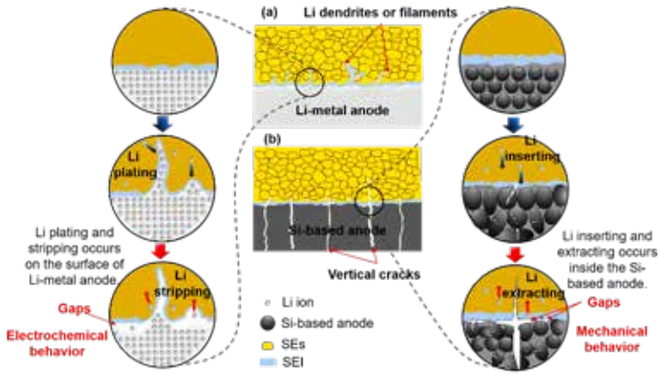


Fig 1
Mechanisms of the interfacial gaps formed by (a) Li-metal anodes and (b) the Si-based anodes with the SEs, respectively.

Li-metal and Si are two of the most impressive anode materials for ASSBs, as both have extremely high specific capacities of 3860 and 3590 mAh g^{-1} at room temperatures, respectively. However, both materials form gaps at the interface with solid electrolytes (SEs) during charging/discharging, resulting in increased impedance and uneven current density distribution. In this perspective, we elaborate in detail the different mechanisms of formation of these gaps. For Li-metal anodes, Li-ions are repeatedly stripped and unevenly deposited on the surface, leading to gaps and Li dendrite formation, which is an electrochemical behavior and unavoidable. For Si-based anodes, Li-ions inserting/extracting within the Si-based electrode causes volume changes and a local separation from the SE, which is a mechanical behavior and avoidable by mitigating the strain mismatch of thin-film bonding between anode and SE. We also describe Si electro-chemical-mechanical behaviors, including recrystallisation, different lithiation mechanisms, irreversible expansion and electrochemical sintering, and recommend strategies to synergistically decrease Si-based electrode strain, including Si materials, Si-based composites and electrodes. These three aspects correspond to three scales, encompassing microscopic, mesoscopic, and macroscopic.

Finally, the massive mechanical stresses caused by volume expansion and contraction of anode and cathode electrodes can lead to rupture and pulverization of the electrodes, resulting in the separation of solid-solid interface and the damage of SEs, especially for the anode electrode with higher capacity and greater volume variation. We suggest to choose a composite polymer-inorganic SE with favorable elastic properties and high ionic conductivity and to form it directly on the Si-based electrode, which are beneficial for increasing SE strain to accommodate stack pressure and the stability of the interface. Thus, this perspective sheds a light on the development and application of Si-based ASSBs.

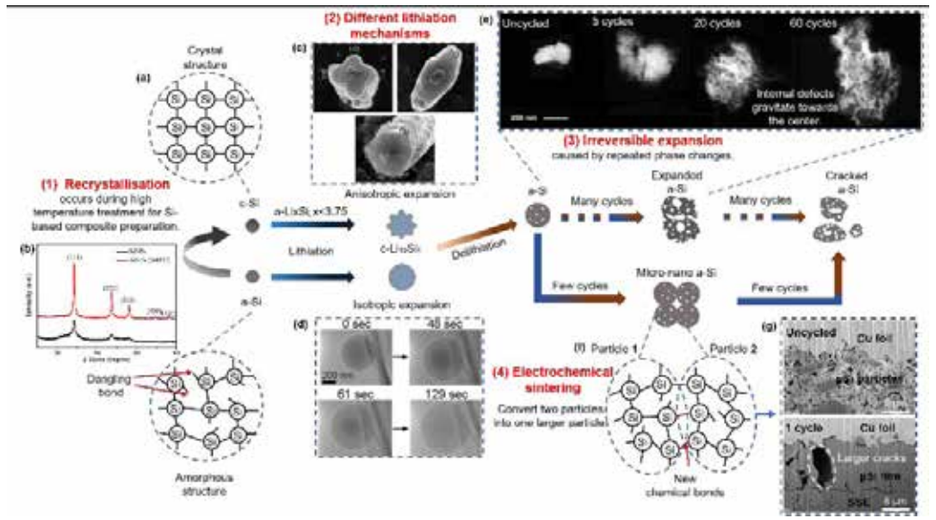


Fig 2
Electro-chemical-mechanical behaviors of Si materials, including (1) Recrystallisation, (2) Different lithiation mechanisms, (3) Irreversible expansion and (4) Electrochemical sintering.

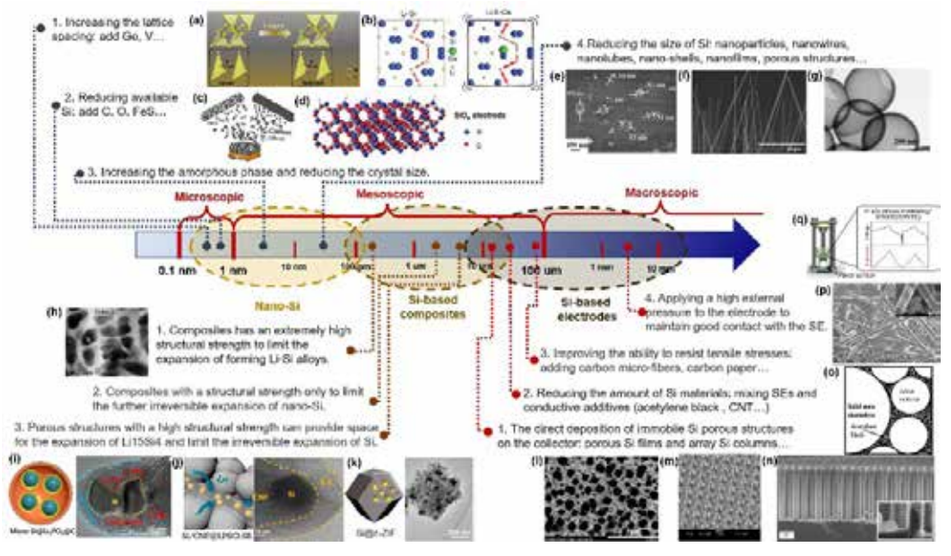


Fig 3
Schematic diagram of strategies for reducing Si-based electrode expansion. This objective necessitates considering not only Si itself, but also its composites and electrodes. These three aspects correspond to three scales, encompassing microscopic, mesoscopic, and macroscopic.

Interface tweaking of perovskite solar cells with carbon nitride-based 2D materials

Naveen Harindu Hemasiri, Muhammad Ashraf, Samrana Kazim, Robert Graf, Rüdiger Berger, Nisar Ullah, Muhammad Nawaz Tahir, Shahzada Ahmad , Nano Energy, Volume 109, 2023,108326

Two-dimensional van der Waals layered materials display strong Coulomb interactions, which in can be used to tune the interface of devices including optoelectrical, and their delineation is of paramount importance. We engineered the interface with carbon nitride at hole transport layers and perovskite, so it can eliminate defective charge build-up and suppress the charge carrier recombination rate to induce accelerated photo-induced charge transfer. The carbon nitride-based 2D materials will serve as an effective interfacial layer for long-term reliability in photovoltaics.

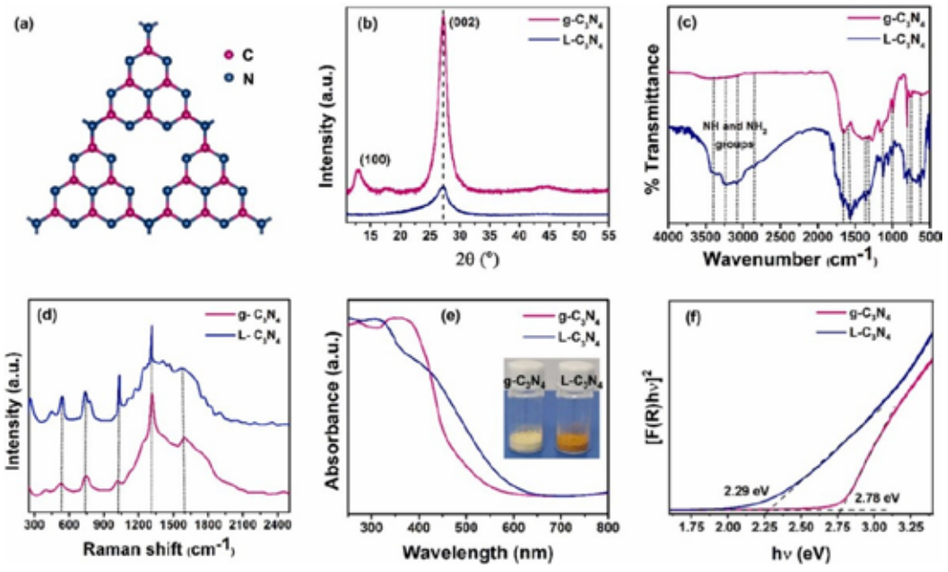


Fig 1
(a) Chemical structure of Tri-8-triazine-based graphitic-C_3N_4, (b) XRD pattern, (c) FTIR spectra, (d) Raman spectra, (e), DR-UV-Vis spectra and inset represents the obtained powders of g-C_3N_4 and L-C_3N_4 and (f) [F(R)h]2 vs. h plot for g-C_3N_4 and L-C_3N_4.

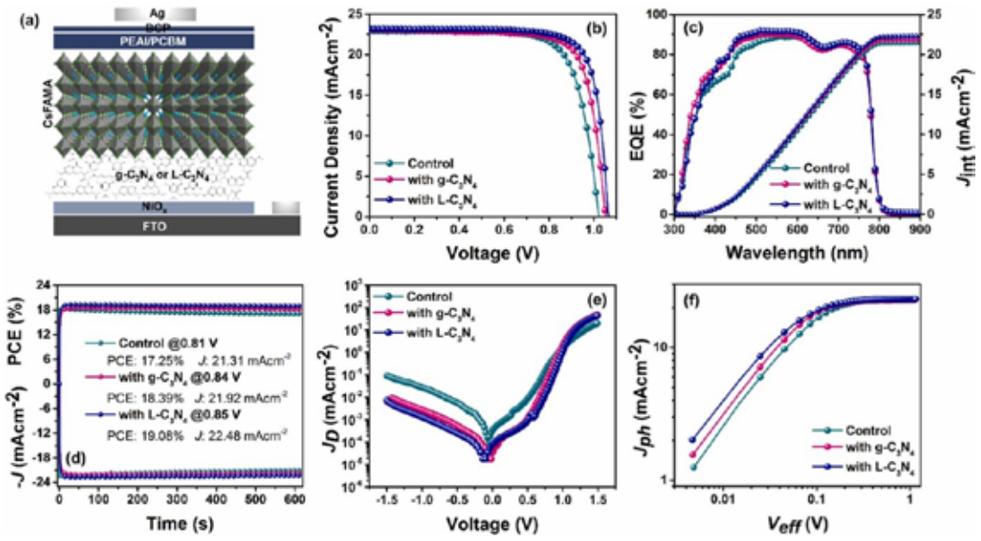
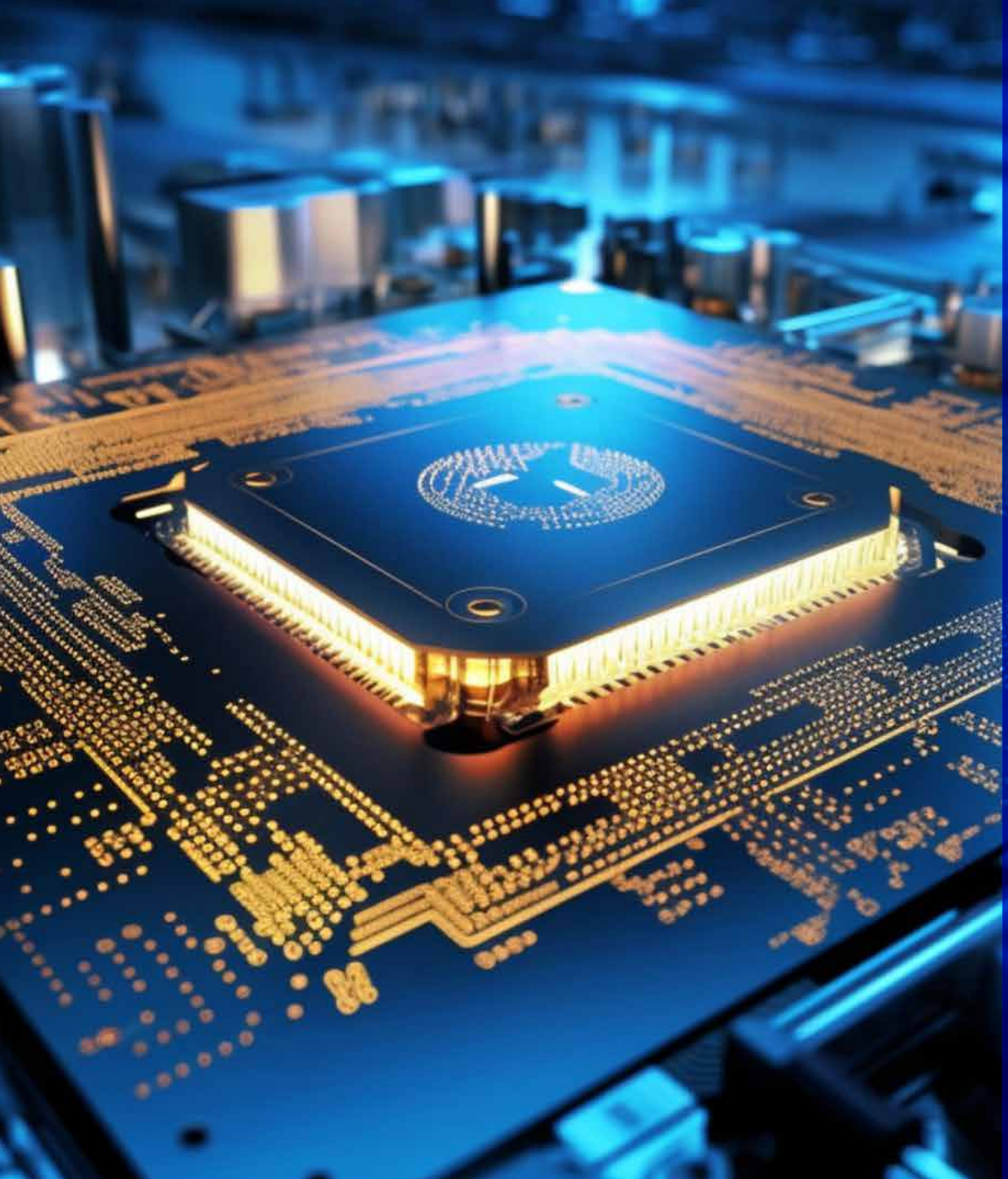


Fig 2
(a) Device configuration, (b) J-V curve of the champion devices without and with g-C_3N_4 or L-C_3N_4 interface layer measured in reverse scan under simulated AM 1.5G illumination, (c) IPCE and integrated current density of the corresponding devices, (d) steady-state power output of PSCs. (e) dark J-V curves and (f) photo-generated current density vs. effective voltage of PSCs.

Lead halide-based perovskite solar cells (PSCs) have revolutionized the field of emerging photovoltaics and shown rapid progress. Here, we have synthesized two graphitic carbon nitride 2D-polymeric materials by solid-state (g-C_3N_4) and solvothermal (L-C_3N_4) synthesis and probed their potential as an interface layer with inorganic hole selective layers in inverted planar PSCs. We investigated the interaction with perovskites and deduced that the coordination of FA-amine and MA-ammonia groups provides a favorable interaction at the interface between C_3N_4 and perovskite. The enhanced photo-induced charge transfer dynamics and attenuated charge recombination behavior upon 2D-carbon nitrides led to improved performances in the PSCs. Subsequently, the low bandgap L-C_3N^4-modified interlayer-based PSCs gave 19.33 %, whereas with high bandgap g-C_3N_4 delivered a PCE of 18.58 %, surpassing the control PSCs performance and reliability. Such PCE are notable values with the use of NiO as hole selective layers and suppressed redox reaction at NiO_x/perovskite interface.

The 2D graphitic-carbon nitride framework is composed of tri-8-triazine connected through planar tertiary amines (Figure 1), which display two different colors depending on the synthesis method; i.e, solid-state synthesis (g-C_3N_4) is milky yellowish and solvothermal (L-C_3N_4) is orange in color. The g-C_3N_4 shows two absorption peaks at around 280 and 375 nm relevant to ϖ-ϖ^* transition in the conjugated polymeric network and n-ϖ^* transition between nonbonding orbitals of nitrogen and aromatic ring, respectively. Notably, L-C_3N_4 shows a strong absorption shoulder with a red-shifted absorption edge at 650 nm compared to g-C_3N_4 (absorption edge at 575 nm), and the optical band gap of the exfoliated C_3N_4 in iso-propanol/ethanol solution, and the optical bandgap was calculated to be 3.3 and 2.5 eV for g-C_3N_4 and L-C_3N_4, respectively.

We fabricated the PSCs using g-C_3N_4 and L-C_3N_4 as interface layers in-between NiO and perovskite absorber layers (Figure. 2). Through C3N4-based engineered interfaces we achieved an improvement in device performance and reliability, measuring a power conversion efficiency of 19.33 %, with complete suppression of the device hysteresis using inorganic NiO. Our investigation distinctly illustrates the advancement of 2D-based materials as an interface layer to uplift the reliability of the PSCs, which will pave the way for the industrial endeavor.



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.

Sustainable antibacterial collagen composites with silver nanowires for resistive pressure sensor applications

Andonegi, M., Correia, D.M., Pereira, N., Fernandes, M.M., Costa, C.M., Lanceros-Mendez, S., de la Caba, K., Guerrero, P. Sustainable antibacterial collagen composites with silver nanowires for resistive pressure sensor applications (2023) European Polymer Journal, 200, art. no. 112494.

The development of new smart materials with advanced functionalities is receiving an increasing demand. In this regard, silver nanowires (Ag NWs) were incorporated into a collagen matrix to develop biocomposites that preserve the triple helix structure of the polymer matrix, enhancing thermal and electrical properties. The resulting biocomposites presented suitable resistance variations under pressure and bending, allowing the development of sustainable multifunctional sensing composites with antibacterial activity, which can be applied in the next generation of touch sensing electronic devices.

The materials obtained from the combination of natural polymers (e.g. collagen) with functional fillers (e.g. Ag NWs) can lead to the development of biocomposites with improved sustainability while maintaining high levels of functional performance. In this work, Ag NW content was varied from 0 to 6 wt %, resulting in collagen biocomposites that showed a fibrillar structure (Figure 1a) with Ag NWs dispersed in the matrix (Figure 1b). The values of glass transition and denaturation temperatures increased from 46.9 °C and 94.2 °C for collagen to 51.4 °C and 105.1 °C for the biocomposites with 6 wt % Ag NWs, indicating the thermal stability improvement. Furthermore, the enthalpy value decreased from 275.7 mJ/g to 136.6 mJ/g when 6 wt % Ag NWs were added. These results are in agreement with the decrease of the free and bound water content with the addition of Ag NWs. Additionally, the electrical conductivity of Ag NW/collagen biocomposites was obtained through I-V curves, which showed increasing slope with increasing Ag NW content. Since the best thermal properties, the highest electrical conductivity (0.0515 S·cm-1) and the greatest antibacterial activity against gram-positive and gram-negative bacteria was obtained for the biocomposites with 6 wt % Ag NWs, these biocomposites were selected to develop a resistive sensor (Figure 2). The sensor response showed the resistance variation of the 3 sensors when 2 different events occurred: pressure applied directly on top of the sensors (Figure 3a) and bending movement applied on a cylinder-shaped object (Figure 3b). The resistance varied as a function of time for the pressure and bending events (Figure 3c). In both events, the sensor allowed the identification of the pressure and bending variation on multiple sensors at the same time for mechanical tactile buttons and when the sensors array was bent, allowing to detect a bending motion that can be also used in touch and finger flexing detection in robotic applications, among others. In sum, this work demonstrates the potential of sustainable multifunctional composites with antimicrobial properties for electronic devices based on bio-based resources.

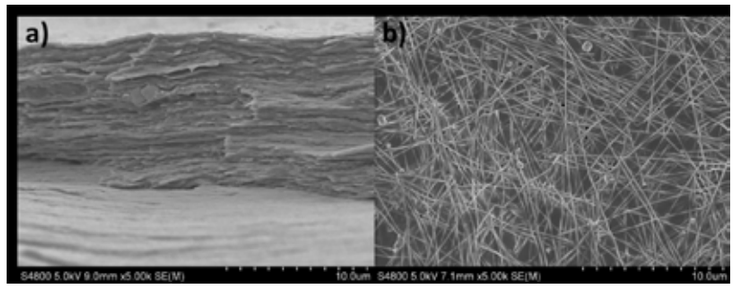


Fig 1
SEM images of a) the cross-section and b) the surface of collagen biocomposites with 6 wt % Ag NWs.

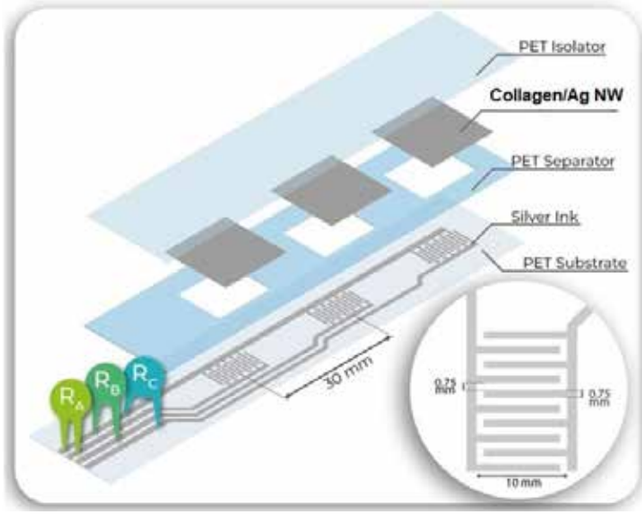


Fig 2
Assembly process of the pressure sensitive collagen/Ag NW film sensors.

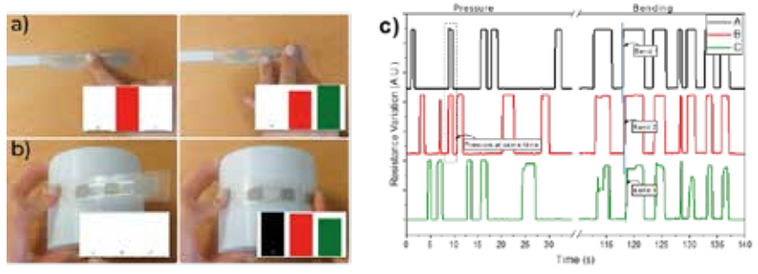


Fig 3
Resistance variation of the 3 pressure sensors: a) Pressure event directly on top of the sensors, b) bending of the sensors on top of a cylinder, and c) corresponding resistance variation as a function of time.

Environmentally Friendlier Printable Conductive and Piezoresistive Sensing Materials Compatible with Conformable Electronics

Naveen Harindu Hemasiri, Muhammad Ashraf, Samrana Kazim, Robert Graf, Rüdiger Berger, Nisar Ullah, Muhammad Nawaz Tahir, Shahzada Ahmad , Nano Energy, Volume 109, 2023,108326

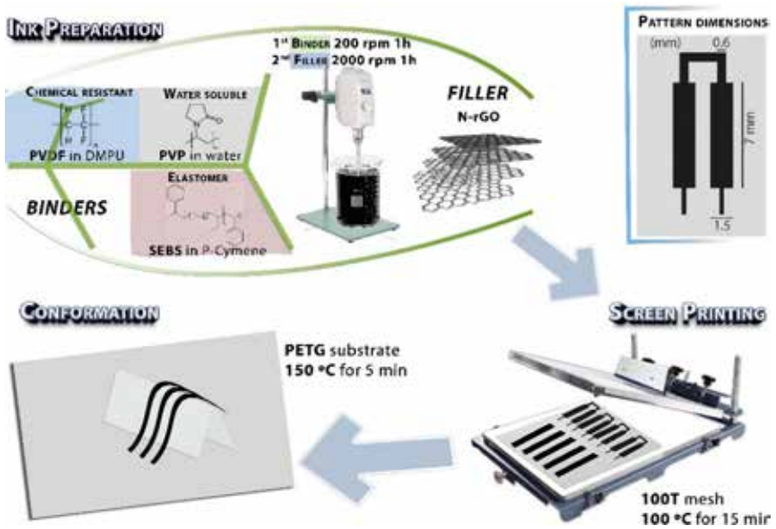


Fig 1
Experimental procedure for N-rGO based inks and films preparation using PVDF, PVP, and SEBS as polymer binders. The films were screen-printed in 20 × 20 mm squares and (1.5 × 70 mm) pads.

The Internet of Things (IoT) and Industry 4.0 revolutionizes the requirements for sensing and functional materials in terms of increased performance, reduced environmental impact, and simplified processing and integration. Additive manufacturing technologies are thus increasingly being established to develop smart and functional materials with tailored properties for electronic applications, leading to new generations of lightweight multifunctional materials with improved integration. The printing technologies can be combined with additional processing strategies to further tailor electronic devices with innovative geometries. In particular, the thermoforming process allows the development of curved-shape electronics with high-precision geometry and fast processing. Nevertheless, for this technique to be sustainable on a large scale, processing and the materials used for composite development must rely on materials that present low toxicity for human health and the environment. Therefore, it is urgent to avoid the use of toxic solvents and to explore greener alternatives. Herein, the polymer binders were dissolved in low-toxicity solvents (PVP in water, SEBS in P-cymene, and PVDF in dimethyl propylene urea) and mixed in different ratios filler:binder with with N-rGO to obtain graphene dispersion (Figure 1). The conductive materials were then obtained by screen-printing and the electrical sheet resistance of the films was evaluated. Further, the effect of the number of printed layers on the electrical conductivity was evaluated (Figure 2). The minimum resistance

Flexible and conformable conductive composites have been developed using different polymers, polyvinylpyrrolidone (PVP), polyvinylidene fluoride (PVDF), and styrene–ethylene–butylene–styrene (SEBS) reinforced with nitrogen-doped reduced graphene oxide (N-rGO) and manufactured by screen-printing using low-toxicity solvents. The printed films showed a sheet resistance lower than Rsq < 100 Ω/sq, being biocompatible and support bending deformations up to 10 mm with piezoresistive performance up to 100 bending cycles. These conductive materials open a path for developing sustainable and functional devices for printable and conformable electronics.

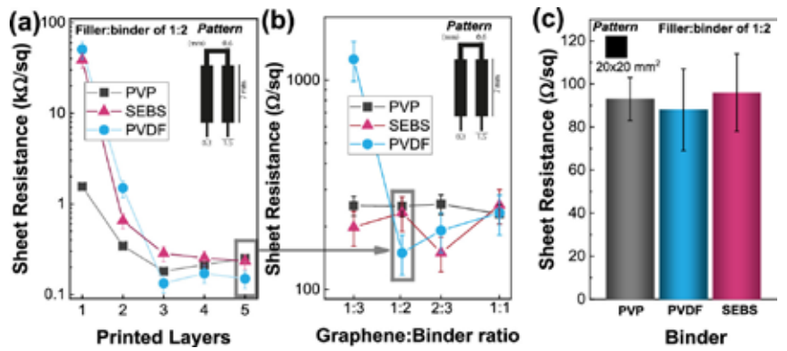


Fig 2
Sheet resistance of the screen-printed pads for PVP-, SEBS-, and PVDF-based films: (a) for pads as a function of the number of printed layers; (b) for pads as a function of the filler:binder ratio for 5 printing steps; and (c) for a 20 mm square obtained after five printing steps using a filler:binder ratio of 1:2.

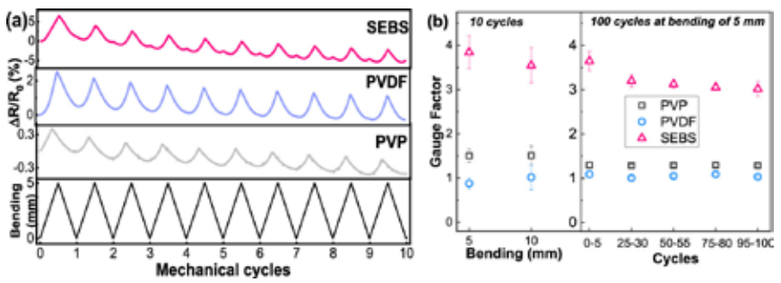


Fig 3
(a) Electrical resistance variation under applied maximum bending of 5 mm over 10 cycles for all samples. (b) Piezoresistive GF for 5 and 10 mm of bending for 10 cycles and as a function of the number of bending cycles for 100 cycles at a maximum deformation of 5 mm.

obtained is similar for all materials near 100 Ω/sq. The pattern area also has a slight influence on the electrical properties, increasing for smaller areas. The multifunctionality of the printed materials was demonstrated for piezoresistive sensing applications. Piezoresistive tests were carried out with simultaneous measuring of the electrical resistance variation (Figure 3). The variation of the electrical resistance follows the applied stimulus and is stable for over 100 cycles. In all cases, the electrical resistance varies linearly with the applied bending deformation. The samples with SEBS binder show a GF = 3.8, decreasing to 0.8 < GF < 1.5 for samples with PVDF and PVP. Overall, the developed printed conductive materials tolerate mechanical bending with no significant electrical resistance variation degradation, being able to self-sensing evaluate that bending through the piezoresistive response.

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.

Magnetic Polymer Actuators with Self-Sensing Resistive Bending Response Based on Ternary Polymer Composites

Ander Garcia Díez, Nelson Pereira, Carmen R. Tubio, Jose Luis Vilas-Vilela, Carlos M. Costa, and Senentxu Lanceros-Mendez. ACS Appl. Electron. Mater. 2023, 5, 6, 3426–3435

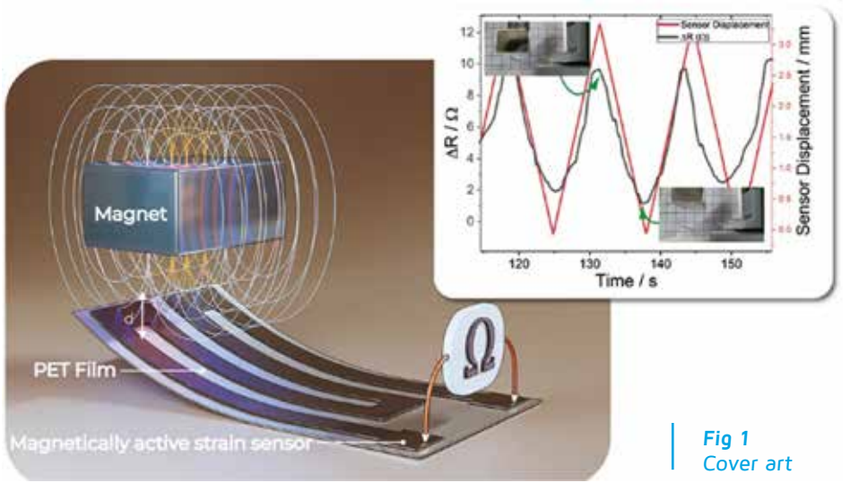


Fig 1
Cover art

Ternary multifunctional composites with both magnetic and electrical response have been developed for advanced applications. The composites were produced by solvent casting technique based on poly(vinylidene fluoride) (PVDF) matrix with a combination of cobalt ferrite ($CoFe_2O_4$, CFO) nanoparticles and multiwalled carbon nanotubes (MWCNT) as fillers. CFO nanoparticles have been selected due to their excellent saturation magnetizations and ability to retain these properties, while MWCNT present excellent electrical conductivity. The composites have been prepared at a fixed weight concentration of 20 wt% for the CFO, varying the MWCNT content between 0 and 3 wt% allowing the development of conductive composites. The experimental results prove that the microstructure of these composites is compact without pores and without aggregates where both fillers are well dispersed. Furthermore, the filler content and type do not affect the polymer phase, the degree of crystallinity, melting and degradation temperatures, and the magnetic behavior. On the other hand, the mechanical and electrical properties strongly depend on the MWCNT content, and a maximum d.c. electrical conductivity value of 4×10^{-4} S/cm have been obtained for the composite with 20 wt% CFO and 3 wt% MWCNT, which is accompanied by a 11.1 emu/g magnetization. Finally, the magnetic strain actuator sensing capability has been demonstrated for the 20wt%CFO-0.5wt%MWCNT/PVDF sample with excellent response and reproducibility through the combination of magnetic and electrical response. The magnetic strain actuator shows a resistance variation of approximately 8 Ω for a bending displacement of around 3 mm at the tip of the magnetic strain gauge. Thus, this work validates the suitability of developing multifunctional materials based on two different fillers with tailored magnetic and electrical responses for the next generation of actuator devices

Aiming to design a new multifunctional polymer-based composites for IoT-related applications, this work shows the development of a novel ternary multifunctional composites with both magnetic and electrical response. The composite were based on poly(vinylidene fluoride) (PVDF) polymer matrix with cobalt ferrite oxide (CoFe2O4) and multiwalled carbon nanotubes (MWCNTs) as fillers, allowing to combine magnetic and electric responses. The suitability of this composite for magnetic strain actuator with self-sensing strain characteristics is demonstrated with excellent response and reproducibility.

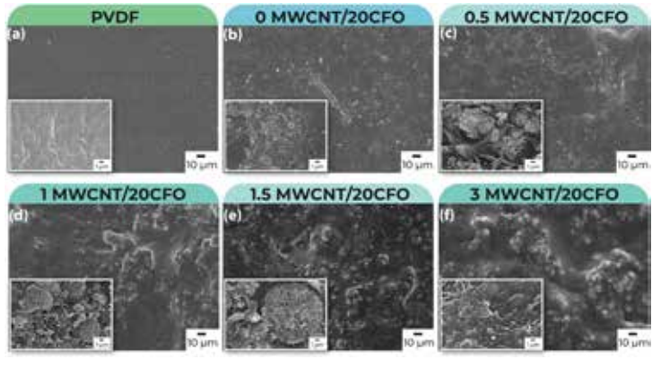


Fig 2
Cross-section and surface SEM images of PVDF/20CFO composites with different MWCNT contents (a–f). The scale bar represents 1 and 10 µm for the cross-section and surface images, respectively.

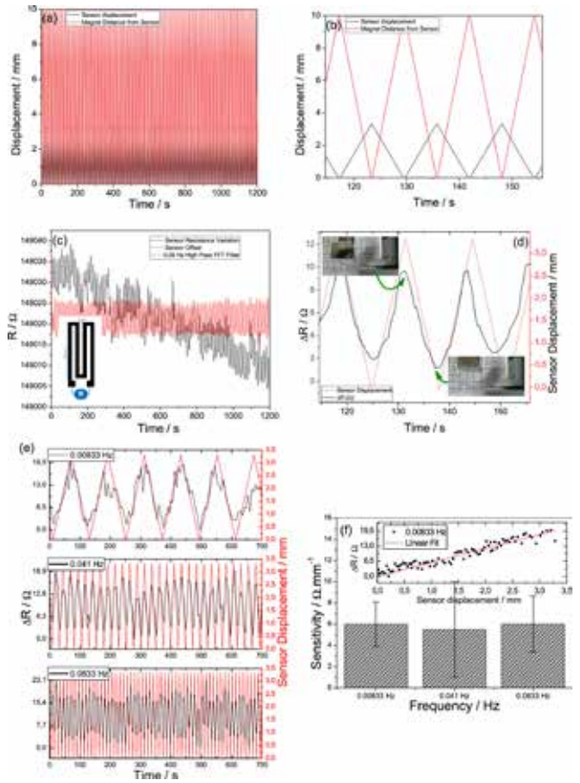


Fig 3
(a) 100 cycles of displacement of the magnet to the actuator and extrapolated bending deformation of the actuator based on video footage. (b) Magnification of some of the bending cycles. (c) Raw and filtered resistance variation over 100 cycles of magnetic displacement, (d) resistance variation correlation with the magnetic actuator displacement after correction of the low-frequency offset, (e) cycles performed at 0.00833, 0.041, and 0.0833 Hz, and (f) sensitivity of the sensor (insert: resistance variation as a function of the sensor displacement for determination the sensitivity value).

Magnetically responsive melt electrowritten structures

G. Saiz, P., Reizabal, A., Luposchainsky, S., Vilas-Vilela, J.L., Lanceros-Mendez, S. and Dalton, P.D. (2023). Adv. Mater. Technol., 8: 2202063.

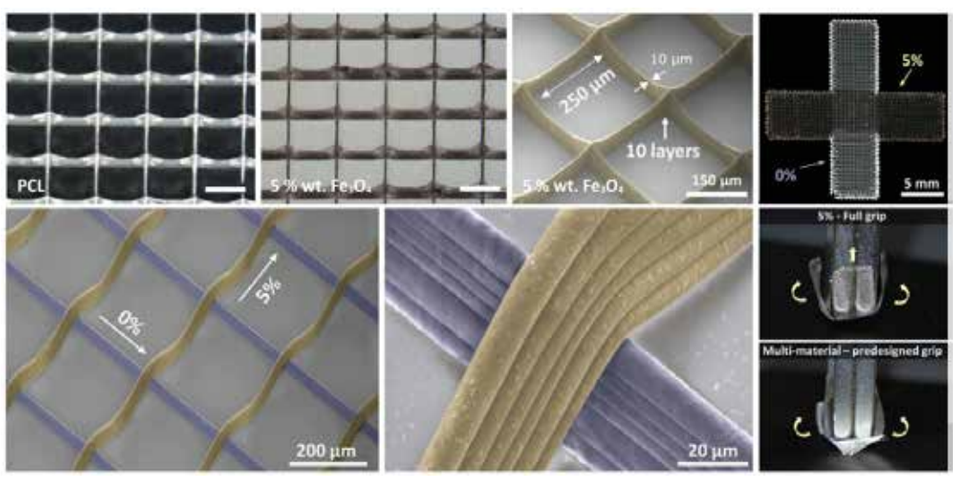


Fig 1
Images of cross-shaped magnetoresponsive MEW samples and their response under an external magnetic field.

Additive manufacturing (AM) is established as a technology capable of solving challenges across many applications. Adapting to specific applications and requirements, different AM technologies have emerged, each with its strengths and weaknesses. To achieve high-resolution 3D printing, melt electrowriting (MEW) has emerged as a novel electrohydrodynamic technique that allows the deposition of continuous polymeric fibers in a very precise way. The microscale and nanoscale perspectives, combined with a solvent-free approach, have allowed MEW to establish itself as one of the most promising techniques for fabricating high-resolution scaffolds with highly controlled porosity and shape.

Despite its advantages, MEW was not discovered until 2011. Thus, as a young AM technology, there are exciting possibilities for exploring new types of advanced materials to be printed by this technique, including new polymers and different composites. Most structures designed by MEW are based on poly(-caprolactone) (PCL), although other polymers are starting to be employed for this purpose as well. In addition, the use of fillers within the MEW-processed structures to promote active properties is limited. This holds the key for 4D printing, where MEW-processed structures can be stimulated into movement by introducing functional additives.

In that context, this work reports an analysis of the printing capacity of MEW for magnetic responsive structures based on poly(-caprolactone) (PCL) and magnetic nanoparticles (Fe_3O_4). The results show that magnetic composites with up to 5%wt. of Fe_3O_4 could be successfully printed in different complex structures without affecting the quality of the scaffolds (Fig. 1). Using a rotatory collector, tubular scaffolds with different magnetic responses are also printed (Fig. 2). The scaffolds actuate toward an external magnetic field, and the control of their microstructure allows tuning this response (Fig. 3). This allowed the design of magnetic clamps with a predesigned grip, butterflies with a controlled beating of their wings, and tubes with preferential magnetic orientation. Besides, they present high cell viability, having high potential applications in areas such as biomedicine.

Melt electrowriting (MEW) leverages electric fields and 3D printing to craft fibrillar structures with micrometer-scale features. Predominantly used in tissue engineering, MEW holds great promise in electronics, robotics, and more. This study focuses on enhancing MEW's capabilities through the printing of magnetoresponsive structures using inks with up to 10 wt. % iron-oxide (Fe_3O_4) nanoparticles. Additionally, we explore the ability to control the response of the processed flat and tubular structures by harnessing their magnetic actuation and micro/macro design.

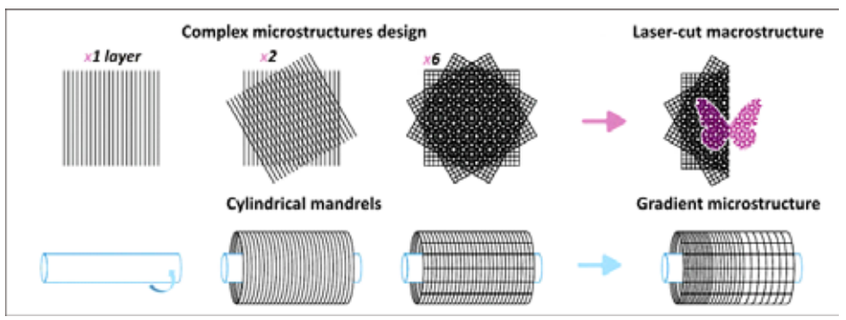


Fig 2
Schematic of the different printing approaches: laser cut butterfly-shaped macrostructures, and tubular shapes with a gradient microstructure.

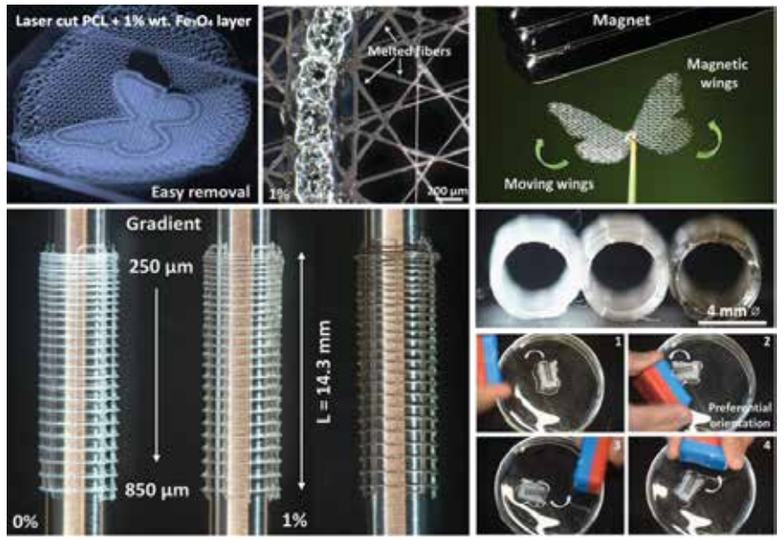
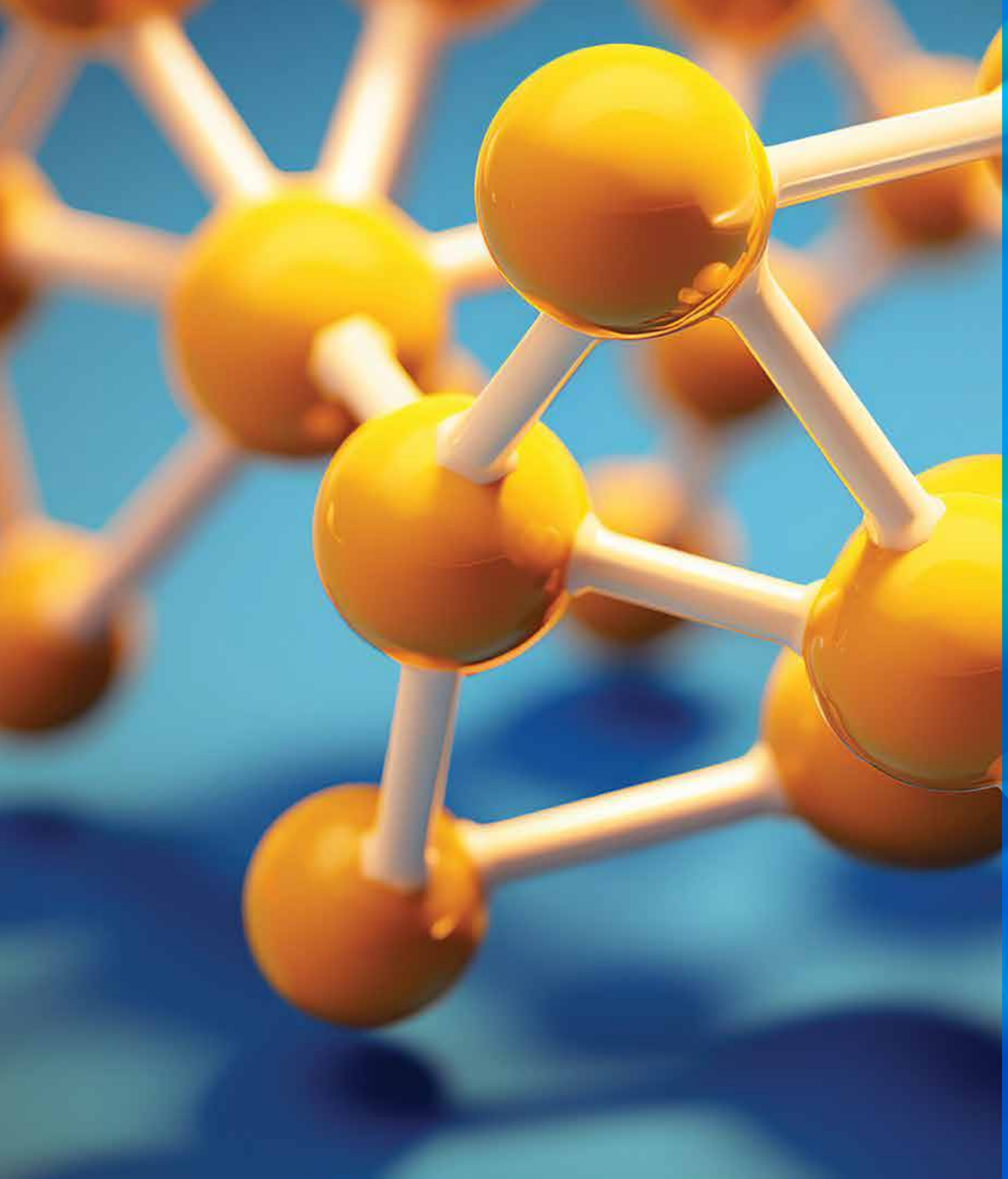


Fig 3
Photographs of laser-cut butterfly-shaped magnetic samples, magnetic tubes with gradient microstructure, and their active response.



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.

Magnetic sustentation as an adsorption characterization technique for paramagnetic metal-organic frameworks

Barroso, N., Andreo, J., Beobide, G., Castillo, O., Luque, A., Pérez-Yáñez, S., Wuttke, S. (2023) Communications Chemistry, 6 (1), art. no. 4,

> New sensing method based on the magnetic properties of metal-organic frameworks (MOFs) containing paramagnetic metal centres, which stands out for the rapidity, low cost and in situ direct measurement of the incorporated adsorbate within the porous material. Our simple and efficient method allows the direct determination of the adsorbed mass, as well as the measurement of adsorption isotherm curves, which will greatly advance the study of adsorption processes in solution.

In this paper we present a direct and low-cost characterization technique taking advantage on the intrinsic magnetic properties of paramagnetic metal-organic frameworks (MOFs) for the in situ study of adsorption processes in solution (Fig. 1). This method does not rely on the complex magnetic interactions that usually only emerge at temperatures well below room temperature. Instead, it is based on the weak attraction exerted by an external magnetic field on paramagnetic materials measured at room temperature.

We have developed the theoretical equations that guide magnetic sustentation experiments to better understand the process and experimentally verify its feasibility using paramagnetic MOFs. On the one hand, water-stable MIL-88A(Fe) was selected, demonstrating that the critical magnetic field it is not influenced by particles size in the range 1-6 μm. The adsorption of different organic molecules (Fig. 2) was quantified, and it was confirmed that there is a linear relationship between the critical magnetic field and captured mass. In order to prove the versatility of this new technique, the same experiments were recorded in ethanol using MOFs that are not water stable, isostructural Cu(II)- and Co(II)-MOF-74 and ZIF-67(Co).

All in all, this technique allowed obtaining adsorption isotherms curves, which altogether provides the advantage of performing a direct and in situ measurement of captured molecules and without the need for any sample preparation that conventional techniques such as ultraviolet spectroscopy usually require.

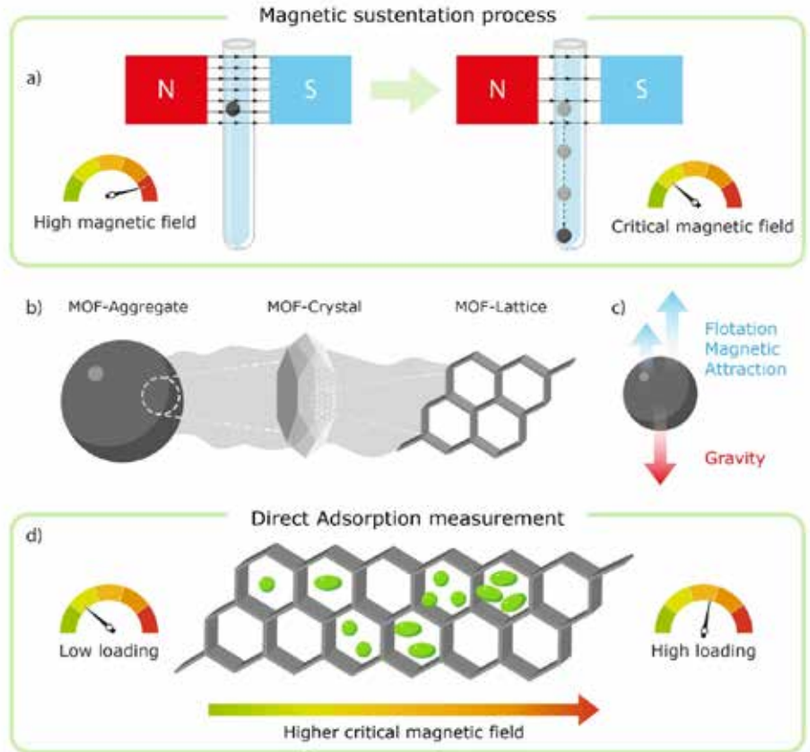


Fig 1
Magnetic sustentation process. a From high magnetic field (suspended aggregate) to the critical magnetic field (aggregate dropping); b the MOF aggregate composition; c forces acting on the aggregate; and d effect of the guest loading on the critical magnetic field.

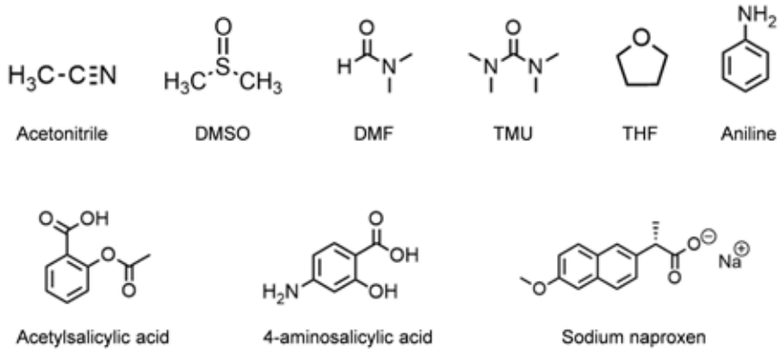


Fig 2
Organic compounds. Selected organic compounds for the adsorption measurements.

Alignment of Breathing Metal-Organic Framework Particles for Enhanced Water-Driven Actuation

G. Saiz, P., Reizabal, A., Luposchainsky, S., Vilas-Vilela, J.L., Lanceros-Mendez, S. and Dalton, P.D. (2023). Adv. Mater. Technol., 8: 2202063.

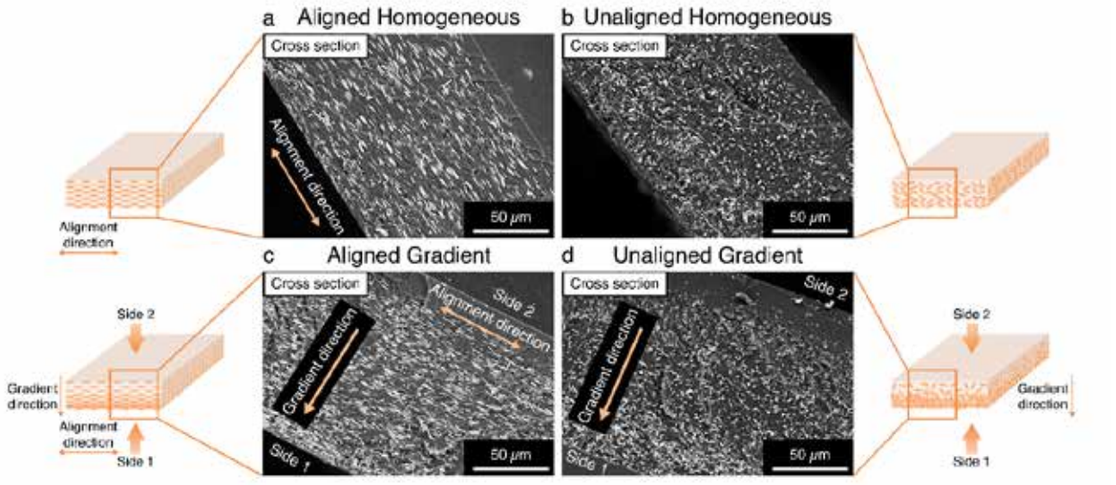


Fig 1
Selected SEM images of a) aligned and b) unaligned films with homogeneous distribution of MIL-88A; c) aligned and d) unaligned gradient distribution of MIL-88A particles with magnification 800x (more SEM images in SI 2.5).

Reticular chemistry has opened up avenues for the design of crystalline porous metal-organic frameworks (MOFs) at the molecular level, allowing precise control of nano and microcrystalline MOF materials. However, the translation of the anisotropic properties of single crystals into macroscale objects is still insufficiently addressed. This translation beyond MOF lattices is of great interest in order to efficiently utilize those materials for diverse applications, ranging from adsorption and sensing to electronic and ion conduction.

In this work, we investigated the effect of harnessing anisotropy at the micro and macro scale on the water-driven actuation of MIL-88A@PEGDA film composites (Fig. 1). We demonstrated that the alignment of breathable MOFs propagates their directional expansion to the macroscale, thus increasing directional folding of the films. The use of an E-field to rapidly achieve large areas of particle orientation, was showcased as a new tool for fabricating anisotropic MOF materials. Furthermore, we show and discuss how the enhanced actuation due to the translation of the MIL-88A expansion results in an increase in mechanical work as evidenced by the dynamometer measurements (Fig. 2). Moreover, by choosing a hydrophilic polymer as the film matrix we were able to improve movement speed and avoid the need of intervention to reactivate MIL-88A for each adsorption cycle (Fig. 3), further improving the applicability of these systems.

In the bigger picture, the translation of the anisotropic MOF properties from the individual microcrystals to the macroscale object opens the door to bridging the gap between the functionality of ordered molecular MOF lattices and MOF-based composites.

As the majority of known metal-organic frameworks (MOFs) possess anisotropic crystal lattices and thus anisotropic physicochemical properties, a pressing practical challenge in MOF research is the establishment of robust and simple processing methods to fully harness the anisotropic properties of the MOFs in various applications. We address this challenge by applying an E-field to precisely align MOF microcrystals and generate aligned MOF@polymer films and demonstrating the improved macroscopic properties compared to unaligned MOF@polymer films.

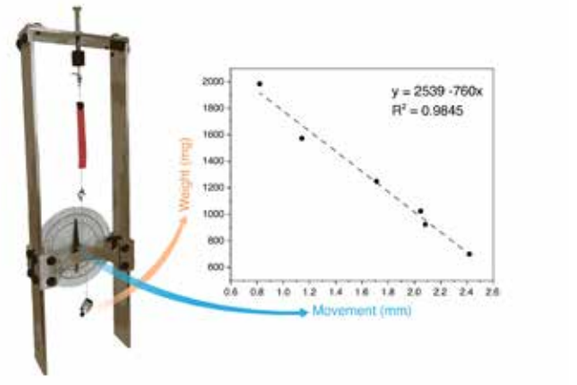


Fig 2
Mechanical strength of the aligned-gradient-large films measured by a self-constructed dynamometer.

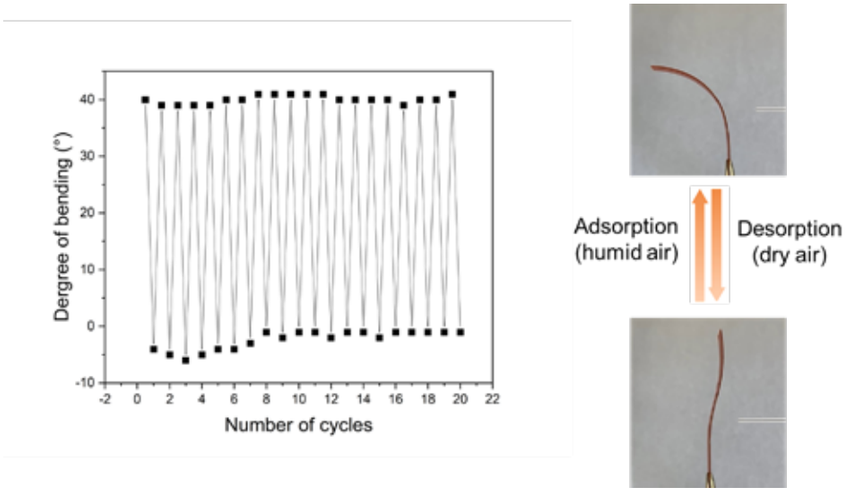
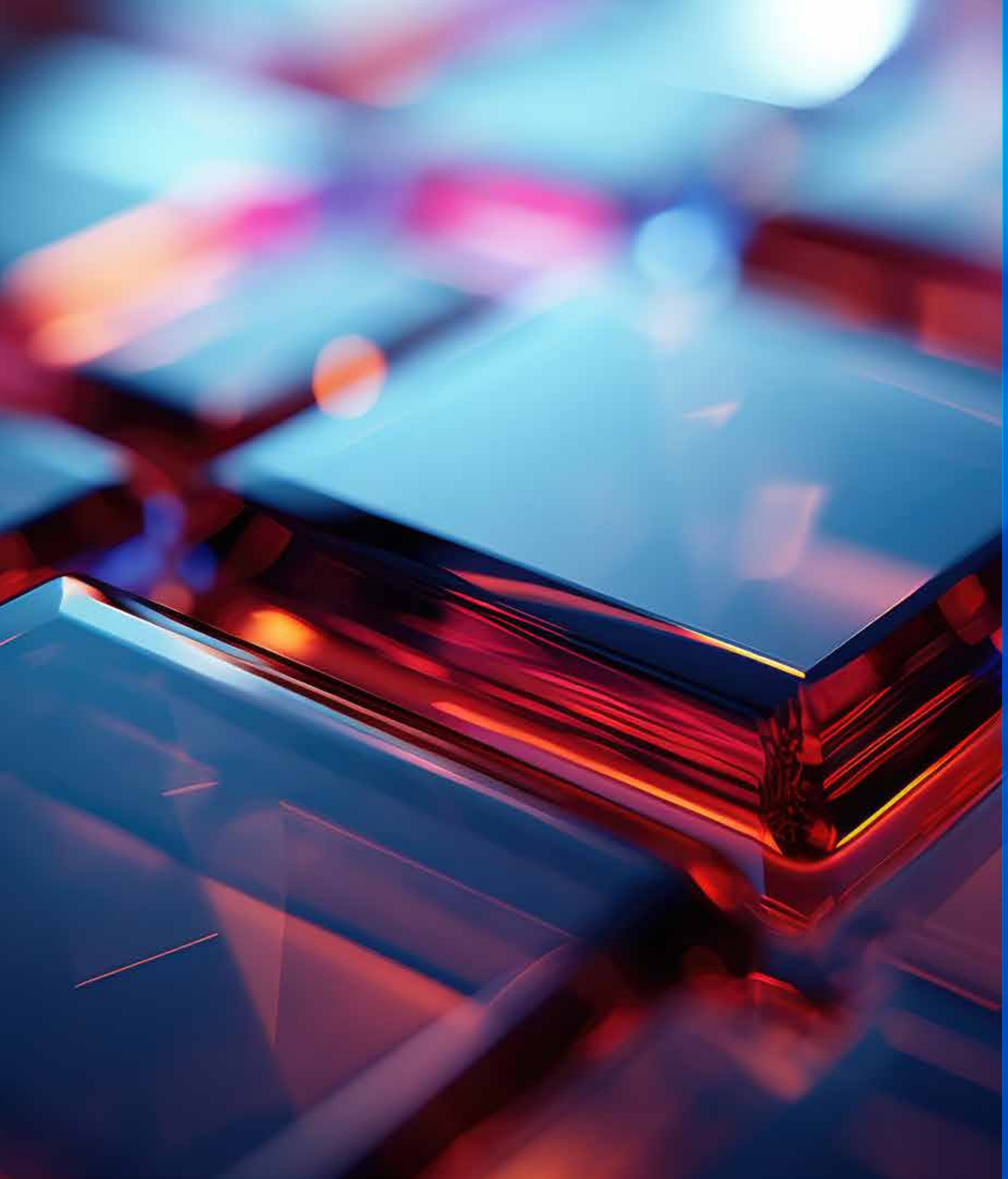


Fig 3
Cyclability of the aligned-gradient-large film upon exposure to humid/dry air.



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.

Shape memory and elastocaloric properties of melt-spun NiMn-based Heusler alloys

Elena Villa, Francesca Villa, Bosco Rodriguez Crespo, Patricia Lazpita, Daniel Salazar, H. Hosoda, V. Chernenko. J. Alloys and Compounds 965 (2023) 171437.

In the present work, five melt-spun ribbons of NiMn-based Heusler ferro- and meta-magnetic shape memory alloys (FSMAs and MMSMAs) have been prepared. Their martensitic transformation (MT) and thermomechanical properties have been studied. Whereas FSMAs ribbons showed a conventional stress-strain behavior at MT and conventional elastocaloric effect (eCE), MetaMSMAs ribbons, in turn, exhibited highly pronounced inverse stress-strain and inverse eCE characteristics at MT. The abnormal thermomechanical behavior of the MetaMSMA ribbons is produced by the presence of significant internal stresses due to appropriate amount of quenched-in defects. These results can serve as a guide for the design of new eCE-efficient materials in the form of ribbon.

Cooling/heating temperature dependences of the strain for tensile loaded ribbons of Heusler –type $Ni_{49}Mn_{20}Ga_{23}Cu_6Fe_2$ FSMA and $Ni_{34}Mn_{48}Sn_8Co_7Fe_3$ MetaMSMA were measured by using DMA Q800 of TA Instruments Co. The results of stress – strain measurements performed under different constant stresses are shown in Figs 1a and 2a. The curves exhibit the following anomalies produced by the martensitic transformation (MT): (i) FSMA ribbon elongates along applied tensile stress at the forward MT and actuates against the stress recovering its length during the reverse MT which is a clear manifestation of the normal shape memory effect; (ii) in turn, the mechanical behavior of MetaMSMA ribbon at MT is strikingly unusual, i.e., exactly opposite to the one of FSMA ribbon: instead of the elongation under tensile stress the ribbon is contracted at the forward MT. The curves shown in Figs. 1a and 2a were served for calculation of the temperature dependences of stress-induced entropy changes at reverse MT by the Maxwell relationship applied for eCE. Figs. 1b and 2b show calculated eCE curves. Whereas FSMA ribbon demonstrates conventional eCE (negative minimum), MetaMSMA ribbon exhibits eCE (positive maximum) which is termed as an inverse eCE. The inverse stress –strain and inverse eCE are resulting from the influence of the internal stresses occurring due to a high concentration of defects in the less-stoichiometric MetaMSMA. Generally, eCE in SMAs originates from two contributions: MT latent heat, , and the entropy change caused by the inelastic and elastic deformations of a sample. Although in studied MetaMSMAs λ is much larger than in FSMAs, the experiment reveals eCE signal about four times smaller (Figs. 1b,2b). This fact can be explained by the different sings of the aforementioned contributions. Indeed, the strain – temperature curves of these materials show opposite signs of slopes at MT. Hence, the entropy caused by a straining of MetaMSMAs should have opposite sign with respect to latent heat whereby reducing total value of eCE. In FSMAs these two contributions have the same sign.

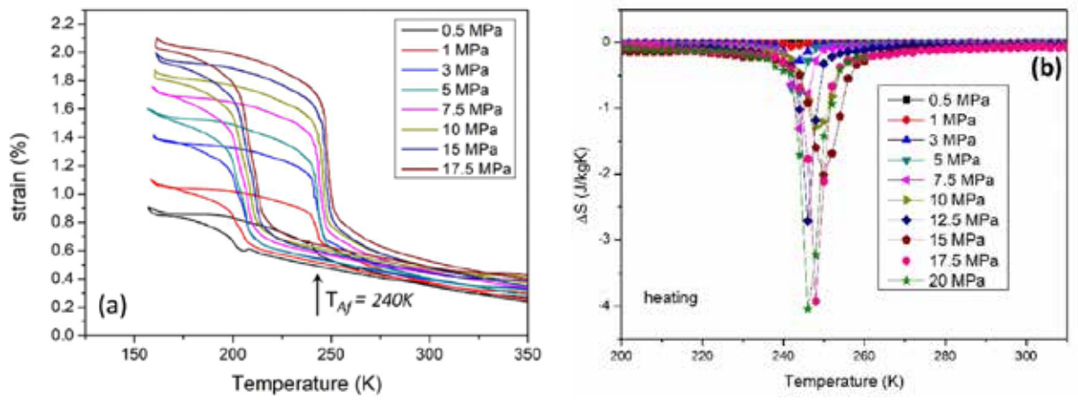


Fig 1
(a) Cooling/heating temperature dependences of the tensile strain for the FSMA ribbon recorded under constant applied tensile stresses. (b) Heating temperature dependences of the stress-induced entropy change, ΔS, of the FSMA ribbon calculated by Maxwell relationship using data from Fig.1(a).

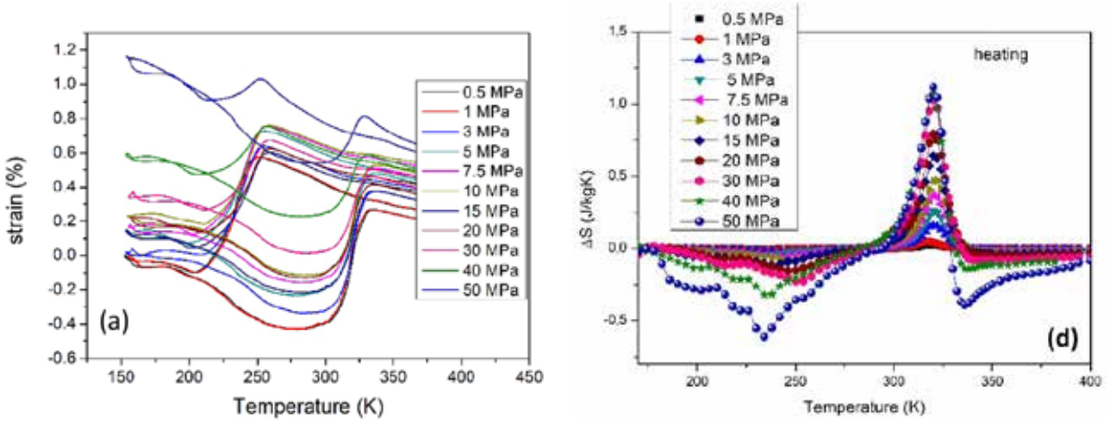


Fig 2
(a) Cooling/heating temperature dependences of the strain for the MetaMSMA ribbon recorded under constant tensile stresses. (b) Heating temperature dependences of the stress-induced entropy change, ΔS, for MetaMSMA ribbon calculated by Maxwell relationship using data from the graphs in Figs. 2(a).

Optimization of UV-C pulsed radiation strategy for a high-efficiency portable water sterilizer

Ruiz-Díez, C., Navarro-Segarra, M., Barrena, R., Gea, T., Esquivel, J.P. (2023) Environmental Technology and Innovation, 31, art. no. 103199

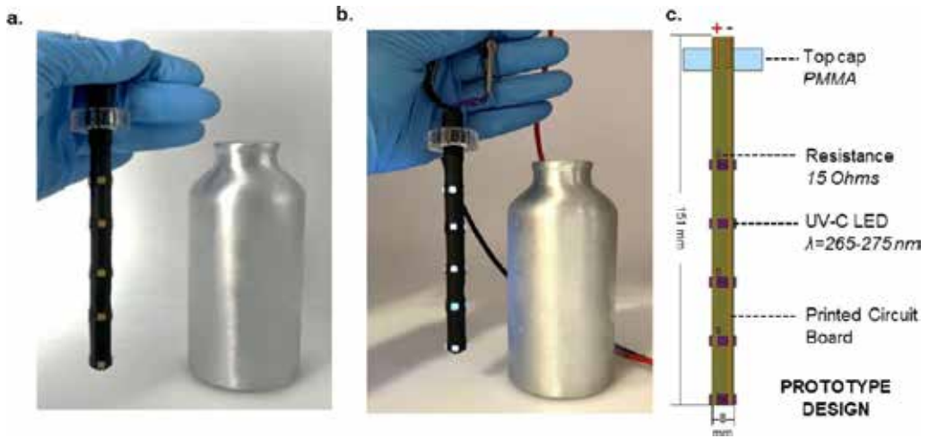


Fig 1
Image of the prototype and one of the 355 mL water vessels used for the sterilization experiments (a. with LEDs OFF and b. with LEDs ON); c. Schematic diagram of the device and its main components.

In many places of the world, the lack of municipal facilities for water sanitation and purification makes self-treatment at a familiar scale, the only realistic solution to ensure continuous access to drinking water. In this context, UV disinfection treatment is a portable and efficient alternative to conventional methods, however, its power need is hindering its implementation in remote off-grid households.

This work presents a portable water sterilizer device using UV-C LEDs, conceived for its direct implementation in isolated rural communities. Pulsed radiation operation has been studied as strategy to reduce the device energy demand. Most relevant parameters affecting the device operation and performance, namely voltage, radiation time, frequency and duty cycle; are thoroughly studied using the Design of Experiments methodology to optimize energy consumption and Escherichia coli removal from polluted water.

The optimal conditions, found for pulsed radiation, showed a noteworthy reduction of 68 % of the energy consumption while improving the sterilization effectiveness, compared with continuous radiation. Furthermore, the efficiency of sterilization of the optimized prototype was benchmarked against a commercial device using river water samples. The presented prototype achieved higher E. coli disinfection effectiveness using a fraction of the energy consumption.

The presented water sterilization device is an example of a technological improvement that satisfies performance requirements while prioritizing energy efficiency and technology accessibility. Energy is an increasingly valued resource, therefore, electronic devices of the future should be designed to run from renewable sources and have minimal resource consumption in order to ensure equitable technology access. To succeed in this, together with other present and future challenges, multiple areas of science and society must jointly develop the new era of technological solutions, all in all promoting a sustainable thrive which is only possible by applying a holistic and environmentally conscious grounded vision.

A portable water sterilizer device using UV-C LEDs to prevent health-risk diseases. Energy efficiency was placed as core priority during the prototype development. Design of Experiments methodology was used to optimize energy consumption. Using pulsed radiation strategy a reduction in energy demand of 68% was achieved. The prototype was benchmarked against a commercial device using river water samples.

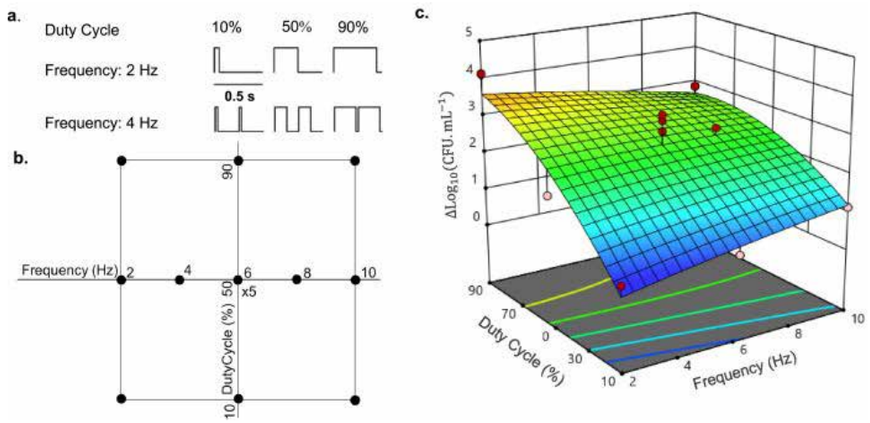


Fig 2
a. Example of pulses of 2 and 4 Hz at different duty cycles; b. Board of experiments of second sterilization assay; c. Reduction in E. coli population (log10 CFU mL). Experimental results are shown as red and pink dots. The mathematical model is presented as the heat-map surface.

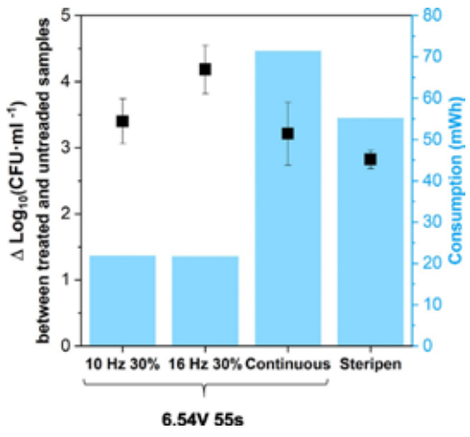


Fig 3
Comparison of bacterial inactivation and energy consumption for most favourable points (pulsed and continuous) and SteriPEN® commercial device. Bacterial inactivation is shown in dots and energy consumption in bars.

Overcoming Limitations in Water–Ethanol Sprayed Superstrate Solar Cells by Compositional Engineering of $Cu_2CdSn(S,Se)_4$

David Payno Zarceño, Maxim Guc, Samrana Kazim, Alejandro Pérez-Rodríguez, and Shahzada Ahmad
ACS Appl. Mater. Interfaces 2023, 15, 25684–25692

The increasing demand for solar energy requires materials from earth-abundant elements. We report solar cells based on $Cu_2CdSn(S,Se)_4$, deposited by spray pyrolysis using environmentally benign solvents, in a superstrate architecture. This reduces the potential cost of upscaling, the environmental hazards, and enabling its use in semi-transparent or tandem solar cells. The fabricated solar cells with $Cu_2CdSn(S_{2.8}Se_{1.2})$ gave a 3.5% power conversion efficiency, which is on par with the chalcogenides and the first report using $Cu_2CdSn(S,Se)_4$, paving the way for environmental friendly solar cells.

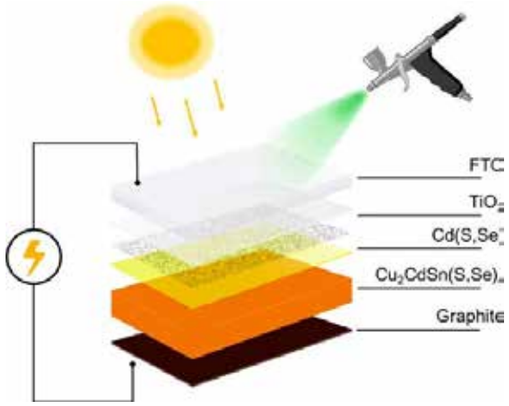


Fig 1
Water–Ethanol sprayed superstrate solar cells.

The current opportunities in the photovoltaic (PV) sector are constrained, mainly due to the requirements of optoelectronic properties and the quality of materials. A suitable bandgap, high conductivity, large charge diffusion length, slow bulk and interface charge recombination, and rational band alignment of the electron and hole transport layers are some of the key prerequisites that demand considerable scientific effort during the optimization of materials to yield high efficiency. We reported the first proof of concept of functional superstrate CCTSSe solar cells using spray pyrolysis from a simple molecular solution with benign solvents for the preparation of the absorber film. We showed that the introduction of Se into a Cu_2CdSnS_4 composition allows the control of the band gap while improving the required properties for their use as a light harvester (Figure 1). The transmittance of the substrate is 75% in the wavelengths above the bandgap of CdS, which is calculated to be 2.39 eV (Figure 2). The slight difference can be due to the changes in the crystalline quality and/or possible doping by Cu or Sn atoms coming from the absorber

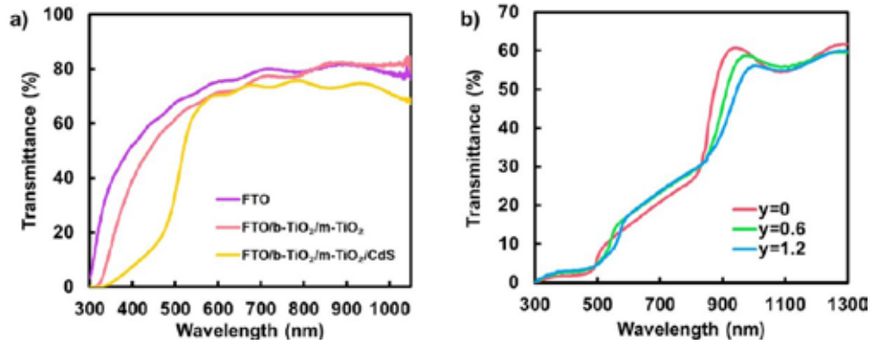


Fig 2
a) Transmittance spectra of the substrate after depositing each layer, and b) of the solar cells with different Se content.

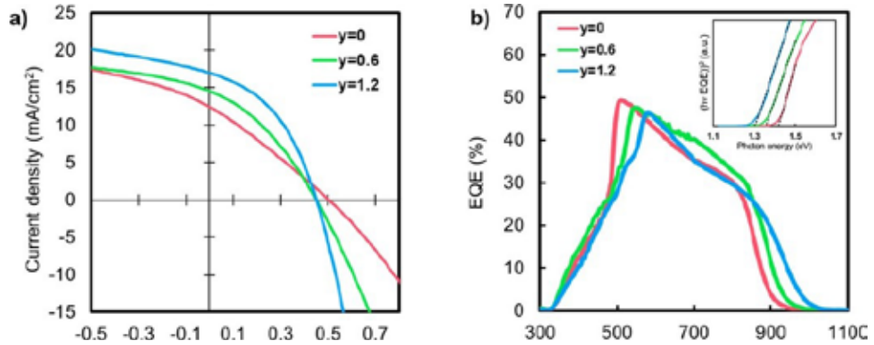


Fig 3
a) J–V curves of a device with the different conditions under 1 Sun illumination and b) EQE graph. The inset shows the band gap calculation from the band edge.

to the CdS during the absorber synthesis. The change of the band gap with the composition obeys Vegard's law for a Cd(S, Se) solid solution, suggesting a homogeneity in the absorber. A higher content of Se improves the fill factor (FF) owing to a reduction in the series resistance while presenting a lower Voc deficit. The FF is almost doubled with the introduction of 30% of Se/(S+Se) relative content, measuring a power conversion efficiency of 3.5%, a state-of-the-art value reported for quaternary materials in a superstrate architecture and comparable to similar materials used in a substrate architecture. Improving the crystallinity could promote such solar cells as a green and cost-effective alternative to the current PV technologies and, simultaneously, avoid the use of critical or scarce elements. The fabricated solar cells showed a broader EQE in both short and long wavelengths (Figure 3). The band gap of the absorber can be tuned from 1.4 eV to lower values depending on the Se content. Our results suggest that Se addition increases the diffusion length of the carriers and reduces the resistance, reaching suitable properties for efficient superstrate solar cells.

Influence of magnetic relaxation on magnetoelastic resonance-based detection

B. Sisniega, J. Gutiérrez, J.M. Barandiaran, J.M. Porro, A. García-Arribas. 2023 J. Phys. D: Appl. Phys. 56 105001

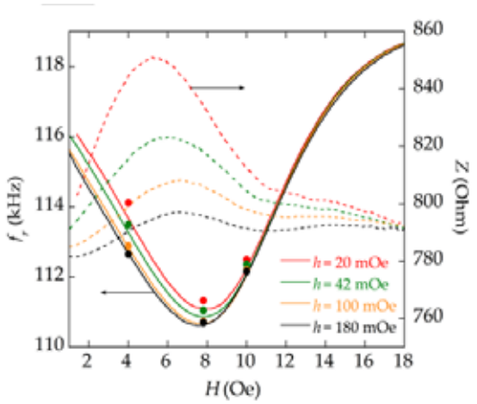


Fig 1
Influence of the bias field on the resonance frequency (solid lines) and maximum impedance (dashed lines) of the resonance curves for different values of the excitation amplitude h. Dots correspond to the relaxed values of the resonance frequency (calculated through the parameters fitted to equation (4) of the manuscript) for the different excitations and bias fields selected in the relaxation measurements.main components.

In the present study, we investigate the magnetic relaxation behaviour that takes place in amorphous ferromagnetic ribbons when they are used as magnetoelastic sensors. The study reveals that the effect of this relaxation on the sensor signal is considerable under certain conditions of the experiment, being the amplitude of the excitation a key factor that influences this process (Fig.1). Using an excitation amplitude of of h=20 mOe, relaxation times of about =2300 s and relaxation amplitudes of up to I=420 Hz (for applied bias field of 4 Oe) are observed. It is fundamental, therefore, to select the excitation and the operation point (bias field) in order to minimize the effect of the magnetic relaxation on the magnetoelastic sensor, always considering the compromise with the quality of the signal. It can be said that moderate excitation amplitudes (h ≥100 mOe) are, in general, suitable for measuring with these sensors, resulting in reasonably low relaxation times and relaxation amplitudes (<460 s, I <77 Hz). Since the origin of magnetic relaxation is based in sudden rearrangements of the magnetic domain structure in the material, we studied the magnetic domains formed in the ribbons at different applied fields through Magneto Optic Kerr Effect microscopy (Fig.2), which fully support the measured relaxation magnitude of the magnetoelastic resonance frequency.

Depending on the specific interest of each application, it will be necessary to evaluate whether to give priority to the speed of the measurement or, on the contrary, to the precision in the determination of the change in the resonance frequency associated with the measurand. If the measurement requires it, and the experimental procedure allows it, it could be convenient to wait a certain time (relaxation time) for the magnetization to relax in order to be able to make accurate quantitative measurements, which would be in this case less perturbed by this effect. Alternatively, if a post-processing is feasible, it can be possible to fit the sensor blank behaviour and subtract the relaxation in the operation conditions. It has been shown that this approach allows to reach the expected resolution of 1 µg in the mass detection experiment of CaC_2 O_4 precipitation performed in this study (Fig.3). In addition, annealing treatments of the amorphous ribbons have demonstrated to reduce the magnetic relaxation by relaxing the material reducing its density of structural defects and internal stress regions (disappearance of stress pattern domains). These treatments should be considered when using these materials as magnetoelastic sensors if good performance is to be achieved. Finally, as the resonance frequency of these sensors has been found to be very sensitive to this phenomenon, the measurements of magnetic relaxation performed by magnetoelastic resonance provide a novel, simple and accurate method of general interest to be employed in the study of magnetic relaxation processes of amorphous ferromagnetic materials.

Magnetic relaxation in amorphous ferromagnetic alloys can result in an undesired time evolution of the magnetization that produces serious drawbacks in the use of these materials in sensor applications. Here we analyse the influence of magnetic relaxation on the performance of an amorphous ferromagnetic ribbon, in which the resonance frequency increases with time in a typical relaxation behaviour with a relaxation amplitude and a relaxation time that depend on the excitation conditions. The influence of this relaxation on the sensor performance and the possible approaches to overcome this problem are evaluated and applied to the case of a magnetoelastic sensor, operating as mass sensor, for monitoring a chemical precipitation reaction.

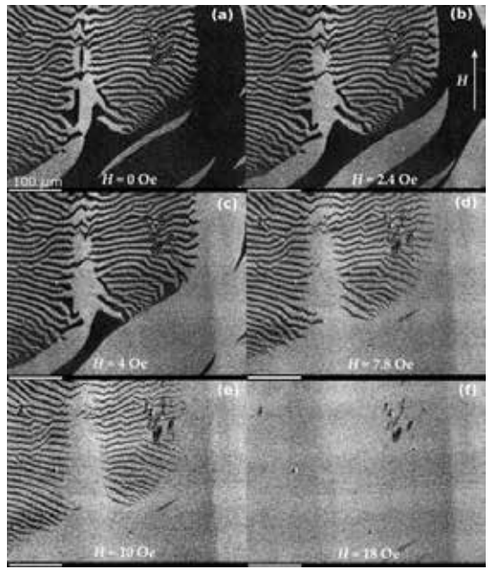


Fig 2
Kerr effect magnetic domain images of a representative zone of the surface of the ribbon at different applied fields (applied in the longitudinal direction of the ribbon): (a) 0 Oe, (b) 2.4 Oe, (c) 4 Oe, (d) 7.8 Oe, (e) 10 Oe and (f) 18 Oe..

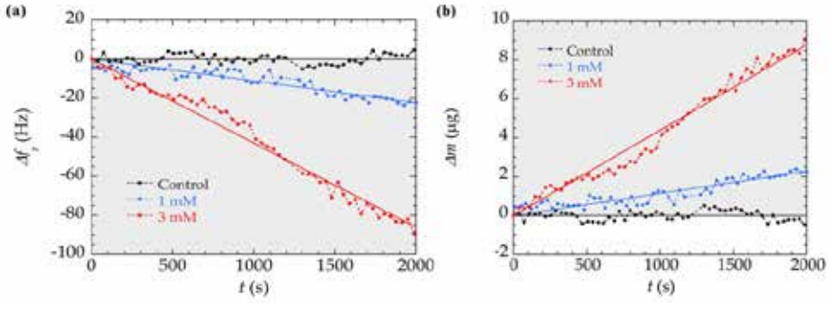
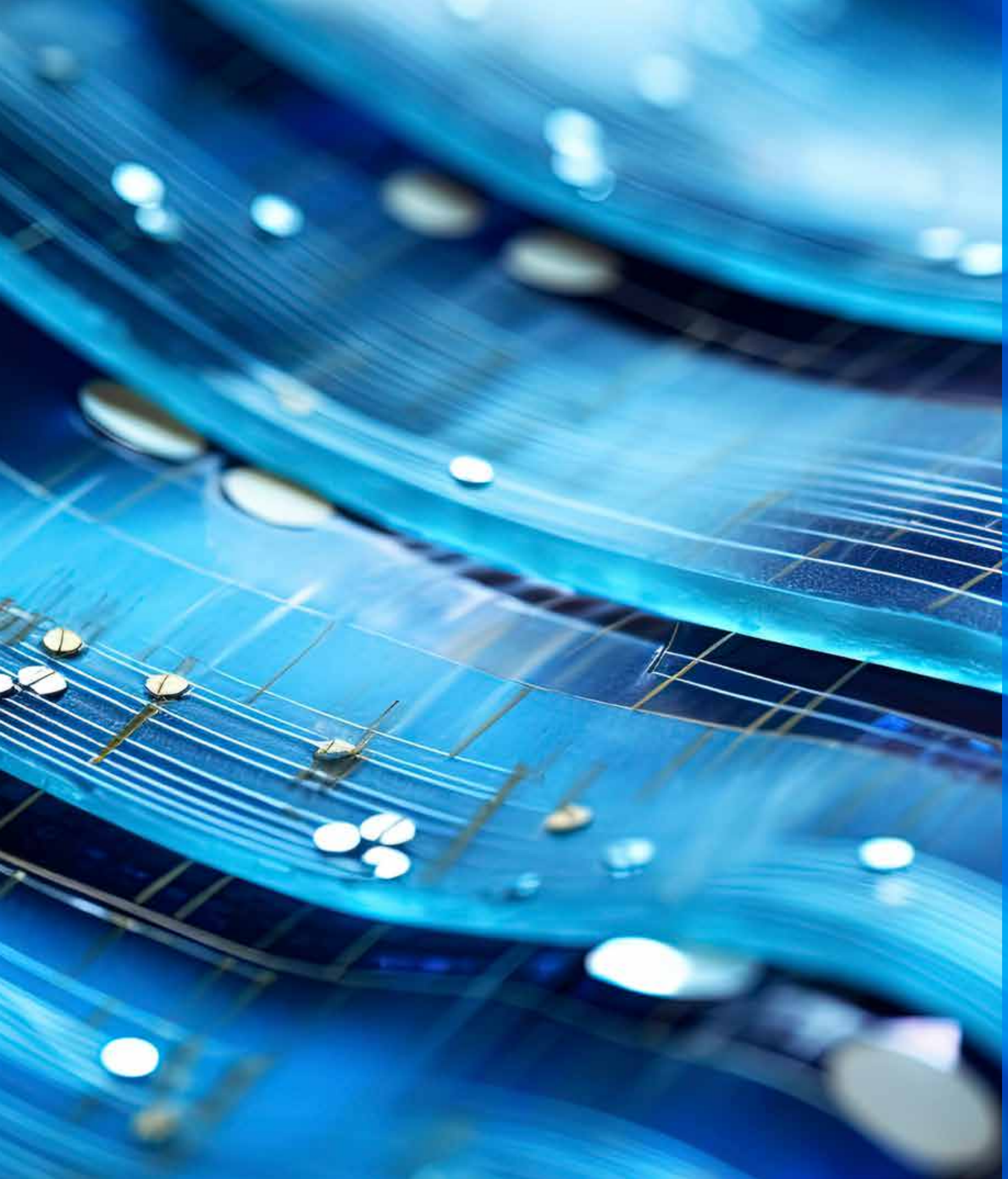


Fig 3
(a) Change of frequency and (b) estimated increment of the sensor mass during the measurement of CaC_2 O_4 precipitation, after correction of the magnetic relaxation. As seen, a sensitivity below 1µg is achieved.



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.

Screen-printed nickel hydroxide electrodes: Semiconducting, electrocatalytic, and electrochromic properties

A. Sánchez, A. E. Shalan, M. Rosales, I. Ruiz de Larramendi, and F. Javier del Campo. Journal of Electroanalytical Chemistry, vol. 928, p. 117052, Jan. 2023, doi: 10.1016/j.jelechem.2022.117052.

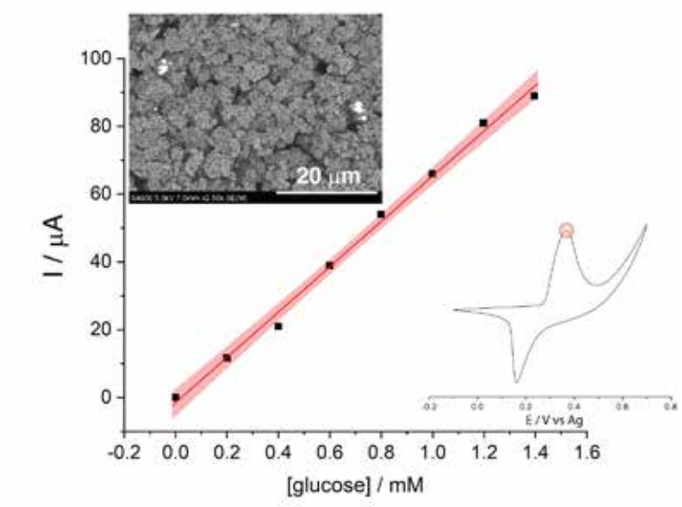


Fig 1
Screen printed Nickel Hydroxide electrodes catalyse the oxidation of glucose, thus enabling enzyme-less biosensing.

We have reported a highly active, screen-printable nickel hydroxide material that may find application in energy storage and electrocatalysis. $Ni(OH)_2$ has been grown by co-precipitation on the surface of conducting particles. Morphologic study by SEM and TEM images have allowed us to determine that these $Ni(OH)_2$ deposits differ in structure and thickness, depending on the synthesis conditions. Providing a larger surface area through the use of more conduction particles during synthesis leads to thin coatings that display better properties.
Regarding the electrochemical behaviour of the screen-printed ATO/$Ni(OH)_2$ electrodes, it has been observed that for low ATO: Ni precursor ratios, the voltammetric response obtained is sluggish and poor, but as the nickel layer becomes thinner and electrons can travel throughout the layer, the voltammetric response becomes better defined and with higher currents. The electrocatalytic properties of the screen-printed $Ni(OH)_2$ electrodes were also studied on the oxygen evolution reaction, OER, and the direct oxidation of glucose, demonstrating the suitability of these materials for electrolysers and for future enzyme-less glucose sensors.
The observed trends are also matched by the electrochromism of the materials, which seem to display an optimum response for the 10:1 – 15:1 ATO to Ni precursor weight ratio-paste electrodes.

This work introduces a method for creating metal-oxide inks for screen-printing, focusing on nickel hydroxide growth on conducting microparticles. Electrodes printed with this ink present and optical bandgap (4.06-4.15 eV) determined by diffuse reflectance spectroscopy, and can oxidise water at 0.7-0.8 V vs Ag, making them suitable for electrolyzers.
In addition, these electrodes enable direct glucose oxidation below 0.6 V vs Ag, suggesting enzyme-less biosensing applications, and exhibit electrochromism with a charge efficiency of 50 cm^2 C^{-1}. Additionally, they possess an This approach is extendable to other metal oxides, expanding the possibilities for screen-printed semiconductors and catalysts.

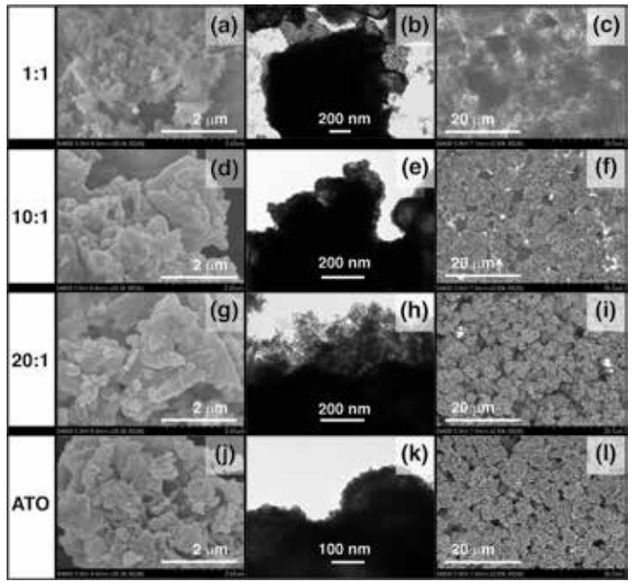


Fig 2
Nickel hydroxide supported on antimony-tin oxide microparticles. Nickel hydroxide content, and hence functionality, can be controlled through synthetic conditions. Deposit thicknesses in the range between 50 and 200 nm can be achieved.

Color efficiencies up to 50 cm^2 C^{-1}, in line with other reports for NiO electrodes, have been recorded. Although the contrast ratio was generally around 2, which is on the low side for visible electrochromic materials, the presented materials enable the fabrication of printed displays that may be suitable for disposable devices, such as smart tags.
The results presented here provide further evidence that for metal oxide films to be effective electrocatalysts, they need to be in the low nm range, and supported by a suitable electronic conductor. Last, it has also been shown that the bandgap of the printed structures may be adjusted by controlling the thickness of the semiconductor material on the supporting conducting particles, which may be useful in the development of printed electronics devices. Last, it is important to note that the approach presented here can be extended to other metal oxides, extending the scope of applications enormously.

Immuno-battery: A single use self-powered immunosensor for REASSURED diagnostics

Galyamin, D., Liébana, S., Esquivel, J.P., Sabaté, N.; (2023) Biosensors and Bioelectronics, 220, art. no. 114868

> This paper presents for the first time a self-powered immunosensor that makes use of a sample-independent chemistry to generate power upon the presence of a biomarker and provide operation voltages above 1.55 V. In particular, the device – which has been named Immuno-Battery – makes use of magnesium as anode and the widely employed HRP enzyme as antibody label as cathodic catalyst to detect C-reactive protein (CRP) presence in artificial samples. This work demonstrates a significant step forward towards the development of standalone POC self-powered devices with relevant opportunities for affordable and sustainable diagnostic.

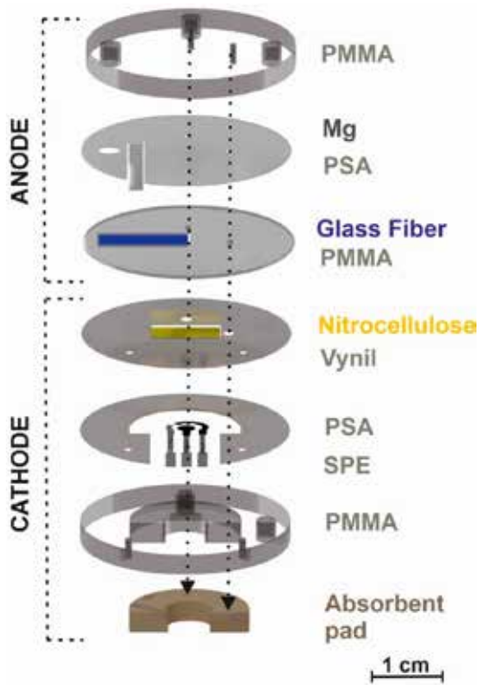


Fig 1
Exploded vision of the immuno-battery different layers.

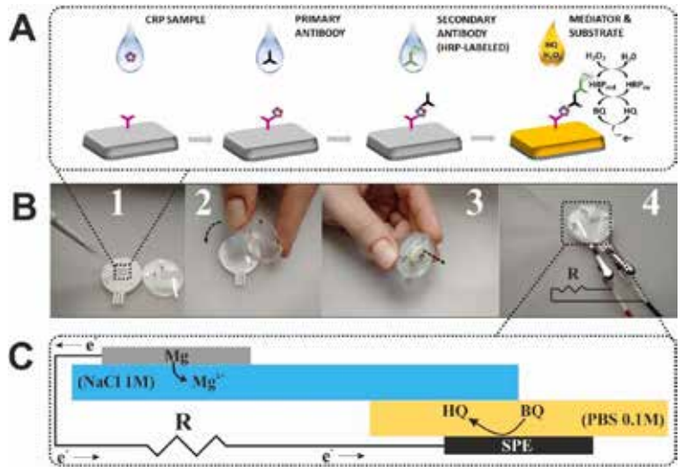


Fig 2
A) Immunoassay steps performed on the nitrocellulose layer located on top of the screen-printed cathode. B) Overview of the immuno-battery working principle: 1) Open device; 2) Anode and cathode sections are connected by magnetically closing the device; 3) Pins on the anode layer eject the absorbent pad located underneath the screen-printed cathode, and 4) Addition of saline electrolyte connects anode and cathode allowing for power generation and readout. C) Cross-section of the device showing anode and cathode reactions.

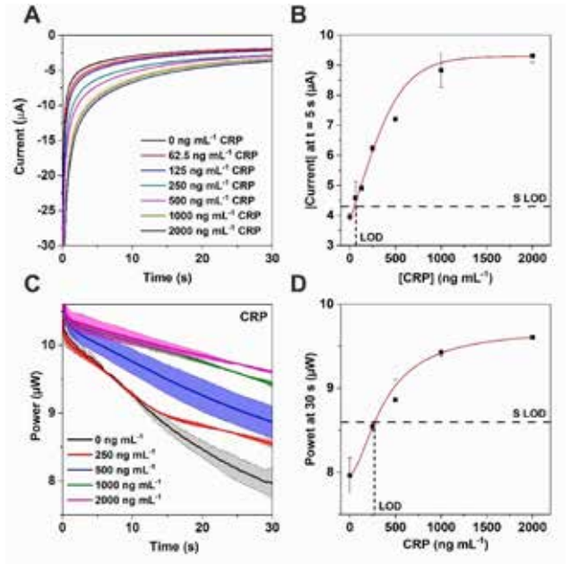


Fig 3
A) Chronoamperometric curves obtained for CRP concentration ranging from 62.5 to 2000 ng mL^{-1}. Potential applied 0.2 V vs. Ag/AgCl for 30 s. B) Fitting plot for amperometric currents taken at 5 s. C) CRP concentration dependent power changes across the battery under the influence of 270 kΩ resistor for CRP concentration ranging from 250 to 2000 ng mL^{-1}. D) Plot of the power generated at 30 s for the different CRP concentrations. In all cases, n = 3.

In the last decade, in-vitro diagnostics industry has invested significant resources to achieve the digitalization of rapid immunoassay tests that can help to remove ambiguities in the interpretation of the result and at the same time, unfold the possibility of data tracking and analysis at large scales (something that has proven to be particularly necessary in pandemic scenarios). Different strategies have been followed to achieve this objective.

In this work, we present a novel self-powered approach totally independent from any external energy source. We have developed a self-powered paper-based immunosensor that generates energy in the presence of the biomarker in the sample. In particular, the device – which has been labeled as Immuno-Battery – makes use of magnesium as anode and the widely employed HRP-labeled antibody as cathodic catalyst to detect C-reactive protein (CRP) presence in artificial samples. Feasibility of self-powered sensing is proved by submitting the immuno-battery to a resistive load. In this regime, the sensor provides operation voltages above 1.55 V and maximum power densities from 40 to 571 μW cm^{-2} that allow for future implementation of an electronic readout circuit. We have demonstrated that sensitivity of the system is not compromised by the self-powered mode operation, as the LOD value delivered by our battery (20 ± 2 ng mL^{-1}) is compliant with LOD values reported for protein detection in paper-based electrochemical immunoassays with chronoamperometric methods. Moreover, as a case study, a LOD of 269 ± 39 ng mL^{-1} is obtained for CRP detection, in accordance with available commercial high-sensitivity CRP detection kits.is proof-of-concept opens the path towards the development of digital diagnostic devices in a sustainable and affordable manner.

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.

Photocurable hybrid materials with high magnetodielectric coupling

Cristian Mendes-Felipe, Rui Carvalho, Pedro Martins, Oleksandr Igorovych Ivankov, Ivan Bobrikov, Viktor Petrenko, Jose Maria Porro, Marco Sangermano, Senentxu Lanceros-Mendez. ACS Applied Polymer Materials 5 (9), 7631-7641, 2023.

> Magnetodielectric materials are crucial for IoT devices enabling magnetic control of dielectric response. Together with the strong efforts to obtain magnetodielectric materials with high dielectric constants or low losses, there is still a big issue to be tackled in this field: how to achieve a large magnetodielectric coefficient (MD %) near room temperature. Here, photocurable magnetic hybrid materials can be interesting candidates but the study of how filler type, content and dispersion affect their properties is mandatory. In this way, maximum MD as large as 28% can been obtained.

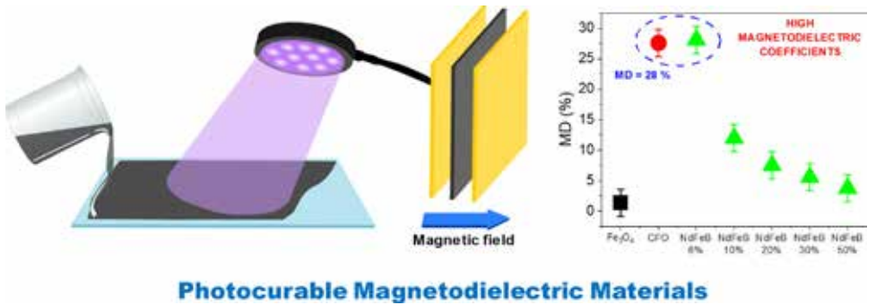


Fig 1
Schematic representation of the magnetodielectric sample preparation by photopolymerization process, magnetodielectric measurements and magnetodielectric coefficient (MD %) results.

IoT devices have undergone an important evolution in terms of materials, ranging from classic conductive or dielectric materials to more complex coupling of properties, such as magnetodielectrics, where dielectric permittivity variates under an applied magnetic field. Generally, the maximization of this magnetodielectric effect is desirable for different IoT components such as four-state memories or tunable filters. Together with the strong efforts to obtain magnetodielectric materials with high dielectric constants or low losses, there is still a big issue to be tackled in this field: how to achieve a large magnetodielectric coefficient (MD %) near room temperature.

One promising approach to overcome this issue, is the use of hybrid systems composed of dielectric and magnetic materials. Particularly, photocurable polymer-based composites are of high interest, as photopolymerization presents numerous advantages with respect to temperature curing including high production velocities, room-temperature processing, and the fabrication of a large variety of specific shapes with high spatial resolutions. Thus, the present work reports on polymer-based magnetodielectric composites, where photocurable polyurethane acrylate (PUA) is combined with different magnetic micro- and nanoparticles, including cobalt ferrite oxide (CFO), magnetite (Fe_3O_4), and a neodymium iron boron alloy (NdFeB).

It was shown that the presence of magnetic particles

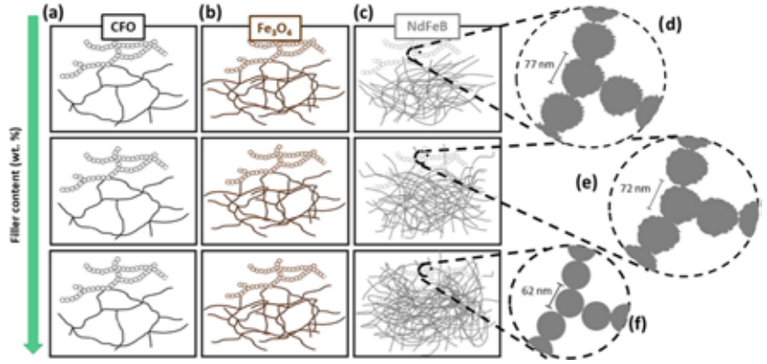


Fig 2
Scheme of the complex structural organization of inorganic magnetic particles within the polymer for CFO/PUA (a), Fe_3O_4/PUA (b), and NdFeB/PUA (c) composites. Surface-fractal organization as well as the characteristic size of the scattering objects for both Fe_3O_4/PUA and NdFeB/PUA composites (d–f).

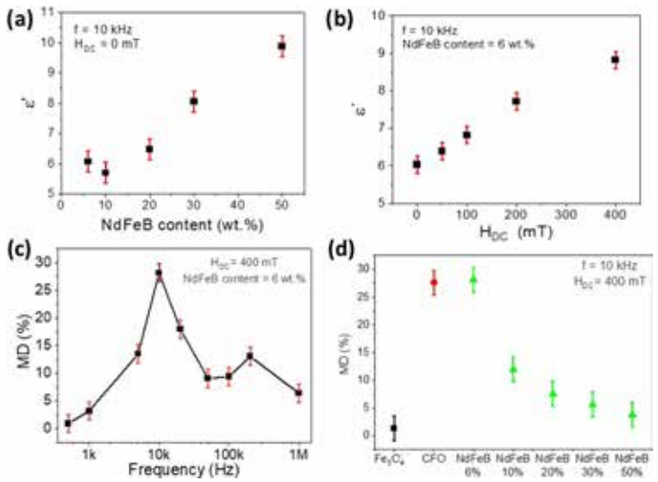


Fig 3
Dielectric constant (ε') as a function of the NdFeB wt. % at 10 kHz and 0 mT (a), ε' as a function of the DC magnetic field (HDC) at 10 kHz (b), magnetodielectric coefficient (MD %) as a function of the frequency at 400 mT (c), and MD (%) for different composite samples at 10 kHz and 400 mT (d).

influences negatively the photopolymerization of PUA. Furthermore, no new chemical interactions between the magnetic particles and the polymer are observed and particles do not suffer relevant variations either in structure or in crystallinity when they are incorporated into the PUA matrix. The dielectric constant (ε') and the AC electrical conductivity (σAC) of the composite films are dependent on the filler type, which is also related to the different structural organization of each filler along the polymer film as confirmed by SANS. Complex fractal-like aggregations were observed by scattering methods, and different structural parameters of mass and surface fractals were obtained for various fillers in the composites. Finally, MD values as high as 28% have been obtained for samples containing 6 wt. % content of CFO and NdFeB fillers, making these magnetic composites of paramount interest for the fabrication of magnetodielectric devices in the context of the digital transition.

Micelle Formation in Aqueous Solutions of the Cholesterol-Based Detergent Chobimalt Studied by Small-Angle Scattering

Artykulnyi, O.P., Siposova, K., Kriechbaum, M., ...Almásy, L., Petrenko, V. Molecules, 2023, 28(4), 1811

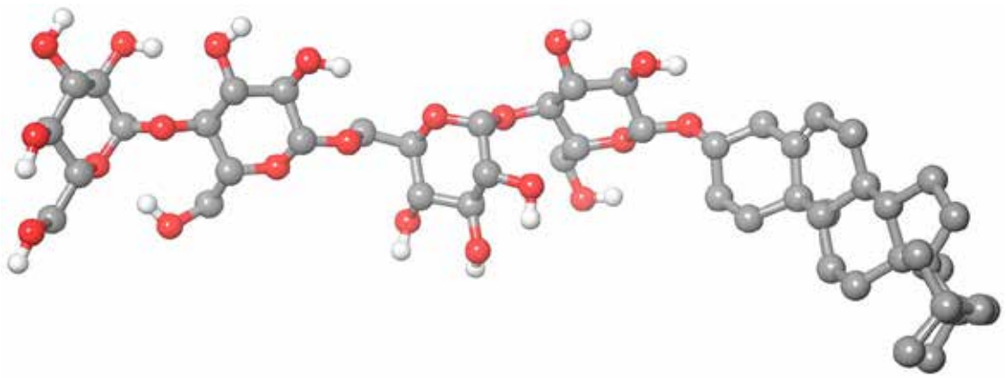


Fig 1
Three-dimensional chemical structure of Chobimalt molecule.

To study hydrophobic membranes or integral proteins in vitro, a special group of amphiphilic compounds called detergents (amphiphilic materials) comes to the rescue. Detergents micelles are used for the solubilization of membrane proteins during purification, crystallization, and a further in vitro analysis. The development of novel cholesterol-based detergents with an improved membrane-protein stabilization efficiency is an actual direction of the current research in this area. Knowledge of the detergent properties and, in particular, knowledge of the size and shape of micelles and the intermicellar interaction is necessary for the right choice of detergent and conditions for further work with proteins.

A novel water-soluble derivative of cholesterol named Chobimalt (Figure 1) is soluble form of cholesterol and, therefore, it is used for experimental modelling of the biological activity of cholesterol. In addition, Chobimalt has recently been successfully used to elucidate the effect of a cholesterol-based detergent on amyloidogenesis, and an intriguing dose-dependent effect of Chobimalt on the formation of an insulin amyloid formation has been discovered. Formation of micelles during protein fibrillogenesis should be considered among the factors determining the effectiveness of Chobimalt molecules. However, there is a lack of detailed information about the structural organization of Chobimalt micelles. Such parameters as the detergent micellar size and packing, detergent–detergent interaction, and hydrophilic–lipophilic balance are crucially important for Chobimalt applications and development.

The models of the cholesterol core–maltose shell interacting micelles were applied for both the SAXS and SANS data analyses. Polydisperse spherical or moderately elongated ellipsoidal shapes of the Chobimalt micelles were concluded in the studied concentration range, and the micelle aggregation numbers were determined from the calculated micelle volumes. The presence of HCl in the solvent did not exhibit a visible impact on the structure of the Chobimalt micelles. The critical micelles concentration value of the synthetic surfactant Chobimalt in water and in the acidic aqueous solution was determined by fluorescence measurements and found to be in the range of 2.5–3.0 μM. We can conclude that the present results may serve as reference information in studies of Chobimalt–protein complexes and various sugar-based surfactant solutions.

The structure and interaction parameters of the water-soluble cholesterol-based surfactant, Chobimalt, are investigated by small-angle neutron and X-ray scattering. It is important for further applications of chobimalt in bioscience and biotechnology. The obtained data are analyzed by a model-independent approach as well as considering a model fitting procedure, using a core-shell form factor and hard-sphere structure factor. The analysis reveals the formation of the polydisperse spherical or moderately elongated ellipsoidal shapes of the Chobimalt micelles with the hard sphere interaction.

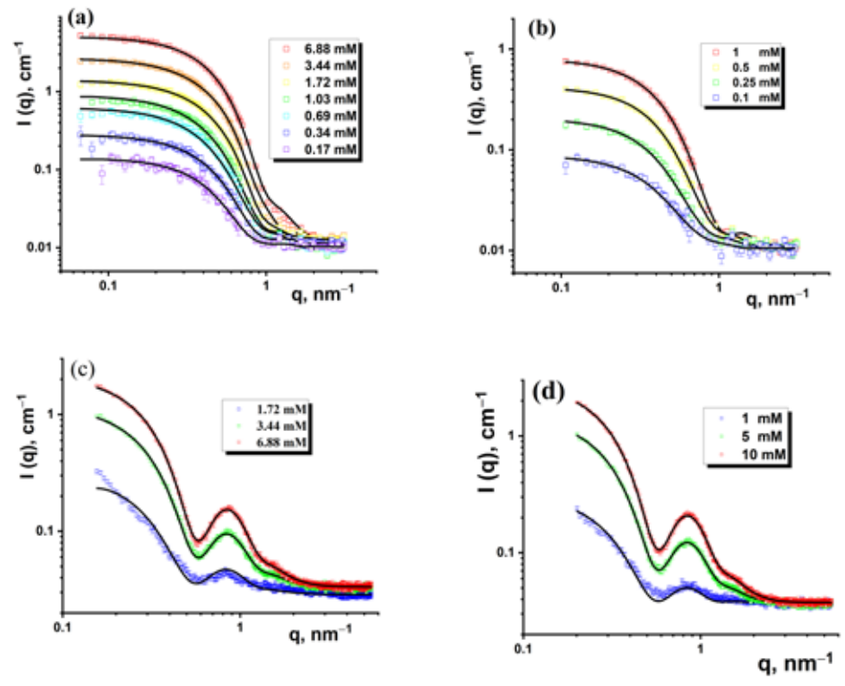
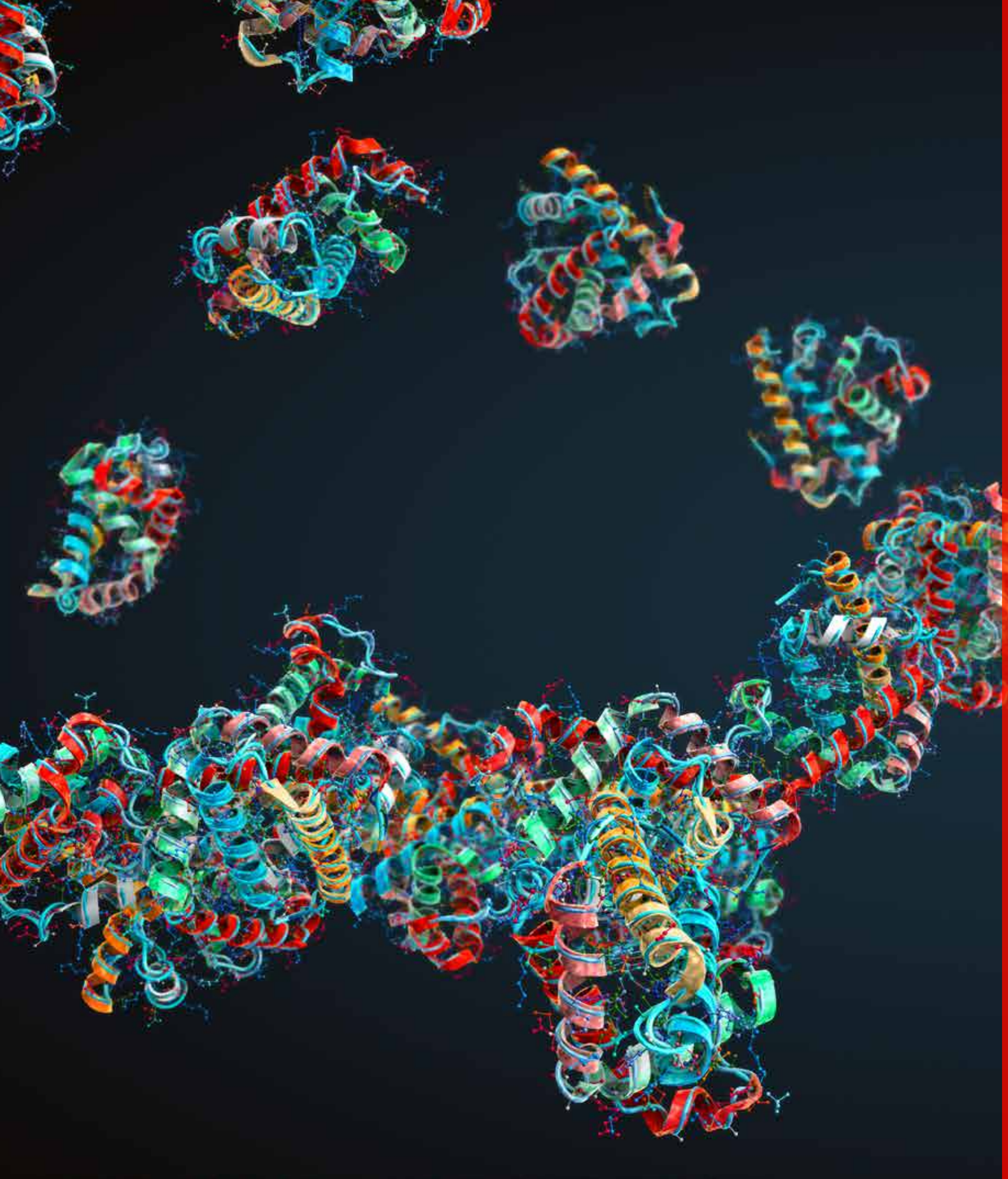


Fig 2
Experimental SANS (a, b) and SAXS (c, d) curves of Chobimalt micelles in water. Solid lines represent the model fits of the spherical core-shell form factor.



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.

Boosting the Photoluminescence Efficiency of InAs Nanocrystals Synthesized with Aminoarsine via a ZnSe Thick-Shell Overgrowth

Dongxu Zhu, Houman Bahmani Jalali, Gabriele Saleh, Francesco Di Stasio, Mirko Prato,Nefeli Polykarpou, Andreas Othonos, Sotirios Christodoulou, Yurii P. Ivanov,Giorgio Divitini, Ivan Infante, Luca De Trizio, and Liberato Manna. Adv. Mater.2023,35, 2303621

InAs-based nanocrystals, compliant with hazardous substance restrictions, show enhanced photoluminescence efficiency through optimized InAs@ZnSe core@shell synthesis. This allows tuning of ZnSe shell thickness to 7 mono-layers (ML), significantly boosting quantum yield to ~70% at ~900 nm. High yields are achieved with a minimum shell thickness of ~3ML. Photoluminescence lifetime varies minimally with shell thickness, while Auger recombination time extends from 11 to 38 ps for 1.5 to 7ML shells. Structural analyses reveal no strain at the core-shell interface, attributed to an In-Zn-Se interlayer, resembling In_2ZnSe_4 structure. Atomistic modeling confirms type-I heterostructure, indicating thick shells (>3ML) can passivate trap states and confine excitons in the core.

Colloidal near-infrared (NIR) emitting semiconductor nanocrystals (NCs) are increasingly important for optoelectronic devices like photovoltaics, LEDs, and biological imaging. While Hg and Pb-based NCs are effective, they are toxic. InAs-based NCs are RoHS compliant and can tune their optical bandgap from ~700 to ~1600 nm, ideal for commercial NIR devices. However, their photoluminescence (PL) quantum yield (QY) and Auger recombination rate need optimization. InAs NCs have low PL emission due to surface defects. Enhancing PL efficiency requires coating them with a material to form a type-I InAs@ shell heterostructure. Standard wider-bandgap semiconductors often don't match InAs's large lattice parameters, limiting shell material choices. CdSe, with minimal lattice mismatch, can achieve high PLQY, but its toxicity is a concern. To avoid toxic elements, ZnSe and ZnS are considered, but they present a high lattice mismatch with InAs, causing strain and low PLQY. Multi-shell NC systems with "buffer" layers reduce this strain. Examples include InAs@InP@ZnSe and InAs@InP@GaP@ZnSe NCs, showing high PLQY. Synthesizing these structures is complex and often involves toxic chemicals. Recent developments in synthesis methods use less toxic precursors like amino-As, aiming to improve control over InAs NCs size and distribution and prepare Cd-free heterostructures with high PL efficiency and low Auger recombination rate.

Our work advanced an amino-As and ZnCl2-based synthesis for InAs@ZnSe NCs, achieving a record PLQY of 42%. We refined this to control ZnSe shell thickness from ~1 to 7 mono-layers (ML). PLQY increased up to ~70% at 3.5ML, then plateaued. PL lifetime remained stable, while Auger recombination time increased with shell thickness. High-resolution STEM and XPS analysis indicated no strain at the core/shell interface and the presence of an In-Zn-Se interlayer.

Our atomistic model based on Density Functional Theory (DFT) aligns with these experimental observations. It suggests the interlayer, composed of In, Zn, Se, and cation vacancies similar to In_2ZnSe_4, reduces strain and supports a type-I heterostructure. The interlayer's complexity results in intermixed core and shell states. Effective surface trap passivation occurs with an overall shell thickness >3ML. This finding contradicts previous beliefs that a thick ZnSe shell would degrade optical properties on InAs NC cores. A thicker shell could reduce environmental leaching of indium and arsenic, positioning these NCs as ideal for commercial optoelectronic devices.

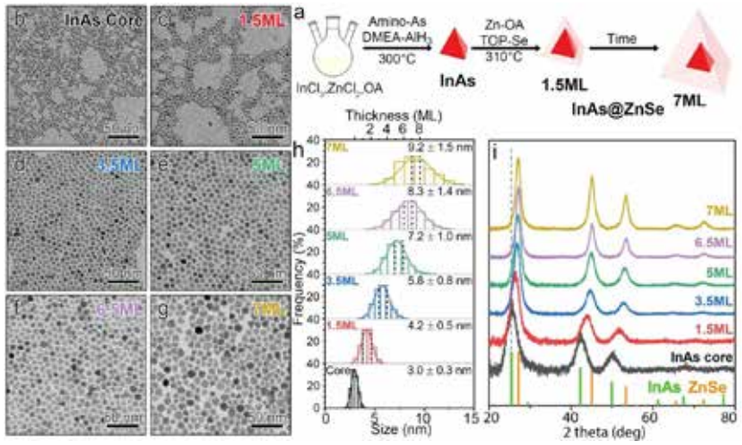


Fig 1
(a) Schematic of the synthesis process. TEM images showing the InAs core and core@shell NCs with shell thicknesses of 1.5ML (c), 3.5ML (d), 5ML (e), 6.5ML (f), and 7ML (g). The size distribution histograms (h) are calculated from TEM images, compared against sizes predicted by a structural/atomistic model, and XRD patterns (i) of InAs and InAs@ZnSe NCs are shown alongside bulk reflections of InAs and ZnSe.

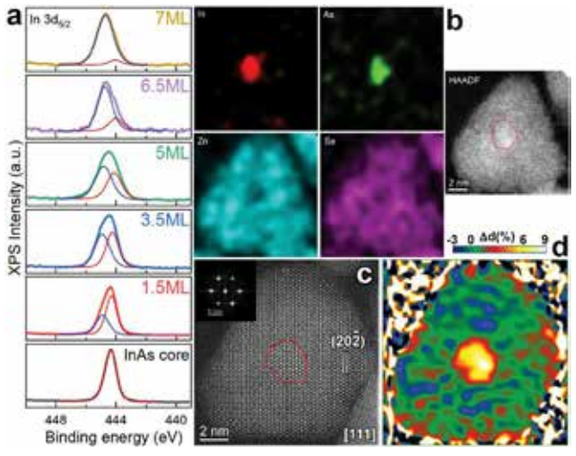


Fig 2
XPS spectra of InAs and InAs@ZnSe NCs and HR STEM characterization of individual 5ML InAs@ZnSe NCs. a) XPS spectral decomposition of the In signal, collected on the core and core@shell samples. b) HR STEM-EDX elemental maps; c) atomic resolution HAADF-STEM image of a core@shell NC oriented along the [111] zone axis and d) the corresponding GPA analysis in which the intensity of each point corresponds to the local value of the interplanar distance for the {220} planes

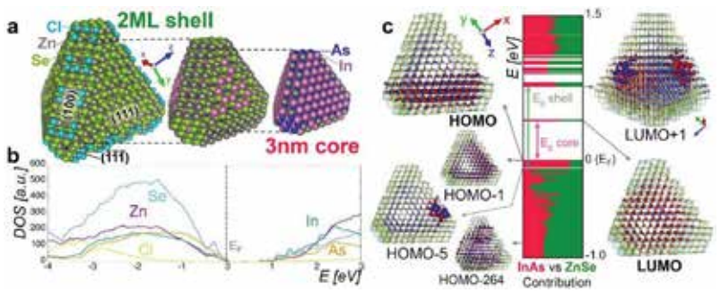


Fig 3
Atomistic structure representation (a) showing the entire core@shell NC, the core with the In-Zn-Se interlayer, and just the core. The density of states (DOS) of the core@shell NC is depicted (b), along with the energy levels of molecular orbitals (MOs) around the Fermi energy (c). The InAs and ZnSe contributions to each energy level are indicated in red and green, respectively. The red and green arrows highlight the core and shell band gaps, respectively.

Ligand dynamics on the surface of CdSe nanocrystals

Cosseddu, S., Pascazio, R., Giansante, C., Manna, L., Infante, I.; Nanoscale, 2023,15, 7410-7419

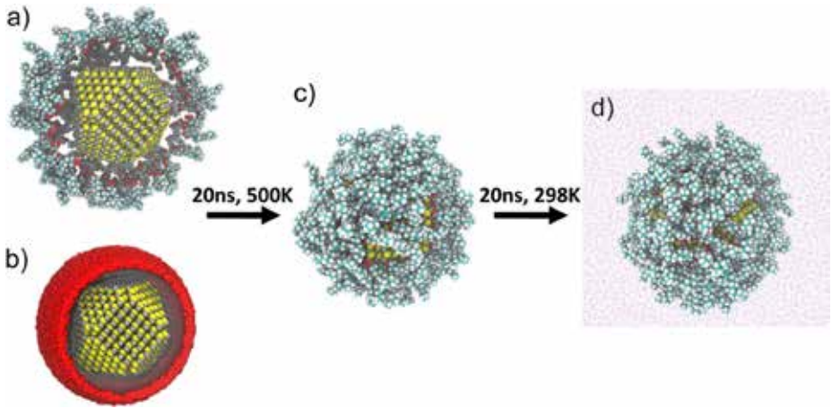


Fig 1
Depiction of a productive run. (a) Initial collocation of oleate ligands on random spheres at 1 nm from the NC surface. (b) Cumulative locations of the ligand oxygen atoms on the spheres. (c) Structural representation of the ligand packing in vacuum after 20 ns in vacuum, NVE ensemble. (d) Structural representation of the ligand packing in solvent after 20 ns of annealing, NpT ensemble

This work delves into the surface chemistry of colloidal semiconductor nanocrystals (NCs), particularly focusing on CdSe NCs. These nanometric particles, often passivated by organic ligands, are crucial in stabilizing NCs in organic solvents and preventing aggregation. The small size of NCs results in a higher surface-to-volume ratio, exposing a large fraction of atoms at the surface. These under-coordinated and mobile atoms may lead to surface defects, introducing "midgap" states that reduce photoluminescence quantum yield (PLQY) and hinder charge transport.

Surface ligands play a vital role in passivating these defects and adjusting energy levels outside the bandgap. While core–shell-type structures with wider bandgap materials have been successful in eliminating midgap states and achieving high PLQY, they also introduce barriers to inter-NC charge transport. An alternative is the use of short organic or inorganic ligands through ligand exchange mechanisms to eliminate surface defects and enhance electronic coupling. Typically, experimental tools like solid-state nuclear magnetic resonance (NMR) and Fourier-transform infrared (FT-IR) spectroscopy are utilized to understand ligand binding modes and coverage on the NC surface. Despite these advancements, controlling PLQY or transport properties through ligand choice remains a challenge, with many variables still not fully understood.

The paper makes a significant contribution by employing classical molecular dynamics (MD) simulations to investigate the inorganic/organic interface of CdSe NCs. The simulations elucidate ligand binding modalities (location, mobility, structure) on the NC surface and their role in stabilizing and optimizing surface coordination. The study reveals that ligand surface coverage is temperature-dependent and facet-specific. Strategies are proposed to improve NC materials, including increasing ligand density to reduce di-coordinated Se, a source of hole traps, and using neutral Z-type metal complexes for better Se-rich facet coordination.

Overall, the work offers new insights and strategies for enhancing the optoelectronic properties of CdSe and other metal chalcogenide NCs, demonstrating the importance of a detailed understanding of NC surface chemistry.

This study explores colloidal semiconductor nanocrystals (NCs) synthesis, focusing on organic ligands' role in stabilizing NCs in solvents. It emphasizes understanding ligand distribution, binding, and mobility on NC facets to prevent defects and enhance optoelectronic efficiency. Using molecular dynamics (MD) simulations, the paper investigates carboxylate ligands on CdSe NC facets, revealing temperature and surface atom coordination number influence ligand behavior. High mobility and structural changes are linked to low Cd atom coordination. Undercoordinated Se atoms, often causing hole trap states, spontaneously form, potentially quenching photoluminescence efficiently.

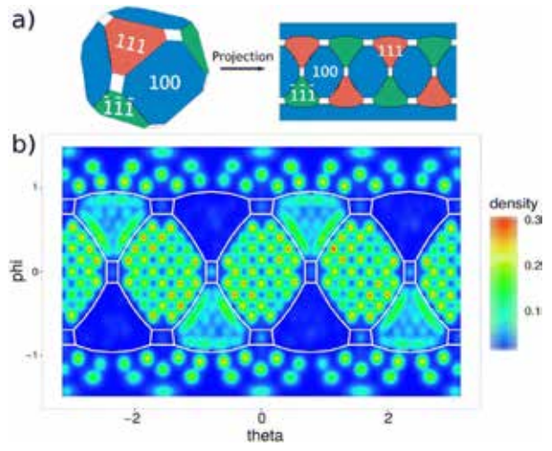


Fig 2
Composition of ligands on the different NC facets. (a) Two-dimensional map of the CdSe NC facets. (b) Density map of the locations of the ligands on the different binding sites of the individual facets.annealing, NpT ensemble

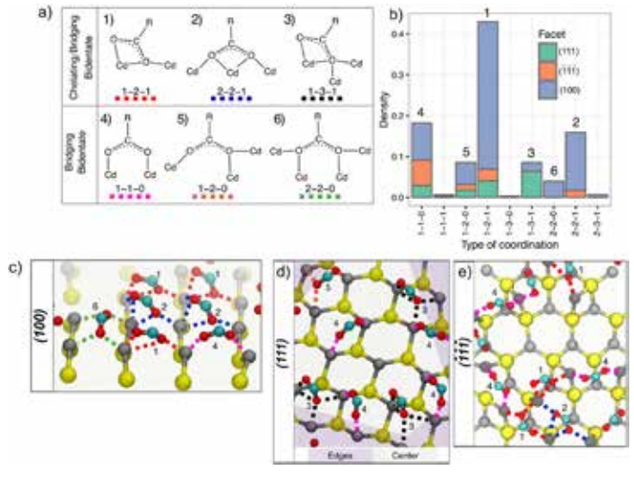
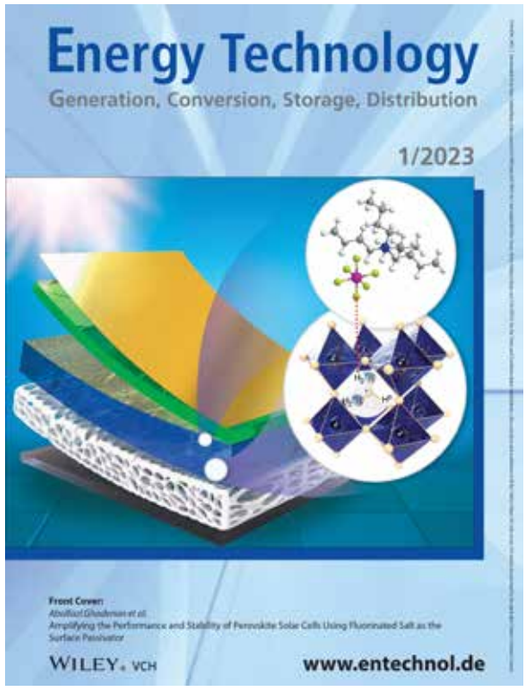


Fig 3
Binding modes of the ligands on the surface of the NC model. (a) Schematic representation of the six most common binding modes. (b) Schematic representation of the density of the different binding modes on the three most packed NC facets, (100), (-1-1-1)and (111). (c) Binding modes on (100) facets. (d) Binding modes on (111) facets. (e) Binding modes on (-1-1-1) facets.

JOURNAL COVERS
SELECTION



Energy Technology

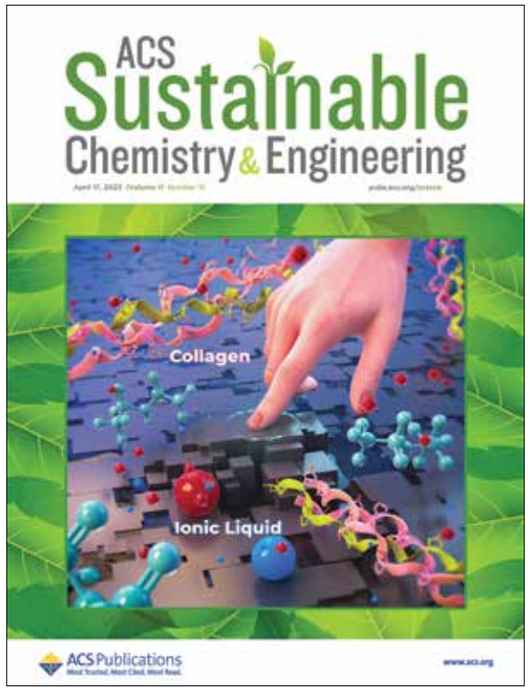
Amplifying the Performance and Stability of Perovskite Solar Cells Using Fluorinated Salt as the Surface Passivator. *Abolfazl Ghaderian, Naveen Harindu Hemasiri, Shahzada Ahmad, Samrana Kazim.*

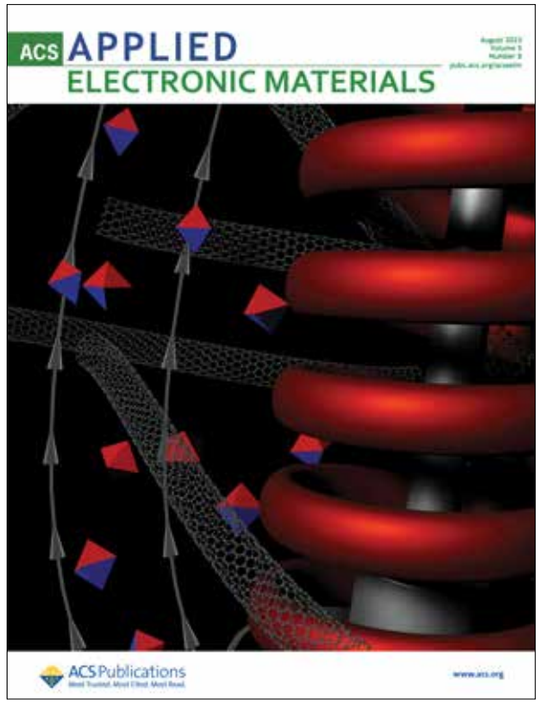
The 3D-halide perovskite-based solar cells have shown outstanding power conversion efficiency, while the layered perovskite is emerging as the advanced version to deliver high stability. Galvanized with the surge of the report of layered perovskites, a common salt tetra-n-butyl ammonium hexafluorophosphate (TBAPF) as a passivating agent between perovskite and hole transporting layer that improves the power conversion efficiency and stability, is explored. The use of TBAPF as a surface passivator mitigates the surface defects and increases hydrophobicity. The fluorine atoms in TBAPF provide hydrogen bonding interaction with the hydrogen of organic ammonium cation in perovskite established by proton nuclear magnetic resonance techniques. Effective charge extraction to the hole transport layer is suggested by steady-state photoluminescence measurements, showing higher quenching with the passivated perovskite compared to the pristine perovskite. The results suggest that TBAPF treatment improves the junction quality and minimizes the defects by virtue of H bonding, which in turn improves the photovoltaic parameters and long-term stability.

Sustainable Chemistry & Engineering

Sustainable Collagen Blends with Different Ionic Liquids for Resistive Touch Sensing Applications. *Mireia Andonegi Mireia Andonegi, Daniela Correia, Nelson Pereira, Manuel Salado, Carlos M. Costa, Senentxu Lanceros-Mendez, Koro de la Caba, Pedro Guerrero.*

Considering the sustainable development goals to reduce environmental impact, sustainable sensors based on natural polymers are a priority as the large im plementation of these materials is required considering the Internet of Things (IoT) paradigm. In this context, the present work reports on sustainable blends based on collagen and different ionic liquids (ILs), including ([Ch][DHP], [Ch][TSI], [Ch][Seri]) and ([Emim][TFSI]), processed with varying contents and types of ILs in order to tailor the electrical response. Varying IL types and contents leads to different interactions with the collagen polymer matrix and, therefore, to varying mechanical, thermal, and electrical properties. Collagen/[Ch][Seri] samples display the most pronounced decrease of the tensile strength (3.2 ± 0.4 MPa) and an increase of the elongation at break (50.6 ± 1.5%). The best ionic conductivity value of 0.023 mS cm−1 has been obtained for the sample with 40 wt % of the IL [Ch][Seri]. The functional response of the collagen–IL films has been demonstrated on a resistive touch sensor whose response depends on the ionic conductivity, being suitable for the next generation of sustainable touch sensing devices.





Applied Electronic Materials

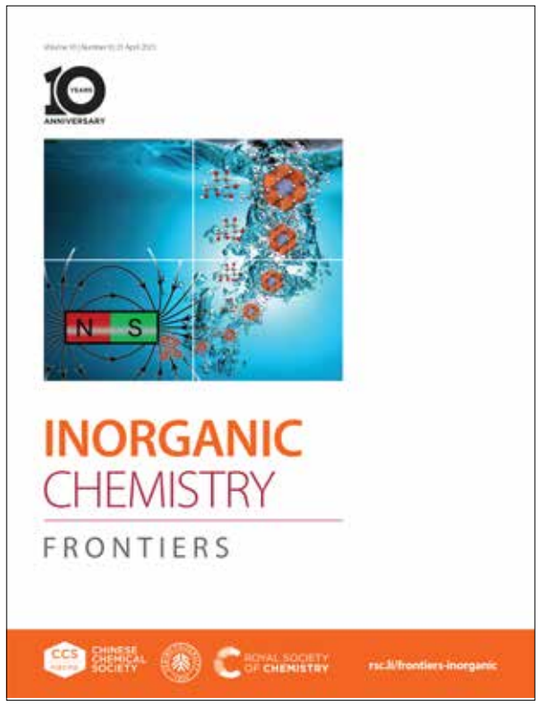
Ternary Multifunctional Composites with Magnetorheological Actuation and Piezoresistive Sensing Response. *Josu Fernández Maestu, Ander García Díez, Carmen R. Tubio, Ainara Gómez, Joanes Berasategui, Pedro Costa, M. Mounir Bou-Ali, Jon Gutiérrez Etxebarria, and Senentxu Lanceros-Méndez.*

Advances in the development and implementation of magnetorheological elastomers (MREs) have demonstrated their potential for vibration control and damping, among others. To increase further the applicability of MREs, the present work reports on MREs with piezoresistive self-sensing characteristics by adding conductive fillers. Multifunctional MREs are thus reported based on the styrene–ethylene–butylene–styrene (SEBS) polymer matrix with embedded Fe3O4 nanoparticles as magnetically responsive materials and multiwalled carbon nanotubes (MWCNT) as conductive fillers. Specifically, SEBS-based composites with a constant 20 wt % Fe3O4 content and different concentrations of MWCNT have been prepared. The effect of MWCNT addition on the morphological, mechanical, electrical, magnetorheological, and piezoresistive properties of the MRE-based composites was explored. Increasing MWCNT filler content leads to an increase of the Young's modulus and maximum elongation of the composite. All samples show a notable MR effect, a maximum MR response of 9% being obtained for the 5 wt % MWCNT sample.

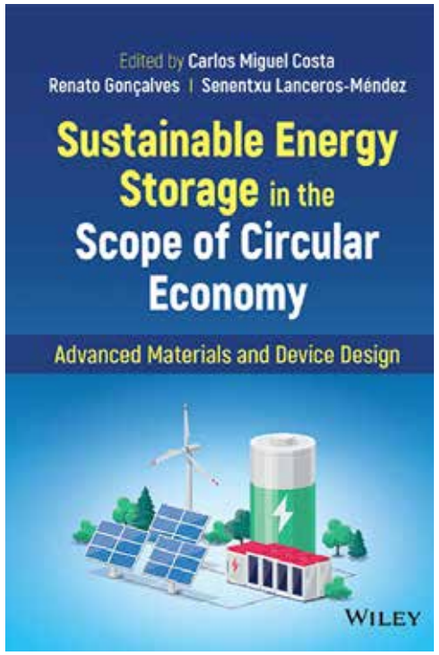
Inorganic Chemistry Frontiers

An in solution adsorption characterization technique based on the response to an external magnetic field of porous paramagnetic materials: application on supramolecular metal–adenine frameworks containing heterometallic heptameric clusters.
Jon Pascual-Colino, Rubén Pérez-Aguirre, Garikoitz Beobide, Oscar Castillo, Imanol de Pedro, Antonio Luque, Sandra Mena-Gutiérrez and Sonia Pérez-Yáñez.

Herein we explore the opportunities arising from combining magnetic properties and porosity in metal–organic materials. In this sense, we have prepared an adenine based homometallic wheel-shaped heptameric [Cu7(μ-adeninato)6(μ3-OH)6(μ-OH2)4]2+ entity containing two metal coordination environments: CuO6 at the core of the wheel with an unusually modest Jahn–Teller distortion and six peripheral CuN2O4 with a more pronounced elongation. The difference in the coordination environments of this compound facilitates the selective replacement of the central metal position by other metal centers (ZnII, NiII, CoII and CrIII) and boosts the magnetic properties of the homometallic heptameric entity. The nature of the central metal modulates the complex net of ferro- and antiferromagnetic superexchange pathways within the heptameric entity to tune the total spin (ST = 3 (Cu6Zn), 5/2 (Cu6Cu), 2 (Cu6Ni), 3/2 (Cu6Co), and 9/2 (Cu6Cr)).



PUBLISHED **BOOKS**



Sustainable Energy Storage in the Scope of Circular Economy: Advanced Materials and Device Design

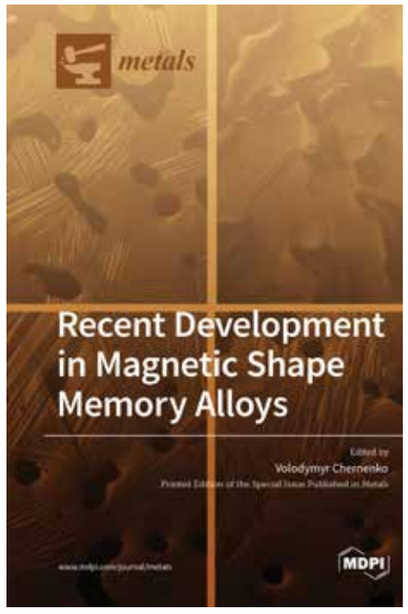
Editors:Carlos Miguel Costa, Renato Gonçalves, Senentxu Lanceros-Méndez

Sustainable Energy Storage in the Scope of Circular Economy reviews the recent developments in energy storage devices based on sustainable materials within the framework of the circular economy, addressing the sustainable design and application of energy storage devices with consideration of the key advantages and remaining challenges in this rapidly evolving research field. Topics covered include:sustainable materials for batteries and fuel cell devices, multifunctional sustainable materials for energy storage, energy storage devices in the scope of the Internet of Things, sustainable energy storage devices and device design for sensors and actuators, waste prevention for energy storage devices based on second life and recycling procedures
With detailed information on today's most effective energy storage devices, Sustainable Energy Storage in the Scope of Circular Economy is a key resource for academic researchers, industrial scientists and engineers, and students in related programs of study who wish to understand the state of the art in this field.

Recent Development in Magnetic Shape Memory Alloys

Editor: Volodymyr Chernenko

Heusler type magnetic shape memory alloys (MSMAs) have gained a strong academic and practical importance during recent decades due to the giant effects they exhibit, particularly magnetostrain produced by magnetic field-induced twin boundaries motion and magneto(elasto)-caloric effects resulting from the magnetic field-induced martensitic transformation.
This book gathers the Special Issue, called Special Issue called Recent Development in Magnetic Shape Memory Alloys, published in the Metals Magazine. The aim of the book is to communicate the latest advances in R&D and theory of MSMAs offering a collection of eleven invited peer-reviewed papers, each detailing a particular aspect in the fundamental and/or applied investigation of MSMAs and related phenomena. The papers are a corpus of up-to-date information on the ongoing studies of MSMAs. It is hoped that this reprint will be useful to physicists and materials scientists, both specialists and graduate students, and enable future technological breakthroughs in engineering.



SELECTED REVIEW PAPERS

Advances in Printing and Electronics: From Engagement to Commitment

Martins, P., Pereira, N., Lima, A.C., Garcia, A., Mendes-Filipe, C., Policia, R., Correia, V., Lanceros-Mendez, S.

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

Self-powered electrochemical sensors

del Campo, F.J.

(2023) Current Opinion in Electrochemistry, 41, art. no. 101356, .

Green Synthesis of Reticular Materials

Desai, A.V., Lizundia, E., Laybourn, A., Rainer, D.N., Armstrong, A.R., Morris, R.E., Wuttke, S., Ettlinger, R.

Adv. Funct. Mater. 2023, 2304660.

Photoreforming of Waste Polymers for Sustainable Hydrogen Fuel and Chemicals Feedstock: Waste to Energy

Ashraf, M., Ullah, N., Khan, I., Tremel, W., Ahmad, S., Tahir, M.N.

(2023) Chemical Reviews, 123 (8), pp. 4443-4509.

Silk Fibroin as Sustainable Advanced Material: Material Properties and Characteristics, Processing, and Applications

Reizabal, A., Costa, C.M., Pérez-Álvarez, L., Vilas-Vilela, J.L., Lanceros-Méndez, S..

(2023) Advanced Functional Materials, 33 (3), art. no. 2210764

PRICES & AKNOWLEDGMENTS

Extraordinary PhD Awards from the UPV/EHU

- Meenakshi Pegu
- Ander Reizabal
- Sheila Maiz
- Cristian Mendes
- Paula González

Visiting Professorship

at the Nanjing University of Aeronautics and Astronautics, and the International School of Materials Science and Engineering, Wuhan University of Technology (WUT), in China

Senentxu Lanceros-Méndez

Expoquimia ‘Best in Class’ award

Juan Pablo Esquivel, Ikerbasque Research Associate at BCMaterials, received, together with the rest of the advisory board of the start-up Fuelium, one of the four “Best in Class” awards with which the Expoquimia fair in Barcelona recognized projects with a highly disruptive profile and business transformation.
Esquivel is co-founder and external advisor of this company devoted to ecodesigned batteries for diagnostic devices, smart sensors for environmental monitoring or wearables.

Senentxu Lanceros-Méndez · Koro de la Caba · Shahzada Ahmad · Stefan Wuttke · Javier del Campo · Volodymyr Chernenko · Qi Zhang · Pedro Guerrero · Erlantz Lizundia

World’s top 2% most influential scientists

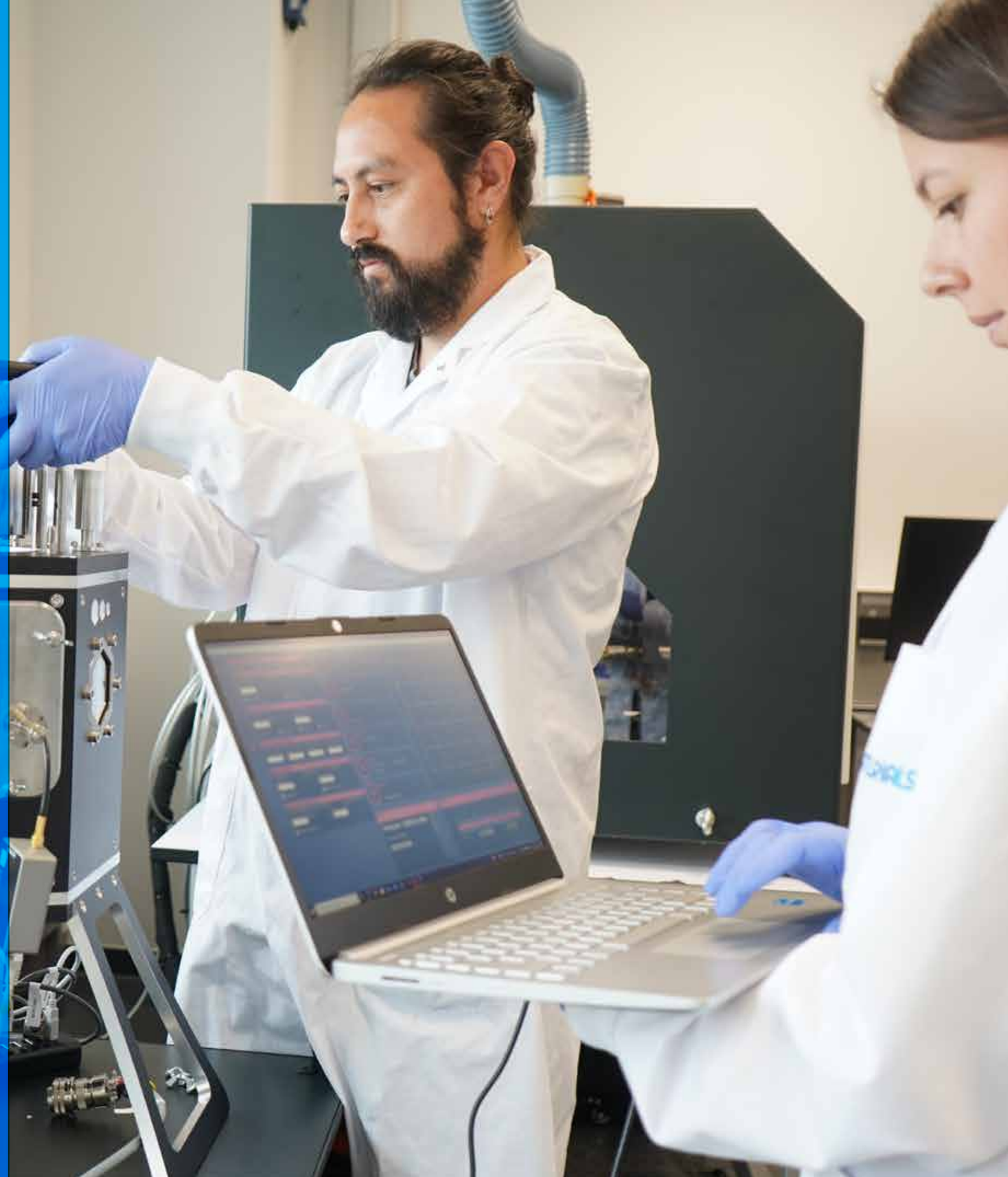
9 BCMaterials researchers in this annual list published by the Standford University (USA).

E-poster presentation award at Puzzle X

Paula González Sáiz obtained the Science Spark E-Poster presentation award at the Puzzle X event held in November in Barcelona. Puzzle X is a hub for ideas, innovation and solutions for Frontier Materials Deep Tech toward the United Nation’s Sustainable Development Goals (SDGs).
This event has international prestigious speakers of cutting-edge science and technology of different disciplines.

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.



20

PHD
Thesis Defended

1. Yara Alvarez Braña
Universal Modular Architectures for Self-powered Microfluidic Devices Based on Polymeric Micropumps and Plastic Cartridges

2. Mikel Arrese-Igor Royuela
Double layer polymer electrolytes enabling high voltage solid state lithium metal batteries

3. Nagore Barroso Garcia
A study of metal-organic framework sorption phenomena in solution

4. Alba Calatayud Sanchez
Microfabricated Tools for Cell Biology Assays: Micropatterned and Microfluidic Biosensors and Optic-fiber Nanoplasmonic Biosensors

5. Beatriz Dias Cardoso
Evaluation of drug loaded magnetoliposomes as multifunctional platforms for advanced cell therapies

6. Dmitry Galyamin
Aspectos clave para el desarrollo de inmunosensores digitales electroquímicos sostenibles

7. Sandra García Rey
Microfluidic Technologies and Sensing Materials for Sample Preparation and Analysis of Biofluids

8. Lorena Germán Ayuso
Microfluidic Technologies and Sensing Materials for Sample Preparation and Analysis of Biofluids

9. Ricardo Jorge Brito Gonçalves Pereira
A new generation of microfluidic platforms based on smart and multifunctional materials

10. Naveen Harindu
Reliability enhancement of perovskite solar cells: Role of low dimensional, materials for interfacial modifications

11. Muhammed Haris Palattuparambil Usman
Phase-stabilization in FAPbI3-based perovskite solar cells via powder engineering and additivisation strategies

12. Maksym Karpets
Impact of magnetic and electric field on structure of magnetic fluids

13. Teresa Isabel Marques de Almeida
Tailored electroactive polymer-based materials for neural tissue engineering applications

14.Jon Mercader
Design, optimization and in vitro evaluation of novel methods for the obtaining of a platelet-rich plasma enriched in platelet and extraplatelet growth factors

15.João Carlos Pacheco Barbosa
Development of three component solid-polymer electrolytes for energy storage applications

16. Maite Perfecto Irigaray
Metal-organic porous materials for carbon dioxide valorization, water adsorption and phtocatalytic hydrogen production

17. Estibaliz Ruiz Bilbao
Polyoxometalate-Based Hybrids with 3d- and 4f-Metal Complexes Bearing Multidentate Organic Ligands - From Magnetoluminescent Molecular Species to Extended Frameworks with Sorption Ability

18. Jon Ander Sarasua
Fisicoquímica de la limpieza por ultrasonidos sin inmersión

19. Ainara Valverde de Mingo
Metal-organic frameworks and their composites for water remediation

20. Fangyuan Zheng
Hybrid photocatalytic materials for contaminants of emerging concern degradation

16

Master
Thesis Defended

20

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.

Universidad del País Vasco · Euskal Herriko Unibertsitatea · UC Universidad de Cantabria

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.

Universidad del País Vasco · Euskal Herriko Unibertsitatea

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.

Universidad del País Vasco · Euskal Herriko Unibertsitatea

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.

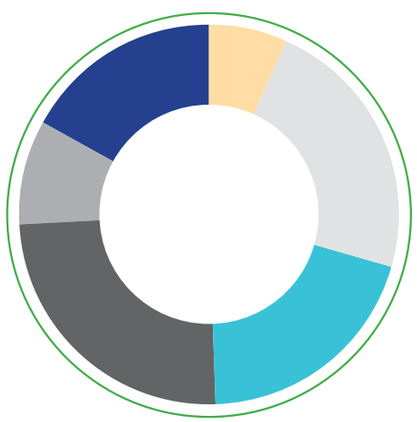
03

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**



7%	Invoicing
23%	Private
20%	BERC
25%	Basque Government
9%	National funding
17%	International

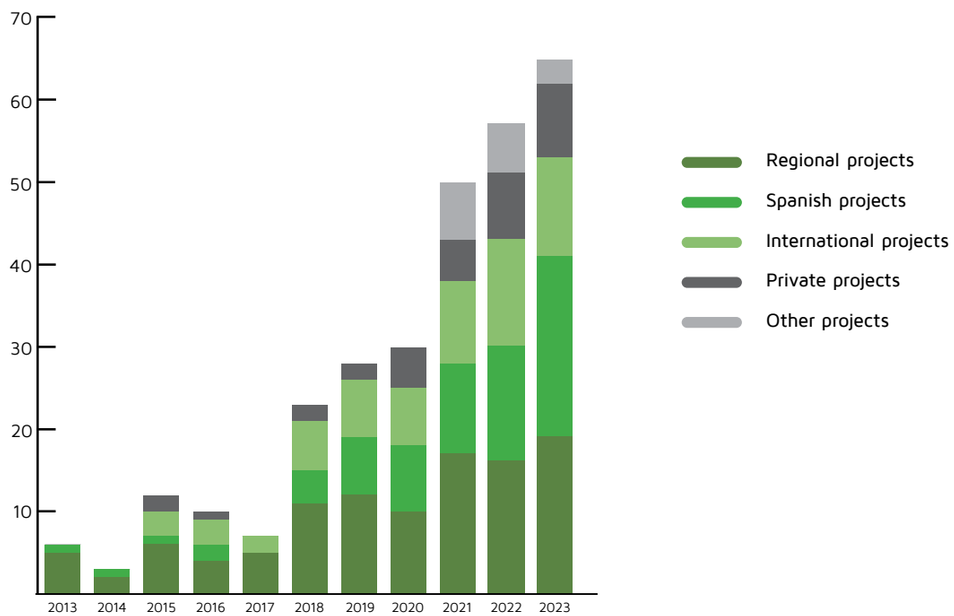
PROJECT **PROPOSALS**

94

PROPOSALS
Submitted

24%	Accepted
11%	Pending
59%	Rejected

ONGOING **PROJECTS**



FINANCIAL **BODIES**

PROJECT MEETINGS & EVENTS

EXPERT PROGRAM FOR PROJECT MANAGERS, *organized by the Centre for Technology and Industrial Development (CDTI), with the participation of Raquel González, Project and Technology Transfer Manager of BCMaterials.* ***Brussels (Belgium), November 2023***

ECLICARE EUROREGIONAL PROJECT WORKSHOP *focused on different aspects of electrochemistry applied to health diagnosis systems through smartphone technology.* ***Bilbao, November 2023***

KICK-OFF MEETING OF THE GIANCE EUROPEAN PROJECT *gather representative of its 23 partners from 10 different countries.* ***Barcelona, October 2023***

INDESMOF EUROPEAN PROJECT WORKSHOP *offered an overview of the results obtained in the development of new filters for the removal of heavy metals from water. These filters are based on metal-organic compounds (MOFs) loaded with specific deep eutectic solvents (DES)..* ***Braga (Portugal), December 2023***

BIDEKO NATIONAL PROJECT CONSORTIUM MEETING *examined the evolution of the work packages' milestones in order to develop ecodesigned batteries.* ***Leioa, March 2023***

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 2023:

- **Sergio Lucarini. Ikerbasque Research Fellow:** "Exploring self-Healing capabilities of Magnetorheological elastomers: modeling and experiments (MagHeal)"
- **Anna Sinelshchikova. Post-Doctoral Researcher:** "Aligned photoactive Ti-porphyrin MOF for enhanced electroconductivity (AlPhoMOF)"
- **Timur Tropin. Post-Doctoral Researcher:** 'Enhancing electrical and mechanical properties of polymer nanocomposites with buckyballs (PNC+C60)'
- **Hugo Salazar. Post-Doctoral Researcher:** "Towards green and sustainable synthesis of MXenes for environmental sensing (MXgreen)"

In September 2023, the 2022 winning projects' leaders presented their results in a session held at the Martina Casiano auditorium.

BASQUE REGIONAL PROJECTS

ADIPRO Investigación en técnicas de fabricación aditiva funcional para la producción de componentes
EJ/GV, ELKARTEK Tipo 2 KK-2022/00104 2022-2023

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

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

ECLICARE Bioensayos Electroquemiluminiscentes para Diagnóstico Personalizado
EJ/GV, EUREG_2021 2021-2023

Ensol3 Investigación en tecnologías avanzadas para el liderazgo de la energía solar fotovoltaica
EJ/GV, ELKARTEK Tipo 1 KK-2022/00067 2022-2023

FRONT22 FRONTIERS 2022 - Superficies multifuncionales en la frontera del conocimiento
EJ/GV, ELKARTEK Tipo 1 KK-2022/00109 2022-2023

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

MAGMETOS Magnetic metamaterials for All Optical Switching phenomena
EJ/GV PIBA PI_2021_1_0051 2021-2023

MIME 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

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 II 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

Prebio2 Policarbonatos renovables, biodegradables y biocompatibles a partir de CO2 para sectores estratégicos del País Vasco
EJ/GV, ELKARTEK Tipo 1 KK-2022/00057 2022-2023

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

ARISE All Inorganic Halide Perovskite Nanocrystals for Thin Film Solar Cells
PROYECTOS I+D+I PID2019-111774RB-I00 2020-2023

BASO Desarrollo de andamiajes biomiméticos activos para el estudio de microentorno de tumor en osteosarcoma
PROYECTOS I+D+I PID2019-106099RB-C43 2020-2023

BIDEKO Biodegradable and compostable batteries for precision agriculture and decentralized energy systems
LINEAS ESTRATÉGICAS PLEC2021-007801 2021-2023

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

HERALD Nuevos grados de abs sus copolímeros y blends termoplasticos con funcionalidades avanzadas para automocion e-mobility
BBVA 2023-2024

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

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

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

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

EUTOPIA European Topology Interdisciplinary Action
COST ACTION CA17139 2018-2023

GIANCE Graphene Alliance for Sustainable Multifunctional Materials to Tackle Environmental Challenges Abstract
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

INDESMOF International Network on Ionic Liquid Deep Eutectic Solvent Based Metal Organic Frameworks Mixed Matrix Membranes
H2020-MSCA-RISE-2017 2018-2023

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

MOLEMAT Molecularly Engineered Materials and process for Perovskite solar cell technology
ERC-COG 2017-2023

MULTIFUN Enabling multi-functional performance through multi-material additive manufacturing
H2020-NMBP-2018 2020-2023

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

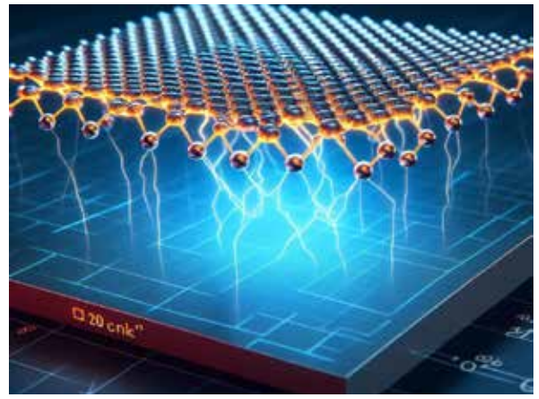
PIEZO 2D Piezoelectricity in 2D-materials: materials, modeling, and applications
HORIZON-MSCA-2022-SE 101131229 2023-2027

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

UNICORN Hybrid Nanocomposite Scintillators for Transformational Breakthroughs in Radiation Detection and Neutrino Research
ERAMIN3 PCI2022-132969 2023-2027

PIEZO 2D

Piezoelectricity in two-dimensional (2D) materials is increasingly important because of its potential in realizing thin yet efficient and flexible piezoelectric devices. The majority of 2D layered piezoelectrics found so far possess in-plane piezoelectricity and require bending of flexible substrates to activate piezoelectric effect. This severely limits their integration with modern Si technology. This project aims at strengthening the piezoelectric activity in 2D materials via interface and stress engineering and bond control. The materials list includes hafnium-zirconium oxide (HZO), transition metal thio/selenophosphates (TPS), graphene on oxide substrates, and polymer PDVF.



GIANCE

GIANCE project aims to design, develop, and produce the next generation of affordable, eco-friendly, lightweight, and recyclable materials based on graphene and related substances (GRM). These materials include multifunctional composites, coatings, foams, and membranes (GRM-bM) with enhanced properties, such as thermal, mechanical, and chemical features. GIANCE will demonstrate and validate the effectiveness of GRM-enabled products through 11 use cases, influencing future technologies across various sectors, including automotive, aerospace, energy (hydrogen economy), and water treatment.

UNICORN

The UNICORN project focuses on the development of an advanced detector to measure the mass of neutrinos by studying Double Beta Decay (0 DBD), an extremely rare nuclear process. This research has the potential to determine the nature of neutrinos as Majorana particles and provide insight into the asymmetry between matter and antimatter in the universe. The project aims to create a scalable, flexible, high resolution, low radioactivity, reliable and cost-effective detector, using nanocrystalline materials. BCMaterials will play a fundamental role by carrying out simulations through its researchers specialized in Computational Materials Science.

OSASUN K0

BCMaterials collaborates with BIOLAN HEALTH in the OsasunK0 project. The goal of the project is to accelerate the development of a new generation of medical devices by creating a km0 framework able to support the design, development, characterisation and validation of these devices.
More specifically, BCMaterials' tasks focus on the characterisation, design and development of new biosensing platforms. With this purpose BCMaterials is working on various instrumental characterization techniques, such as various microscopies, spectroscopies and electrochemical techniques, which are used to understand the factors that control the stability, durability and performance of biosensors.
With this, the aim is to reach a new generation of biomedical devices with optimized performance and production processes."

TOYOTA

To achieve a sustainable future, efficient electrocatalytic materials are crucial for transitioning from a carbon energy-dependent economy to renewable energy schemes. Recent breakthrough results from Lingenfelder's lab have shown that the ultimate level of design and efficiency is possible by controlling the electron spin polarization at the catalyst's surface. This approach allows to double the reaction activity and improve the product selectivity for key reactions in energy conversion devices: such as the oxygen evolution (OER) and the oxygen reduction reaction (ORR). With the support from Toyota Motors Europe, in 2023 we successfully initiated the design and characterization of spin selective electrodes for CO2 electroreduction, based on earth abundant materials.

PRIVATE PROJECTS

CURVE Desarrollo de decoraciones funcionalizadas por tintas transparentes para displays curvos basados en OLCDs
EJ/GV, WALTER PACK ZL-2022/00884 2022-2023

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

INK3D FAGOR. Tecnologías para la impresión de tintas funcionales en superficies poliméricas 3D
FAGOR 2023-2025

INK3D WP Tecnologías para la impresión de tintas funcionales en superficies poliméricas 3D
WALTER PACK 2023-2025

MELEXIS Verifying the feasibility of GMI sensor based on Melexis IMC soft magnetic materials
MELEXIS 2022-2023

OSASUNK0 Nuevos productos de inyección con superficies con capacidad sensorial táctil
BIOLAN 2020-2022

VIBRANTS Investigación en sistemas impresos de respuesta háptica para la mejora de la HMI para el coche eléctrico y autónomo
WALTER PACK 2022-2023

TOYOTA Bioinspired spin-selective electrocatalysis for CO2 conversion
TOYOTA 2023-20XX

PATENT REQUEST

OPTICAL FIBRE INTO A **METALLIC STRUCTURE**

BCMaterials presented in 2023, together with Lortek technology center expert in the digitalisation of manufacturing processes, a patent request regarding a new method and a device for integrating an optical fiber into a metal structure. This innovation allows to improve monitoring sensors integrated into metal structures, capable of measuring the temperature, deformations and vibrations of the structure.

THE GOAL

To integrate an optical fiber into metallic structures, in which the optical fiber, covered with a metallic coating, is arranged in a channel of the metallic structure so that it is integrated to the required depth.

HOW TO

In this method, a molten filler metal is deposited on said channel and on said optical fiber, in such a way that said channel is filled and the optical fiber is covered and in direct contact with the metal throughout its perimeter.

APPLICATIONS

Sensors based on optical fibre integrated into metallic structures can be applied in aircraft or space shuttles, being able to continuously monitor the status of the structure.

Optical fibre sensors are able to monitor the status of metallic structures of planes or space shuttles, for esxample.

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

METALLURGY & CERAMICS

ELECTRICITY & ELECTRONICS

OPTICS & OPTOELECTRONICS

MULTIFUNCTIONAL MATERIALS SYNTHESIS

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 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 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.
- 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.

MATERIALS **CHARACTE-RIZATION**

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

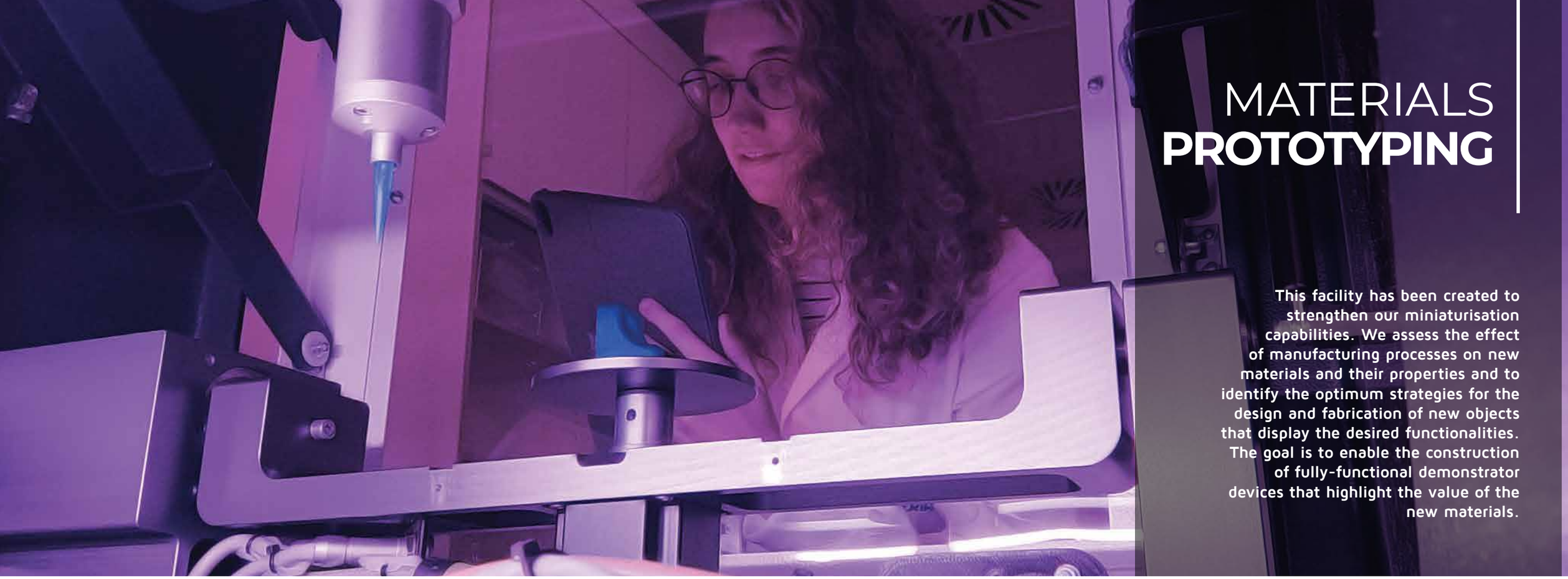
Among many other, our labs offer the possibility to use:

- 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 wire 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.

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.

05

OUTREACH ACTIVITIES

Outreach activities divide 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 to understand BCMaterials.

AT
BCMATERIALS

NEW MATERIALS FOR A BETTER LIFE!

In October, 4th, BCMaterials organized a new edition of its annual 'New Materials for a Better Life!' workshop. This time the event focused on advanced computing, quantum computing and Artificial Intelligence as tools for advanced materials development.
Important Basque and international experts took part in the workshop. The speakers panel was headed by Martin Mevissen, IBM lab manager for IA and quantum technology in Ireland; Ricardo Díez Muiño, director of the Donostia International Physics Center (DIPC) and José Antonio Lozano, scientific director of the Basque Center for Applied Mathematics (BCAM). BCMaterials vision aas represented by our scientific drector, Senentxu Lanceros-Méndez, and the Computational Materials Science research area's scientist.
The event was a total success in scientific and attendance terms.

WORKSHOP **SPEAKERS**

Ricardo Díez Muiño
DIPC

Martin Mevissen
IBM

Adriana Navajas
IBM

Ivan Coluzza
BCMaterials

Mois Ilia Aroyo
UPV/EHU

Ivan Infante
BCMaterials

Karolina Zofia Milowska
CICnanoGUNE

José Antonio Lozano
BCAM

AT
BCMATERIALS

PRINTFUN!
AUTUMN SCHOOL

In September 25th and 26th, BCMaterials organized PrintFun! – Autumn School on Functional Printing Materials and Technologies. Students from different universities, technology and research centers gathered at our headquarters to begin, complete and/or perfect their skills in different functional printing techniques.

The program offered the ideal framework and the perfect environment to work in functional 2D and 3D printing, providing solid training and practical experience in all the steps necessary for successful printing: from ink development to devices design, from physical-chemical to functional characterization, along with the presentation of the most representative and used 2D and 3D printing technologies.

PROGRAM

BACKGROUND & THEORY
- Inks synthesis and formulation
- Printing functional materials.
- Device design: a (printing) process perspective.
- Overview of advanced characterization techniques

HANDS ON SESSIONS
- Inkjet Printing
- Screen Printing
- Stereolithography / UV curation

PRACTICAL CLASSES
- IThermocromic device
- Electrochromic display
- Piezoresistive sensor
- Device testing and characterization

PARTICIPANTS' AFFILIATIONS

- Centre de Recherche Paul Pascal
- CICenergiGUNE
- CIDETEC
- Polymat
- University of Sevilla
- Politechnic Univisersity of Cartagena
- University of Castilla-La Mancha
- University of Córdoba
- University of Oviedo
- University of the Basque Country UPV/EHU

18 EVENTS
8 FORTNIGHTLY SMINARS
4 SOFT SKILLS SESSIONS
7 INVITED TALKS
26 SPEAKERS

SEMINARS & INVITED TALKS

The fortnightly seminars and invited talks program offered by BCMaterials was as intense as in previous years. 2023 was the first years, though, in which we introduced a regular soft-skills sessions schedule.

These soft skills talks aim to enrich the vision and capabilities of our researcher staff, regardless the level or position of each scientist.

Technology transfer and entrepeneurship played a very important role during the 2023 sessions as ways to transcend the basic science made at BCMaterials. At the same time we scheduled talks about preparing succesful European project proposals, since these are essencial to our common project growth as en excellence research center, and also for the particular growth of our scientists careers.

SOFT SKILLS SESSIONS

Raquel González, BCMaterials Project & Technology Transfer manager, gave ttree sessions on how to prepare a succesful European project proposal

'Opportunities for spin-off creation and transfer of results' talk by Zitek, the entrepreneurship support programme at the Bizkaia Campus of the UPV/EHU

Juan Pablo Esquivel, Ikerbasque Research Associate in BCMaterials, offered a researcher's guide to technology transfer and entrepeneurship

OUT

BCMATERIALS

EXTERNAL **DISSEMINATION**

90 INVITED TALKS

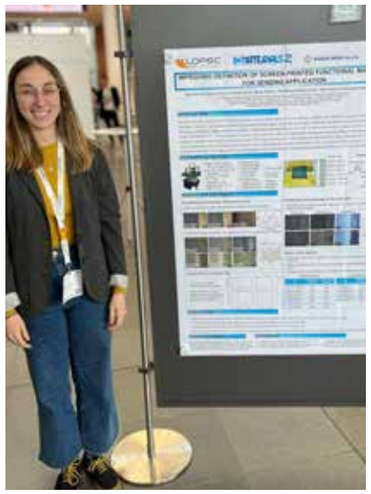
81 ORAL PRESENTATIONS

61 POSTER CONTRIBUTIONS

Senentxu Lanceros-Méndez, BCMaterials scientific director, at the round table of the British-Iberian Bioelectronics workshop (Lisbon, Portugal. February 2023)

Roberto Fernández de Luis, research fellow, during a presentation at the University of Buenos Aires, Argentina (May 2023)

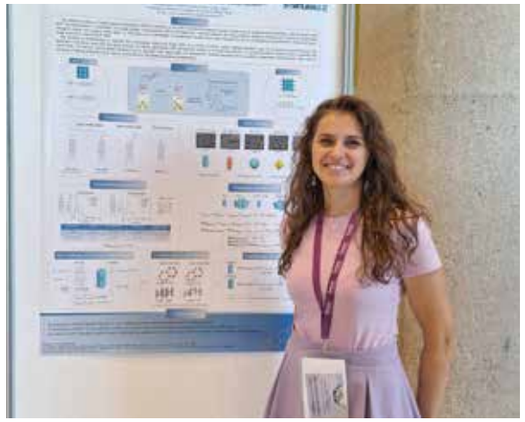
José María Porro, Ikerbasque Research Fellow, during Gordon Research Conference in which he presented the invited talk 'Neutron Scattering for a Sustainable Society'. Ventura USA. (June 2023)



Lía Campos, pre-doctoral researcher's poster at LOPEC conference (Munich, Germany. March 2023)

Javier del Campo, Ikerbasque Research Professor, at the 74th Annual International Society of Electrochemistry Meeting (Lyon, France. September 2023)

Carles Tortosa, post-doctoral reseracher, at Organic Battery Days event (San Sebastian, Spain. June 2023)



Anna Sinelshchikova, post-doctoral researcher, at the EuroMOF Conference (Granada, Spain.September 2023)

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.

IN& OUT

BCMATERIALS

SCIENCE **FOR SOCIETY**

One more year, BCMaterials supported and took part in the 11th edition of **ZIENTZIA AZOKA** *(Science Fair). This outreach initiative aims to promote science vocations among high school students, who present their scientific projects to a contest. Projects are showed to the public every June in Bilbao in a three-day fair. BCMaterials collaborates in the evaluation of the projects and in the mentoring of these young scientists. At the end of the year, some of the winning groups visit our facilities and learn about material science and the work we carry out in our laboratories. This excellent outreach event is organized by Elhuyar Fundazioa.*

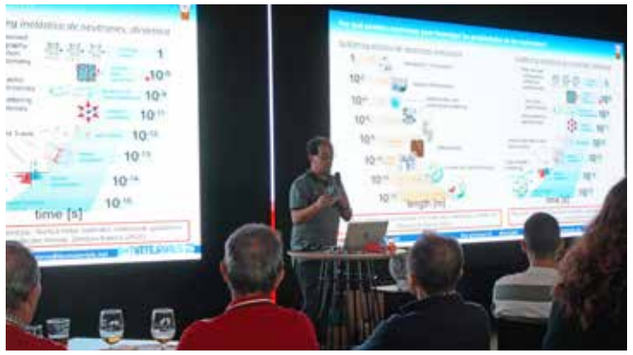
Some of the students that presented winning science projects at Zientzia Azoka were awarded with a visit to BCMaterials. They learned and took part in the making of printed sensors and thermochromic materials.

ZIENTZIA ASTEA (Science Week) is the biggest science outreach event carried out by the University of the Basque Country (UPV/EHU). In 2023 BCMaterials reinforced even more its annual presence participating with not only a science booth in Bilbao during the five days of the event, but also with two workshops in San Sebastian and Bilbao. MOFs, 3D printing for health treatment and environmentally friendly batteries were the experimental areas of our science booth. The two workshops were devoted to obtaining plastic materials from silkworms coccons.

IN& OUT

BCMATERIALS

SCIENCE FOR SOCIETY



José María Porro, Ikerbasque Research Fellow, during his talk on neutronics (Geuria! San Mamés bar. May 22 2023)

Ander Reizabal and Paula González, postdoctoral researchers presented a talk on 3D printing for new materials (Crazy Horse tabern. May, 24 2023)

*BCMaterials had an important role in the series of scientific outreach talks **PINT OF SCIENCE BILBAO**, which took place in May in four bars in the city.*
Our center, in addition to being one of the sponsors of the event, was the coordinating entity of this edition.
BCMaterials researchers also participated by offering two talks out of the twenty-four that made up a complete dissemination program on topics such as health, environment, and new technologies.
The event had a great attendance success and BCMaterials will continue to coordinate future editions in Bilbao.
Pint of Science is an event that takes place in more than 50 Spanish cities and 25 other countries in Europe, America, Asia and Africa.

Along the year we received 6 visits from educational centers in Bizkaia within the framework of the EGIN ETA EKIN initiative of the Provincial Council of Bizkaia for the promotion of entrepreneurial culture among high school students.

BCMaterials had an outstanding participation in the **EUROPE OPEN DAY** celebrated in Brussels in early May as ambassadors of the MSCA-RISE Action in the Water and Oceans Missions stand at the event. Our researchers Roberto Fernández de Luis, María Calles and Leire Celaya represented our center, which acts as secondee and coordinator of the INDESMOF-RISE-MSCA action and partners of Tailing23Green and SOLARSENIC projects.
BCMaterials researchers explained the attendees, using different experiments, how the EU-funded research can help to mitigate the water pollution arising from heavy metals, while in parallel recovering valuable critical raw elements in the process

The 2023 edition of the **EUROPEAN NIGHT OF RESEARCHERS** held in Bilbao in late September,was devoted to the European Union research missions to address important issues like fighting cancer, the climate change, water and oceans... BCMaterials science booth in the event presented three experiments on new materials to treat bone cancer, for water remediation and thermocromic materials for food packaging.

IN& OUT

BCMATERIALS

WOMEN IN SCIENCE DAY

The students that participated in this event had the opportunity to learn about great scientific contributions of women along History, the work developed by BCMaterials female researchers from different countries, and also to create their first scientific posters picturing the future of different science and tehcnology disciplines.

In February 8th and 9th, BCMaterials received students from different high schools in Bizkaia in the outreach activity called 'Woman+Science= a journey through time'. The successful experience from 2022 led the center to keep this format for the central activities framed in the Week of Women and Girls in Science,
Around 100 hundred students took part in this activity.
The aim was, once again, to raise awareness of the important role of women in the history of Science, as well as to promote a scientific vocation among female students and also among their male classmates.

BCMaterials joins the 'Emakumeak Zientzian' initiative

In late 2023, BCMaterials signed the agreement to be part of the 'Emakumeak Zientzian' (Women in Science, in Basque) initiative, a joint effort from more than 30 Basque academical and research institutions and centers to develop an extensive activities program during the International Week of Women and Girls in Science each February.
BCMaterials entered as a coordinating entity to help organizing and promoting the 2024 activities, that add up more than 60 events in the whole Basque Country with hundreds of volunteers.

IN& OUT

BCMATERIALS

MEDIA IMPACT

TV

Juan Pablo Esquivel
3cat (Catalonian Television)
October 2023

Daniel Bacigalupe & Paula González
Onda Vasca
May 2023

Daniel Bacigalupe
Radio Vitoria
May 2023

José María Porro
Radio Euskadi
May 2023

Ivan Infante
Radio Euskadi
October 2023

Senentxu Lanceros
Radio Euskadi
Nobvember 2023

Ander Reizabal
Euskadi irratia
Nobvember 2023

NEWS

Raquel González
Euskotek
March 2023

Campusa
October 2023

WWW

Mapping Ignorance
October 2023

2018-2023

THE YEARS IN WHICH EVERYTHING CHANGED

BCMaterials has grown extraordinarily in the last six years. Thanks to all those who have made up our team and the institutions and partners that paved our way. Places and people may change but not our determination to keep working on new materials for a better life.

TURN THE PAGE
& **SEE**

2018 A TIMELINE TO SUCCESS 2023

STRATEGIC PLAN 2018-2021

This plan defined the reseacrh areas and lines for a 4-year period. It was the turning point for the center's growth, starting from a small but highly motivated reseracher and services staff.

APRIL 2018

DEC 2018

FIRST YEAR WITH MORE THAN 100 PAPERS

Research output boosts with regards to previous years. Plus, the number staff researchers (33) overcomes the number of associates (29) for the first time.

1ST BILBAO NEUTRON SCHOOL

Together with ESS-Bilbao we hosted and coorganized the first neutron scattering school in Europe focused in science and instrumentation for CANS facilities.This was an important step for our future actions related to neutron science and technology, and also with the organization of international events in our center.

JUNE 2019

DEC 2019

NEW HEADQUARTERS

Basque Government President Lehendakari Iñigo Urkullu inaugurates BCMaterials new facilities at the UPV/EHU Science and Technology Park.

OVERCOMING THE PANDEMIC CHALLENGES

The global lockout and later progressive unscale caused by the Covid-19 pandemic did not stop us in our growth. The first Ikerbasque Associate was integrated as well as new groups from the UPV/EHU. Our total number of researchers reached 80. We had 30 ongoing projects and more than 160 national and international partners.

MARCH 2020

BIOREACTOR PATENT

We patented a modular magnetically driven bioreactor system fot cellular cultures and biomedical applications. Bioence spin-off was created by BCMaterials in the area of biomedical devices.

DEC 2020

FEB 2021

NEW LABS DEVOTED TO AREAS

We opened new labs for Energy, Environment, Digitalizatoin and Advanced Technologies, Biomedicine and Biotechnology

THE IKUR STRATEGY IMPACT

The Basque Government´s Education Department's IKUR Strategy's support allowed us to develop new work lines in Neutronics and Computational Materials Science, and to add hihgly motivated and excellent scientis in a variety of areas including quantum technologies, materials for energy storage and biomaterials for neural regeneration, among others.

MAY 2021

JUNE 2022

OUR FIRST 10 YEARS

We celebrated our 10th anniversary reaching numbers that definitely consolidate our center and prepare us for the future, materialized in the new Strategic Plan 2022-2025. We reached more than 100 staff and associate researchers, offered a training program with almost 20 PhD thesis defended each year, was able to organized big events like New Materials for a Better Life! workshop or IMOH2022 conference...

HR EXCELLENCE IN RESEARCH

EXCELLENCE IN HUMAN RESOURCES

We obtained obtained the "HR Excellence in Research", as a seal of our transparent and merit-based recruitment of researchers, the safeguard good working conditions and focus on professional development for researchers at all stages of their careers.

MARCH 2023

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BCMATERIALS
BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES

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