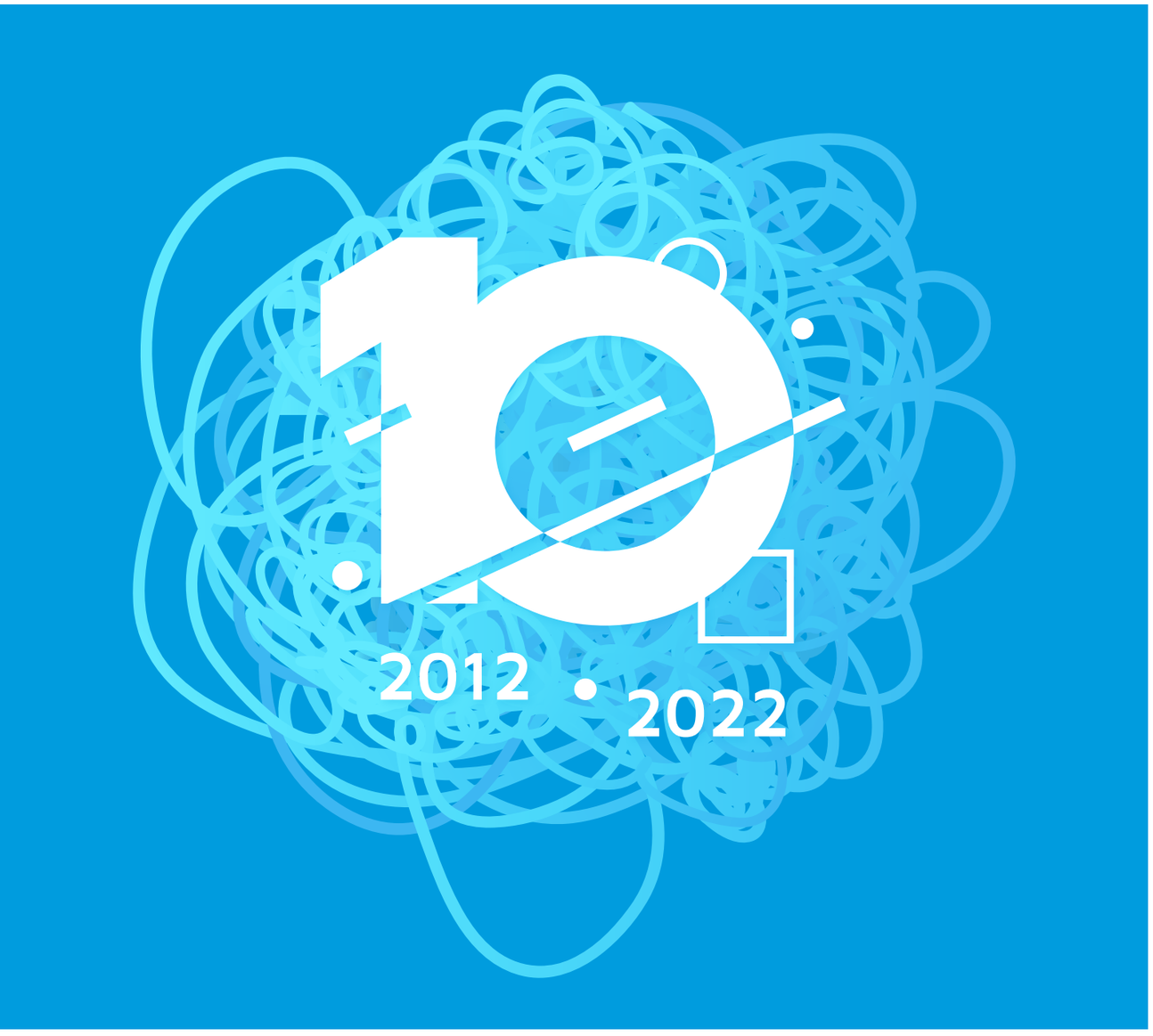
ANNUAL REPORT 2022

BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES

EUSKO JAURLARITZA
GOBIERNO VASCO

ikerbasque
Basque Foundation for Science

Universidad del País Vasco
Euskal Herriko Unibertsitatea



ANNUAL REPORT 2022

BCMATERIALS
BASQUE CENTER FOR MATERIALS, APPLICATIONS & NANOSTRUCTURES
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CONTENTS

SENENTXU LANCEROS-MENDEZ
Ikerbasque Professor / Scientific Director

TEN YEARS AND EAGER FOR THE NEXT TEN

The year 2022 has been quite special for BCMaterials, marked by two events that gave us a sense of fulfilment, illusion, and responsibility.

On the one hand, BCMaterials celebrated its 10th anniversary. Ten years of a collective effort to stablish a centre of reference in advanced materials, applications, and nanostructures. We shared and celebrated the history of the centre, the intense present and the bright and challenging future ahead to contribute to the development, understanding and application of next generation materials for the benefit of the society.

On the other hand, 2022 represents the beginning of a new strategic program full of possibilities and opportunities. We have reformulated the research lines, new research groups have emerged and we are consolidating our capabilities in the areas of Computational Materials Science and Neutron Science.

We have been also continued the implementation of the research facilities that now provide excellent conditions in all our areas of activity.

Both, the celebration of the 10th year anniversary and the beginning of the strategic program provided a the perfect time to reflect and assume our privileged condition to contribute to the many challengers society is facing nowadays.

The echoes and consequences of the recent pandemic situation, the energy and supplies crisis derived from the war in Ukraine, the consequences of climate change on environment and society and the rapid digitalization of the society and the economy, are just current examples proving that new generations of advanced materials, as the ones being developed at BCMaterials, are more urgent that ever.

> **The tree which fills the arms grew from the tiniest sprout; the journey of a thousand li commenced with a single step**
>
> **Lao-Tse,**
> **Tao Te Ching 571 a.C.**

Timely response to the requirements of society and anticipation to the next challenges must be our main drive for development, together with excellence, commitment, solidarity, and responsibility.

The 2022 annual report shows that we are certainly in the right track to become a necessary and reliable player contributing positively to address the aforementioned challenges. The scientific discoveries, the number of publications, the funded projects, works with industry and technology transfer, and the strong national and international collaborations are witnesses of our increasing activity and consolidated research activity. Most important, we have also consolidated our contribution to the formation of next generation of researchers and the commitment to share our work, our science and our passion with society.

We can only be extremely thankful to all that, over the years, have contributed to the creation and growth of BCMaterials: researchers, administration, research associates from the UPV/EHU, the International and Local Advisory Committees, together with the continuous support from the Basque Government, Ikerbasque and the UPV/EHU. We also thank the trust and confidence from all our collaboration partners, all over the globe.

In this appreciation of the past and value of the present, also lays our commitment to continue giving our best to contribute to the next generation of materials … for a better life!

> **All this happened, more or less.**
>
> **Slaughterhouse-Five,**
> **Kurt Vonnegut (1922-2007)**

10TH ANNIVERSARY

TEN YEARS SHAPING THE FUTURE

On November 16, we celebrated our 10th anniversary with a very special edition of our annual workshop New Materials for a Better Life!

This time we made a journey from BCMaterials origins, passing through the current progress of our research and collaborations, and finally looking into the future of materials science, showing our committment to pay an even more important role as an internacional center of reference for our field of research.

It was a great pleasure for us to share this important date with representatives of the key institutions that support BCMaterials, like the Basque Governent, the UPV/EHU and Ikerbasque, along with a significant amount of our partners, collaborators, former staff and those who helped us to reach our nowadays position.

NM4BL 2022
Program

Welcome by academical and institutional representatives

Senentxu Lanceros-Méndez. BCMaterials
"One decade of developing New Materials for a Better Life"

BLOCK 1: FROM THE BEGINNING TO CONSOLIDATION

José Luis Vilas (Labquimac. UPV/EHU)
"Origen, necesidad e historia de BCMaterials"

José Ramón Dios (Gaiker-BRTA)
"The relevance of the local projects and collaborations– Actimat"

Raquel González & Roberto Fernández de Luis (BCMaterials)
"Internationalization at BCMaterials: Increasing impact and excellence"

BLOCK 2: EXPANDING ACTIONS AND INTERACTIONS

Lara Herrera del Val (IIS Biocruces Bizkaia)
"The relevance of advanced materials for biomedical applications"

Koro de la Caba (Biomat. UPV/EHU)
"New generation of advanced materials with improved sustainability"

José María Porro & Viktor Petrenko (BCMaterials)
"Neutrons as an essential tool for materials development and characterization "

Ivan Coluzza & Ivan Infante (BCMaterials)
"Theory as a driving force for materials design, development and understanding"

BLOCK 3: CHALLENGES, OPPORTUNITIES AND NEEDS: THE NEXT TEN YEARS

Amaia Esquisabel (Research Director. Basque Government)
"Retos principales en Ciencia, Tecnologia e Innovacion en el País Vasco"

Enrique Solano (Kipu Quantum / Quanvia)
"Computación cuántica y tecnologías cuánticas: retos y oportunidades"

Olga Martín (Aclima. Basque Environment Cluster)
"Los desafíos de la sostenibilidad: materiales avanzados para un planeta sostenible"

Cristina del Amo Mateos (IIS Biocruces Bizkaia)
"Materiales avanzados en el contexto de la biomedicina y la biompresión"

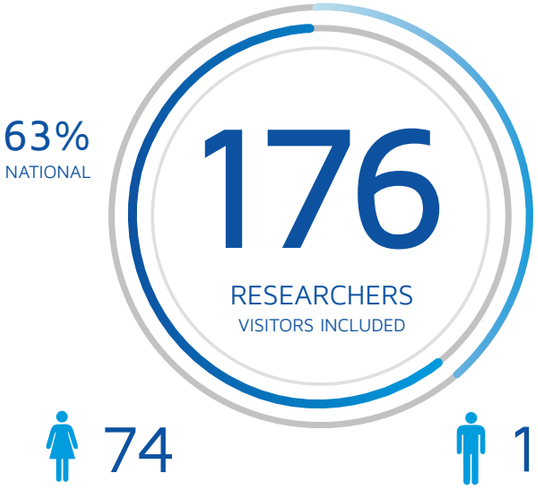
Teófilo Rojo (UPV-EHU)
"Challenges and perspective in Materials for Energy "

01 THE CENTER

BCMaterials, Basque Center on 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



RESEARCH OUTPUT

247
SCOPUS INDEXED ITEMS

64
H INDEX

83%
Q1 PUBLICATIONS

7010
CITATIONS

2
BOOKS

10
BOOK CHAPTERS

PROJECTS AND FUNDING

57
ONGOING PROJECTS

= 4.570.000 €
FUNDING

TRAINING

18
PHD THESIS DEFENDED

22
MASTER THESIS

24
UNDERGRADUTE PROJECTS

OUTREACH

27
SEMINARS & TALKS AT BCMATERIALS

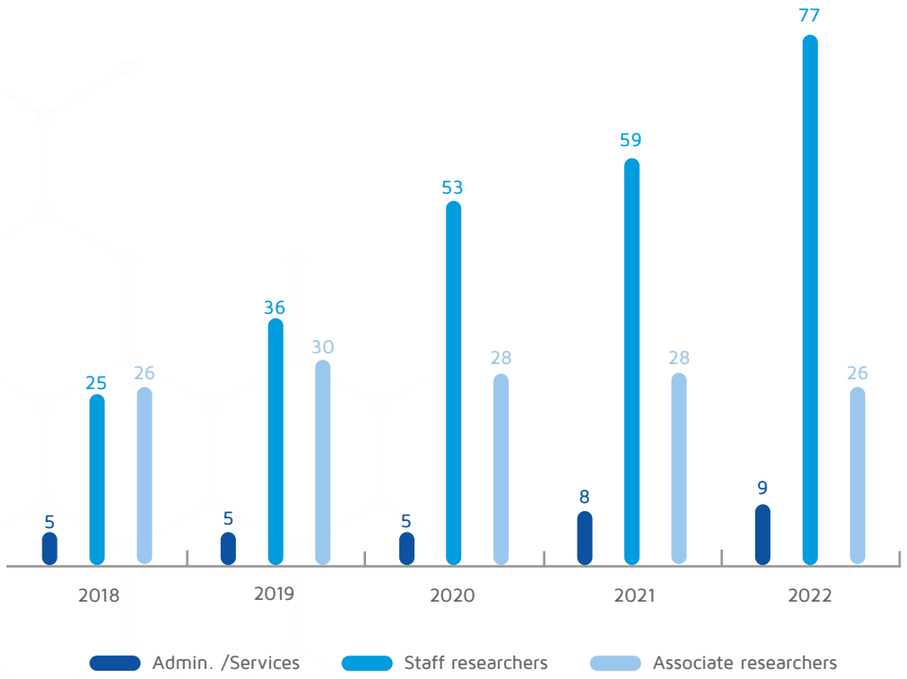
59
ORAL PRESENTATIONS

49
INVITED TALKS

12
OUTREACH ACTIVITIES

BCMATERIALS **COMMUNITY**

6,8%	Ikerbasque Research Professors
1,9%	Ikerbasque Research Associates
3,8%	Ikerbasque Research Fellows
3,8%	Research Fellows
8,7%	Administration / Services
25,2%	UPV/EHU Research Associates
38,8%	Pre-doctoral Researchers
19,4%	Post-doctoral Researchers



BCMATERIALS RESERACHERS

VISITORS

Argentina		1
Brazil		1
Canada		1
Chile		1
China	3	3
Colombia	2	2
Costa Rica	1	1
Cezch Republic	1	
Egypt	1	
France		1
Germany	1	1
India	4	
Iran		1
Italy	3	5
Portugal	5	9
Russia	1	
Slovenia		2
Spain	74	43
Sri Lanka	1	
Tunisia		1
Turkey		6
United Kingdom	2	
Ukraine	3	
USA	1	1
Venezuela		2

RESEARCH **NETWORK**

312
COLLABORATORS

222
INTERNATIONAL

42
COLLABORATIONS
IN SPAIN

48
REGIONAL
COLLABORATIONS

26 RCVT | **6** CLUSTER | **16** 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 • RUSSIA • SERBIA • SLOVAKIA • SLOVENIA • SOUTH AFRICA • SWEDEN • SWITZERLAND • THAILAND • TURKEY •UNITED KINGDOM • UKRAINE • USA • VIETNAM

EXCELLENCE IN **HUMAN RESOURCES**

BCMaterials is fully committed to recruit the better scientists possible 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'. This also reflects in the last years' tendence towards a better balance between gender representation in our center.

HUMAN RESOURCES EXCELLENCE IN RESEARCH

In 2000, the 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 14/07/2022 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.

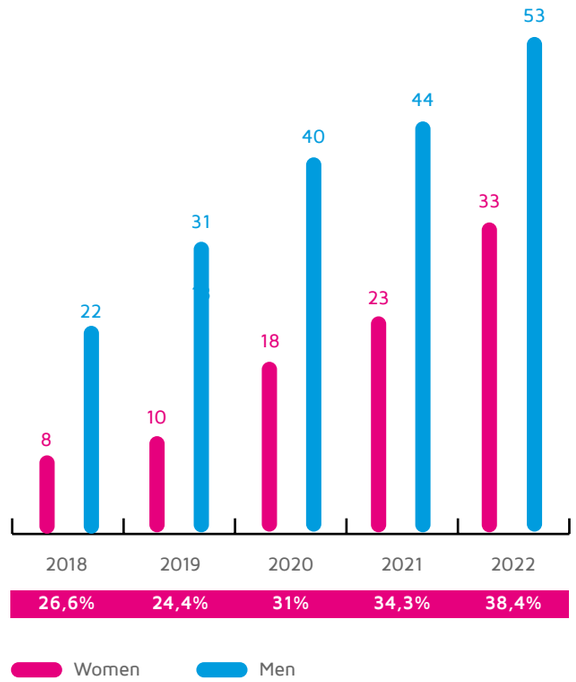
Fundación BCMaterials presented its Application on 18/07/2022 to obtain the "HR Excellence in Research" award, based on the implementation of the HRS4R action plan.

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.

GENDER DISTRIBUTION (STAFF RESEARCHERS)



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 impartial vision and guidance that allows our center 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 bigger and transcendent pointing at new challenges and goals.

Board of trustees

ADOLFO MORAIS

Vice minister of Universities and Research, Basque Government

AMAIA ESQUISABEL

Director of Scientific Policy, Basque Government

FERNANDO COSSÍO

Scientific Director of Ikerbasque

INMACULADA AROSTEGUI

Vice Rector of Research. UPV/EHU

GUILLERMO QUINDÓS

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

AITOR ZURIMENDI

General Secretary of the UPV/EHU

International Advisory Committee

PROF. MARIA VALLET- REGÍ

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

PROF. OMAR M. YAGHI

James and Neeltje Tretter Chair Professor of Chemistry University of California, Berkeley
Co-Director: Kavli Energy NanoSciences Institute at Berkeley California Research Alliance by BASF

PROF. CAROLINE A. ROSS

Associate Head of the Department of Materials Science and Engineering
Toyota Professor of Materials Science and Engineering
Massachusetts Institute of Technology (MIT), USA

PROF. GORDON WALLACE

Director ARC Centre of Excellence for Electromaterials Science (ACES)
Director ANFF (Materials Node)
Director Translational Research Initiative for Cellular Engineering and Printing (TRICEP)

PROF. SABETH VERPOORTE

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

PROF. PHIL WITHERS FRS

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

Local Advisory Committee

PROF. TEÓFILO ROJO

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

PROF. Mª ISABEL ARRIORTUA

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

PROF. LUIS MANUEL LEÓN

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

DR. ELENA GUEDE VÁZQUEZ

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

DR. ANTONIO PORRO

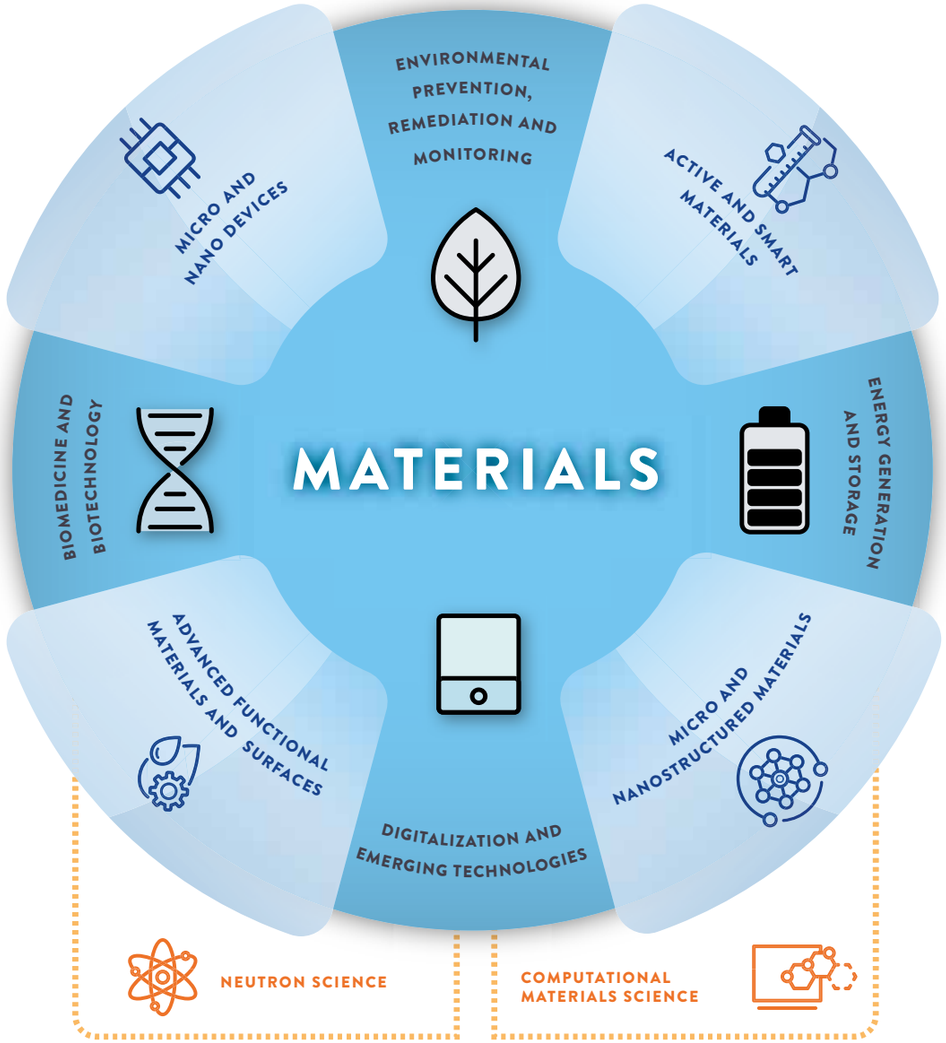
Former Chief Technology Officer and Business Development Director at TECNALIA Research & Innovation, BT Division.
Former member of the Conseil Scientifique et Technologique of NOBATEK-INEF4 (France).

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.

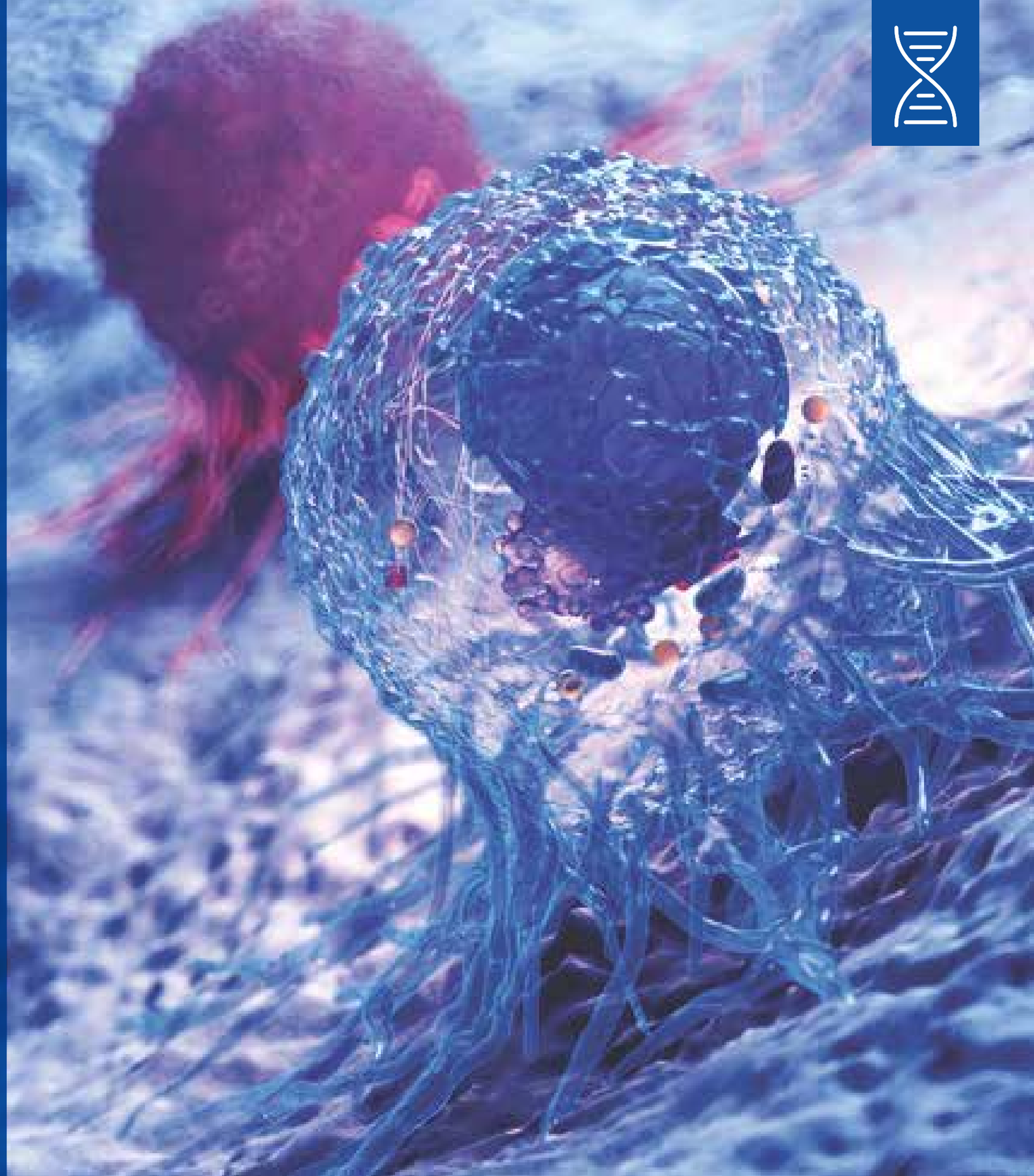
Transverse lines

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.



UNDERSTANDING MYOBLAST DIFFERENTIATION PATHWAYS WHEN CULTURED ON ELECTROACTIVE SCAFFOLDS THROUGH PROTEOMIC ANALYSIS

Sylvie Ribeiro, Clarisse Ribeiro, Vítor M. Martins, Bent Honoré, Maria Teresa Neves, Andreia C. Gomes, Senentxu Lanceros-Mendez. ACS Applied Materials & Interfaces 2022, 14, 22, 26180−26193

Electroactive materials allow to modulate cell-materials interactions and cell fate, leading to advanced tissue regeneration strategies. Nevertheless, their effect at the cellular level is still poorly understood. In this context, the proteome analysis of C2C12 cell differentiation cultured on piezoelectric polymer films with null average surface charge (non-poled), net positive surface charge (poled +) and net negative surface charge (poled -) has been addressed. Protein/pathway alterations for skeletal muscle development were identified comparing proteomic profiles of C2C12 cells differentiated on poly(vinylidene fluoride) with similar cells differentiated on polystyrene plate (control), using label-free liquid chromatography-tandem mass spectrometry (LC-MS/MS).

Some proteins and pathways are required for skeletal muscle tissue engineering applications. This work demonstrates the influence of electroactive poly(vinylidene fluoride) films with different surface charge (no charge, positive and negative polarization) on C2C12 cell differentiation by proteome analysis using LC-MS/MS. It is shown that films with different polarizations lead to cells significantly altering expression of some proteins comparatively to the control used in the study (a polystyrene plate). After 5 days of cell differentiation, it was observed that the significantly expressed proteins were categorized as being involved in binding, of which some were related with calcium binding, which is fundamental for C2C12 differentiation to muscle cells. Comparing both types of polarization, it is concluded that a negative polarization promotes the expression of proteins related with skeletal muscle tissue development, whereas a positively polarized surface induces the expression of proteins involved in muscle contraction, which corrobates previous studies where positive surface charge promotes higher myoblast maturation index.

Specifically, a total of 37 significantly expressed proteins were detected on the C2C12 proteome with PVDF "poled −" at 24 h, whereas on the PVDF "poled +" a total of 105 significantly expressed proteins were considered. At 5 days of differentiation, the number of significantly expressed proteins decreased to 23 and 31 in cells grown on negative and positive surface charge, respectively, being the influence of surface charge more explicit in some proteins. In both cases, proteins such as Fbn1, Hspg2, Rcn3, Tgm2, Mylpf, Anxa2, Anxa6, involved in calcium-related signaling, were highly expressed during myoblast differentiation. Furthermore, some proteins involved in muscle contraction (Acta2, Anxa2, Anxa6) were detected in the PVDF "poled +" sample.

Upregulation of several proteins that enhance skeletal muscle development was detected in the PVDF "poled −" sample, including Ckm (422%), Tmem14c (384%), Serpinb6a (460%), adh7 (199%), and Car3 (171%), while for the "poled +" samples these proteins were also upregulated at a smaller magnitude. Cells cultured on non-poled samples have no differences with respect to the ones culured on the control, demonstrating the relevance of scaffolds surface charge on cell behavior.

Concluding, this study proves the importance of surface charge of piezoelectric polymers to modulate myoblast differentiation and demonstrates the need to further understand how surface charge influences molecular functions to reach successful tissue regeneration approaches.

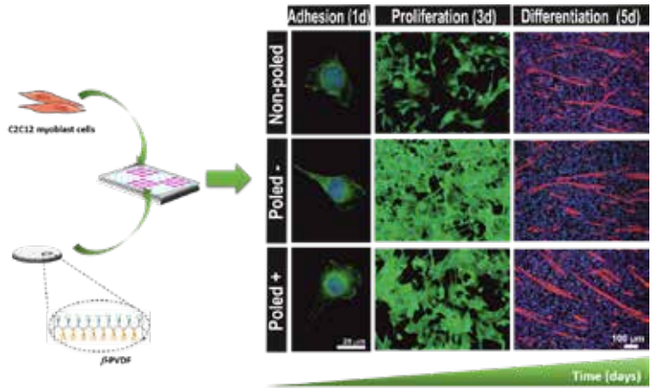


Fig 1
Schematic representation of the results on C2C12 myoblast adhesion (1 day), proliferation (3 days) and differentiation (5 days) on -PVDF films without (non-poled) and with positive (poled +) and negative (poled -) surface charge.

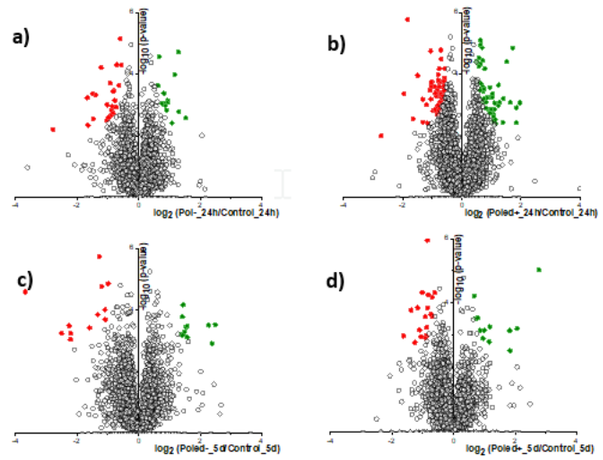


Fig 2
Volcano plots of the LC-MS/MS analysis of C2C12 cells cultured on PVDF films with different overall surface charge after 24 h or 5 days of cell culture. X-axis: log2 of the differences between each material vs control (= material/control); Y-axis: -log10 (p-value) where p values are based on a t-test. The unchanged proteins are indicated with grey circles, the proteins significantly upregulated are indicated as red spots and the downregulated ones as green spots. a) 2865 proteins were identified in PVDF "poled −" after 24 h being 37 significantly expressed; b) 2871 proteins were identified in PVDF "poled +" after 24 h being 105 significantly expressed; c) 2875 proteins were identified in PVDF "poled −" after 5 days being 23 significantly expressed; d) 2874 proteins were identified in PVDF "poled +" after 5 days being 31 significantly expressed.

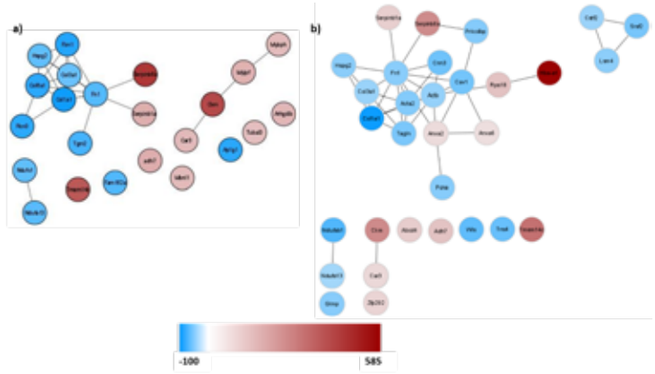


Fig 3
Differentially expressed proteins in C2C12 cells cultured on polarized PVDF samples relative to control: a) "poled -" and b) "poled +", as depicted in their networks by STRING and visualized through Cytoscape. Each dot represents a protein of interest and the lines represent the protein interactions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

GREEN HEMOSTATIC SPONGE-LIKE SCAFFOLD COMPOSED OF SOY PROTEIN AND CHITIN FOR THE TREATMENT OF EPISTAXIS

Jon Jimenez-Martin, Kevin Las Heras, Alaitz Etxabide, Jone Uranga, Koro de la Caba, Pedro Guerrero, Manoli Igartua, Edorta Santos-Vizcaino, Rosa Maria Hernandez.Materials today Bio 15 (2022) 100273

Sponge-like scaffolds based on soy protein and chitin were developed as nasal packs for the treatment of epistaxis, one of most common otorhinolaryngology emergencies worldwide. In addition to their biocompatibility and hemocompatibility, they showed high capacity in vitro for blood clotting and red blood cells and platelets binding. Furthermore, a rat-tail amputation model revealed that these scaffolds could reduce bleeding time in vivo. Therefore, this work demonstrated that a green strategy can be followed to manufacture nasal packs with excellent hemostatic properties using valorized by-products.

Nasal hemorrhage, also known as epistaxis or nosebleed, is one of the most common otorhinolaryngology emergencies worldwide. Although there are currently several treatments available, they present several disadvantages since they act just by physical pressure without any inherent hemostatic effect. This, in addition to the increasing need of employing more environmentally respectful materials, led us to research unexploited opportunities to maximize the valorization potential of biological resources. In this work, natural by-products from the food industry, such as soy protein (SP) and -chitin (CH), were employed to develop a sponge-like scaffold (SP-CH) as a nasal pack for the treatment of epistaxis. To evaluate the potential of SP-CH as a nasal pack, it was compared with two of the most commonly used nasal packs in the clinic: a basic gauze and the synthetic pack Merocel® (Figure 1A). SP-CH presented an interconnected porous microstructure (Figure 1B), which led to higher damping coefficients under compression cycles, indicating its capacity to dampen the impact waves and mechanical forces that may be produced with the pack placed in the nasal cavity. SP-CH pack was shown to be both biocompatible and hemocompatible in vitro (Figure 1C), clearing up any doubt about its safety. Interestingly, it was able to degrade partially within a few days when incubated in blood, losing about a 25% of its initial weight after 48 h, which is enough to relieve the patient discomfort and damage associated to the pack removal, avoiding rebleeding episodes, in contrast to gauze and Merocel®, which were shown to be nonabsorbable nasal packs. Moreover, the hemostatic properties of SP-CH outperformed those of the two commercial nasal packs. SP-CH pack was found to effectively promote blood coagulation in vitro, showing outstanding red blood cells (RBC) and platelet binding (Figure 2), likely due to the intrinsic hemostatic properties of its natural components. Furthermore, a rat-tail amputation model revealed that SP-CH significantly shortened bleeding time in vivo (Figure 3). Therefore, this work, carried out from a material sustainability approach, demonstrates that a green strategy can be followed to manufacture safe and effective nasal packs with better hemostatic properties than the commercial packs in the clinic, using valorized by-products from the food industry as valuable and sustainable sources of biomaterials.

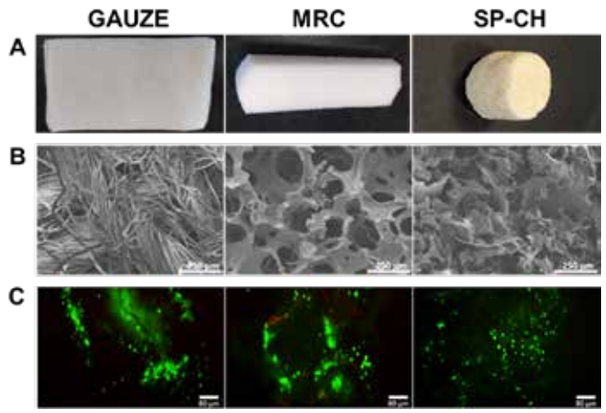


Fig 1
Characterization of the materials. (A) Macroscopic images of the nasal packs: Gauze, MRC, and SP-CH. (B) SEM micrographs of dry materials. (C) Live/Dead micrographs of the cell-cultured materials, with calcein-etidium staining.

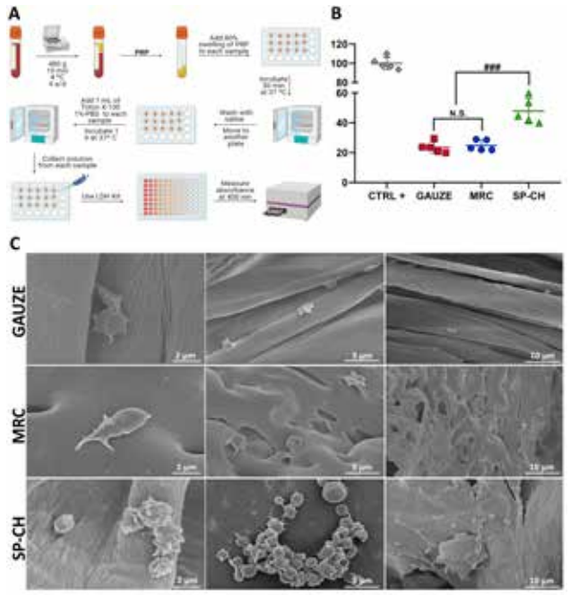


Fig 2
In vitro platelet adhesion. (A) Scheme of the procedure carried out for the determination of platelet adhesion of the materials. (B) Normalized lactate dehydrogenase (LDH) release (%) of the materials. Error bars, mean ± SD. N.S., nonsignificant ($p > 0.05$). ###$p < 0.001$ SP-CH vs the other groups. n=5 independent samples per group. (C) SEM micrographs of platelets adhered to the surface of the materials.

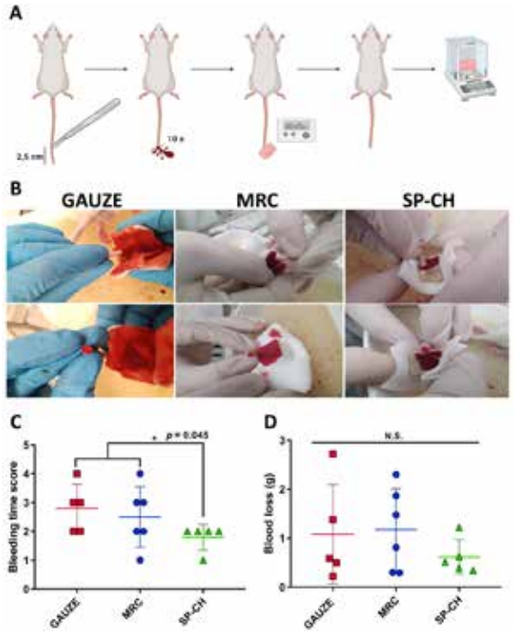


Fig 3
*In vivo hemostatic efficacy. (A) Scheme of the procedure carried out for the rat-tail amputation model. (B) Photographs of the three materials during the experiment. (C) Bleeding time score of the three materials. Error bars, mean ± SD. *$p < 0.05$ SP-CH vs the other groups. (D) Blood loss (g). Error bars, mean ± SD. N.S., nonsignificant ($p > 0.05$).*

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.

REUSABLE NANOCOMPOSITE MEMBRANES FOR HIGHLY EFFICIENT ARSENITE AND ARSENATE DUAL REMOVAL FROM WATER

H. Salazar, P. M. Martin, M. M. Fernandes, P. Costa, , S. Ferdov, G. Botelho, and S. Lanceros-Mendez.
Advanced Materials Interfaces 2022, 9, 2101419

A membrane reactor (MR), combining adsorption and membrane separation processes, represents a new hybrid and promising technology for arsenic-contaminated water treatment. This work reports on nanocomposite filters (NCFs) based on poly (vinylidene fluoride-hexafluoropropylene), PVDF-HFP, containing yttrium carbonate ($Y_2(CO_3)_3$) and magnetite (Fe_3O_4) to adsorb neutral and anionic species of As(III) and As(V), in an up-scaled membrane reactor. Thus, the nanocomposite filters and the up-scaled membrane reactor represent a suitable alternative for a continuous treatment process for As(III) and As(V) remediation in real condition effluents sources.

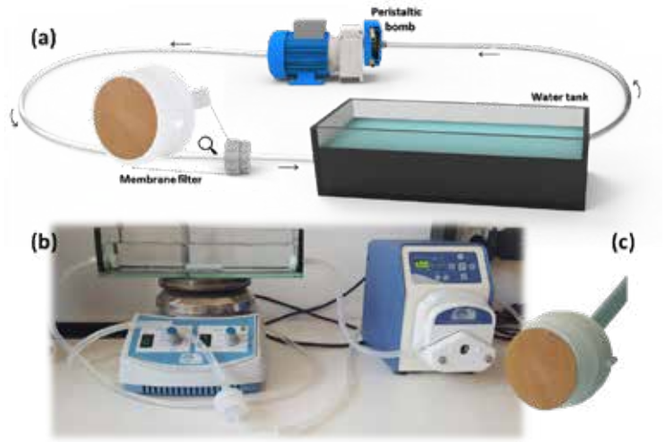


Fig 1
(a) Schematic representation of the membrane reactor, (b) picture of the functional membrane reactor and the corresponding (c) nanocomposite filter holder.

Nanocomposite membranes based on 10 wt.% Y@Fe_3O_4/PVDF-HFP were prepared with 5 wt.% of $Y_2(CO_3)_3$ and 5 wt.% of Fe_3O_4 NPs. The membranes were characterized and implemented in an up-scaled membrane reactor to evaluate their adsorption efficiency over As(III) and As(V). The NCF presented a well-distributed and micrometric porous structure with interconnected porous, with a homogeneous distribution of $Y_2(CO_3)_3$ and Fe_3O_4 NPs in the pore walls. The NCF membranes presented a hydrophobic behavior (contact angle of 126°), good thermal stability (141 °C of melting temperature), 13.7% of crystallinity, and a Young modulus of 60 MPa.
In respect to the removal efficiency of the membranes, it was proven that flow rate and pH of media play paramount roles in the adsorption efficiencies of As(III) and As(V), being lower rates and acidic pH optimal conditions for effective adsorption. The prepared NCF achieved maximum adsorption capacities of 101.9 and 212.8 mg/g for As(III) and As(V). In addition, the evaluation in the up-scaled membrane reactor demonstrated that the prepared NCF allow to remove arsenic species from effluents in the presence of interfering contaminants

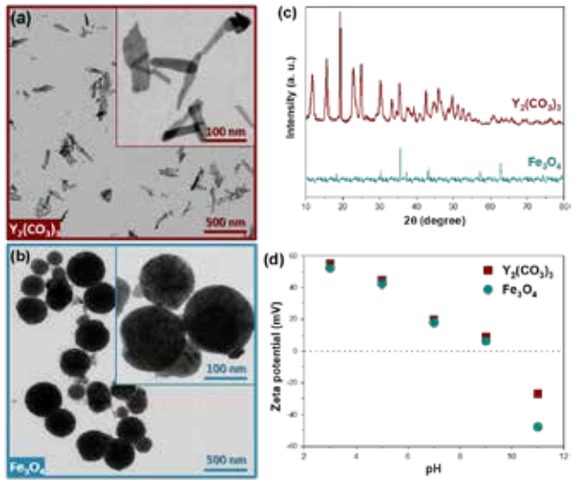


Fig 2
TEM images of (a) $Y_2(CO_3)_3$ and (b) Fe_3O_4; (c) XRD patterns and (d) zeta potential results for $Y_2(CO_3)_3$ and Fe_3O_4 NPs.

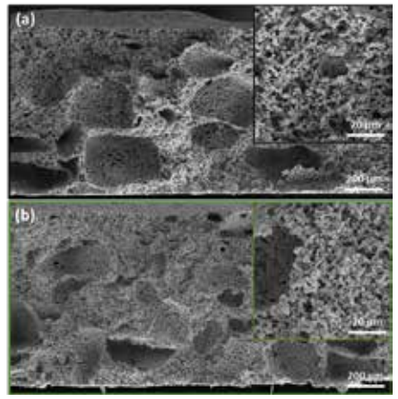


Fig 3
SEM images of (a) PVDF-HFP and (b) Y@Fe_3O_4/PVDF-HFP nanocomposite filter membranes.

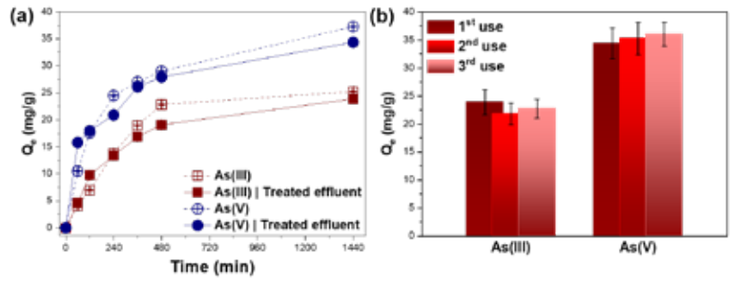


Fig 4
(a) As(III) and As(V) removal experiment on treated effluent sample by NCF, and (b) reusability of the NCF ([As] = 5 mg/L; contact time: 24 h; pH = 7.7; flux: 10 L/h).

with efficiencies of 21.9 and 51.8% for As(III) and As(V), respectively, allowing at least three utilization cycles after membrane regeneration and achieving total removal of As(III) and As(V) after 7 and 3 days, respectively. Adsorption kinetics of NCF followed a pseudo-second-order model, indicating chemical adsorption processes. The Langmuir model's isotherm data confirmed chemisorption as the dominant arsenic uptake phenomenon. Additionally, in good agreement with kinetic and isotherm results, together with post-use characterization, chemisorption appears as the main mechanism for arsenic adsorption.
The prepared Y@Fe_3O_4/PVDF-HFP membranes proved suitable for the long term and dual removal of As(III) and As(V) from water effluents under natural conditions. This work represents a significant advance on novel hybrid materials to remove persistent and hazardous contaminants from water efficiently, such as As and related compounds. This work also opens the avenue for further scalability and getting close to real water treatment for membrane reactors towards efficient and cost-effective treatments.

ENHANCEMENT OF MAGNETIC SURFACE-ENHANCED RAMAN SCATTERING DETECTION BY TAILORING Fe_3O_4@Au NANOROD SHELL THICKNESS AND ITS APPLICATION IN THE ON-SITE DETECTION OF ANTIBIOTICS IN WATER

Leixuri B. Berganza, Lucio Litti, Moreno Meneghetti, Senentxu Lanceros-Méndez, and Javier Reguera.
ACS Omega 2022, 7, 49, 45493–45503

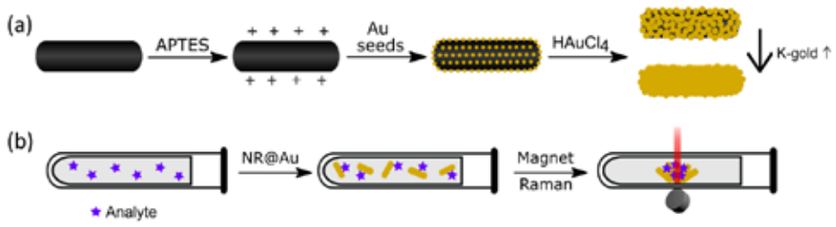


Fig 1
A) Schematic representation of the synthesis procedure, starting with the synthesis of magnetite nanorods, which are modified by electrostatic binding of gold nanoclusters and a final growth of a gold shell. B) Schematic representation of the measurement procedure, by adding the NR@Au to an antibiotic-containing solution, magnetic separation and accumulation, and Raman measurement at the pellet spot. Correlation coefficient, R, was greater than 0.98 in the ranges shown. Grayscale analysis (middle data set) leads to poorer limits of detection than Red channel analysis, but the same linear range.

Novel quick and affordable chemical sensing techniques for on-site monitoring are urgently needed in modern society. Their development underpins the development in fields as important as the environmental pollution control, or the personalized medicine. Here, we have evaluated the use of gold-coated magnetite nanorods as novel multifunctional nanoparticles for chemical sensing, that makes use of magnetic extraction and surface-enhanced Raman spectroscopy as the molecular sensing method. The results show quick magnetic separations and high Raman enhancement with limits of detection up to the nanomolar range for antibiotics such as ciprofloxacin when using portable Raman instruments.

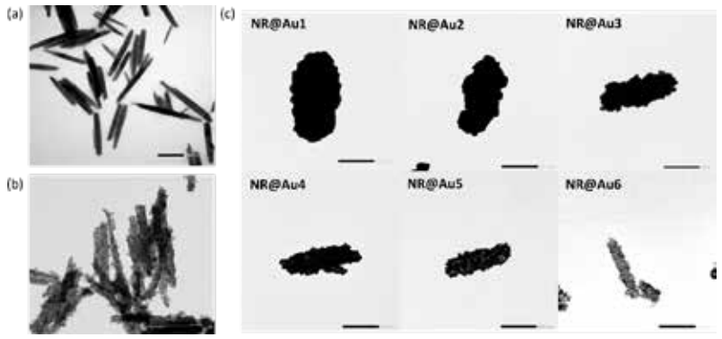


Fig 2
a)TEM image of Fe_3O_4 nanorods. b) TEM image of NR core-satellite structure. c) TEM images of core@shell structures synthesized at different shell growths.

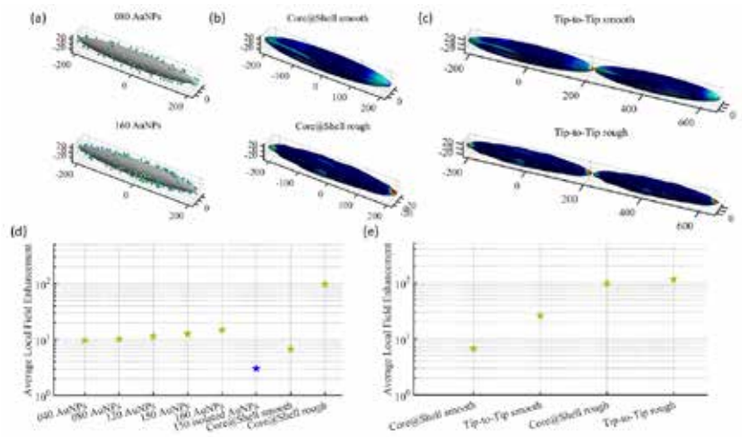


Fig 3
Simulations of different nanoparticles and configurations. a)Fe_3O_4 nanorods functionalized with different amounts of Au nanospheres, b) smooth (top) and rough (bottom) core@shell Fe_3O_4@Au NRs, c) tip-to-tip assembled smooth (top) and rough (bottom) core@shell structures, d) average local field enhancements of the different nanostructures,e) average local field enhancement of assemblies vs. individual nanoparticles.

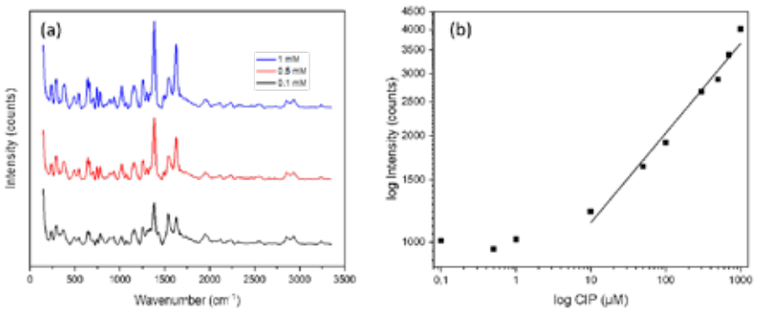


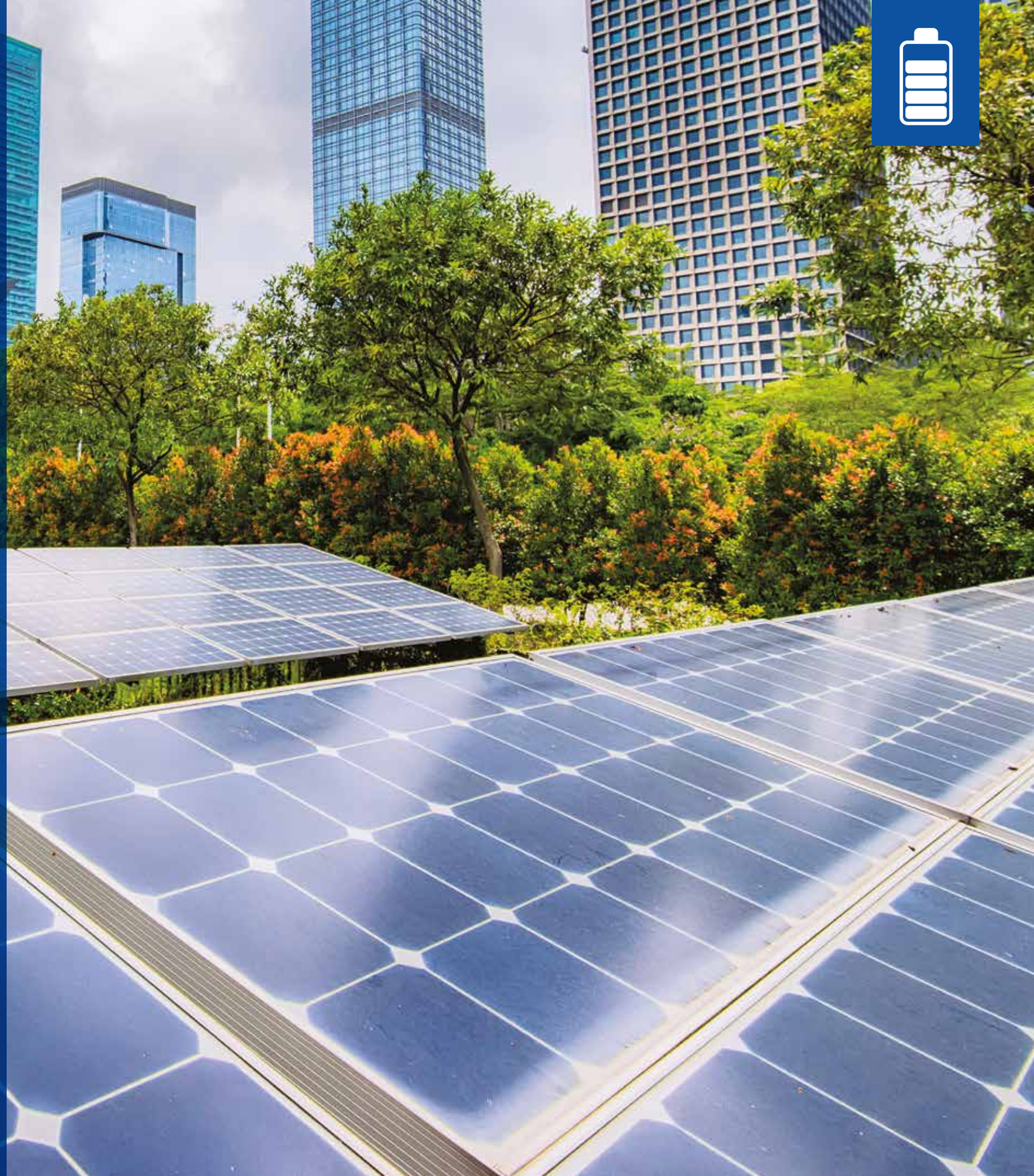
Fig 4
a) Raman spectra of CIP at different concentrations using NR@Au1 as substrate. b) Intensity of one characteristic peak of CIP (1382 cm^{-1}) at different concentrations performed with NR@Au1 structure.

Surface-enhanced Raman scattering (SERS) has become a promising method for the detection of contaminants or biomolecules in aqueous media. The low interference of water, the unique spectral fingerprint, and the development of portable and handheld equipment for in situ measurements underpin its predominance among other spectroscopic techniques. Among the SERS nanoparticle substrates, those composed of plasmonic and magnetic components are prominent examples of versatility and efficiency. These substrates harness the ability to capture the target analyte, concentrate it, and generate unique hotspots for superior enhancement. Here, we have evaluated the use of gold-coated magnetite nanorods as a novel multifunctional magnetic plasmonic SERS substrate. The nanostructures were synthesized starting from core-satellite structures. A series of variants with different degrees of Au coatings were then prepared by seed-mediated growth of gold, from core-satellite structures to core shell with partial and complete shells. All of them were tested, using a portable Raman instrument, with the model molecule 4-mercaptobenzoic acid in colloidal suspension and after magnetic separation. Experimental results were compared with the boundary element method to establish the mechanism of Raman enhancement. The results show a quick magnetic separation of the nanoparticles and excellent Raman enhancement for all the nanoparticles both in dispersion and magnetically concentrated with limits of detection up to the nM range (50 nM) and a quantitative calibration curve. The nanostructures were then tested for the sensing of the antibiotic ciprofloxacin (CIP), highly relevant in preventing antibiotic contaminants in water reservoirs and drug monitoring, showing that ciprofloxacin can be detected using a portable Raman instrument at a concentration as low as 100 nM in a few minutes, which makes it highly relevant in practical point-of-care devices and in situ use.

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 the conversion between solar energy and chemical energy 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.



MICROSTRAIN AND URBACH ENERGY RELAXATION IN $FAPbI_3$-BASED SOLAR CELLS THROUGH POWDER ENGINEERING AND PERFLUOROALKYL PHOSPHATE IONIC LIQUID ADDITIVES

Muhammed P. U. Haris, Samrana Kazim and Shahzada Ahmad
ACS Applied Materials & Interfaces 2022, 14, 24546-24556.

> Perovskite based solar cells have emerged as the potential contender for silicon solar cells in the past decade. In addition to performance-related research and development, long-term stability and device reliability based investigations have attracted the thin film PV community in recent years. We have developed a cost-effective powder methodology of α-$FAPbI_3$ synthesis and further through ionic liquid additivization improved the photovoltaic efficiency along with the high thermal and moisture stability of the perovskite. Our process mitigates the notorious structural and electronic imperfections.

Significant improvements in power conversion efficiency and stability have been made in perovskite solar cells (PSCs), by adopting research direction in fabrication processes, compositional engineering, phase stabilization strategies, strain engineering, additive engineering,and passivation methods. PSCs with formamidinium lead triiodide ($FAPbI_3$) as a photoactive layer are a front runner among the developed perovskites. However, most of the developed engineering protocols induce structural and electronic disorders which impede photovoltaic reliability.

We have demonstrated a powder engineering methodology for realizing a methylammonium and Br-free α-$FAPbI_3$ powder through a cost-effective precipitation route. We investigated their optoelectrical, structural, and photovoltaic properties, and correlated them with that of conventional and δ-$FAPbI_3$. We noted a drastic decrement in microstrain and Urbach energy values which are directly related to the structural and electronic disorders respectively. The reduced microstrain enhanced the stability of the perovskite layer and the Urbach energy decrement helped to improve the PSCs efficiency to 16.37% by lowering the open-circuit voltage deficit. Moreover, our synthetic protocol employing the low-grade PbI_2 could reduce the fabrication cost for the PSCs.

To hinder the moisture induced degradation of the PSCs, we further additivized the perovskite layer with ultra-hydrophobic perfluoroalkyl phosphate-based ionic liquids (ILs) with ethyl- (EMIFAP) and hexyl-functionalized (HMIFAP) imidazolium cations. The IL treatment enhanced the solar cell efficiency from 16.37% to 18.26%. The performance hike was ascribed to the improved crystallinity and absorption coefficient, reduced microstrain and Urbach energy, and a fluorine-Lead (F-Pb) semi-ionic interaction. The stability measurements under shelf-life, thermal stress, and maximum power-point tracking showed that the additivization boosted the PSCs long-term stability along with the performance enhancement.

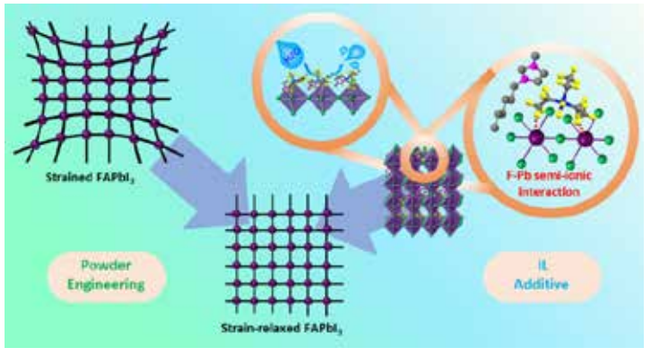


Fig 1
Graphical Abstract of powder engineering and IL additivization method. Fig. reproduced from ACS Appl. Mater. Interfaces 2022, 14, 24546-24556.

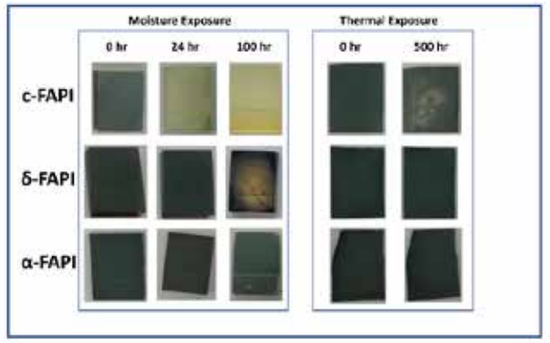


Fig 2
Digital photographs of perovskite thin films upon moisture (45-50% RH) and thermal (85 °C) exposure taken over time. Fig. reproduced from ACS Appl. Mater. Interfaces 2022, 14, 24546-24556.

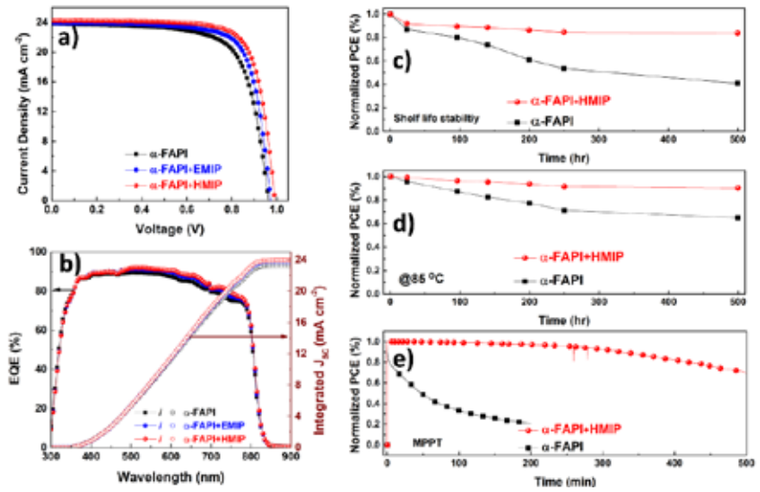


Fig 3
Photovoltaic properties of EMIFAP- and HMIFAP-treated solar cells: (a) J-V curves under forward scan, (b) EQE and integrated photocurrent of corresponding devices,(c-e) normalized stability curves of unencapsulated devices under (c) shelf-life, (d) thermal stress and (e) MPP tracking.
Fig. reproduced from ACS Appl. Mater. Interfaces 2022, 14, 24546-24556.

A PLANT-LIKE BATTERY: A BIODEGRADABLE POWER SOURCE ECODESIGNED FOR PRECISION AGRICULTURE

Marina Navarro-Segarra, Carles Tortosa, Carlos Ruiz-Díez, Denis Desmaële, Teresa Gea, Raquel Barrena, Neus Sabaté, Juan Pablo Esquivel. Energy Environ. Sci., 2022, 15, 2900–2915

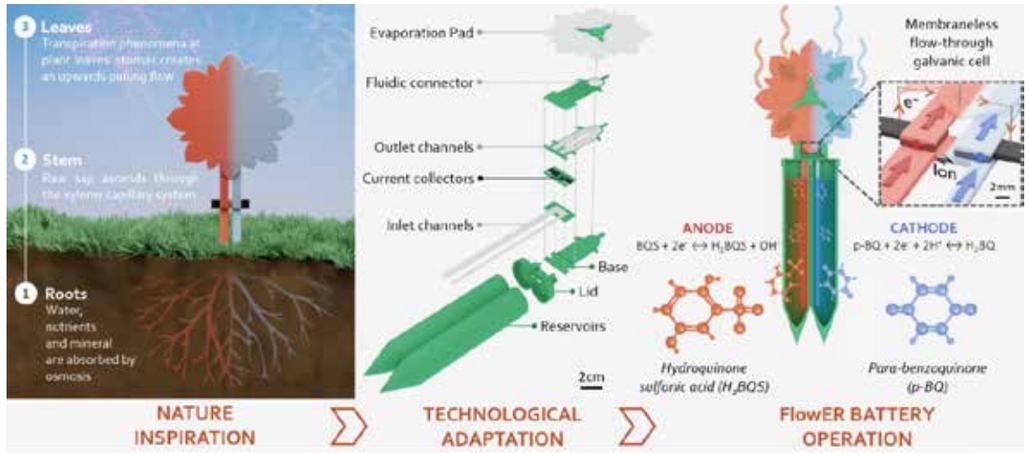


Fig 1
FlowER battery concept evolution from the inspiration, found in the liquid transport in plants, to an operational prototype. The technological adaptation of the FlowER battery concept has been performed through the selection of environmentally harmless materials to produce: two inlet channels acting as roots, from which the device nurtures with dissolved redox species, just like plants take water and nutrients from their surroundings. The main laminated paper core, analogue to a plant steam, includes two porous carbon current collectors and a salt bridge, indispensable components to create a membraneless galvanic cell. The core ends with two outlet channels that transport the fluid towards the top. A rounded leaf-like absorbent pad exposed to the atmosphere keeps wicking the solution by transpiration pull through the battery. Finally, a 3D printed compostable green casing (i.e., reservoirs + lid + base + paper supports) was used to provide mechanical robustness and verticality.

> In this work we show a biodegradable battery inspired in transpiration pull of liquids in plants that has been ecodesigned to follow the life cycle of applications in precision agriculture. The battery meets power requirements of wireless sensors and is composed of benign non-toxic materials that allow, after its operation, to be safely biodegraded or composted, resembling the way a plant comes back to nature at the end of its life cycle.

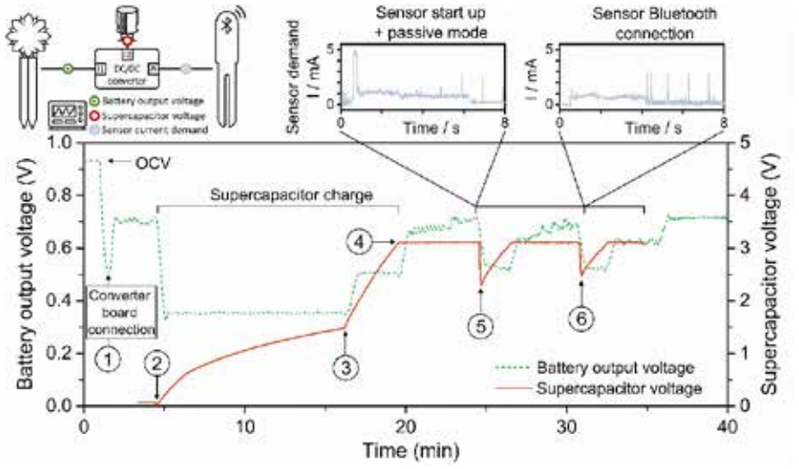


Fig 2
Proof of concept of the evaporation driven flow battery demonstrating the capability of powering the start-up, passive mode and Bluetooth connection of a horticulture caring device.

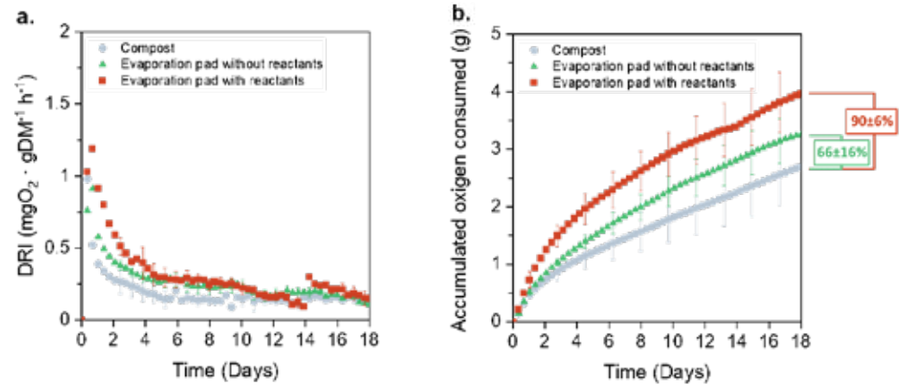


Fig 3
Aerobic biodegradability assessment of the FlowER battery, (N=3). a. Dynamic respiration index (DRI) of evaporation pads with and without reaction products accumulated over 3 days and compost used as a blank; b. Total oxygen consumed by the three samples and level of biodegradation achieved at day 18.

The natural environment has always been a source of inspiration for the research community. Nature has evolved over thousands of years to create the most complex living systems, able to leverage inner and outside energetic interactions in the most efficient way. This work presents a flow battery profoundly inspired by nature, which mimics fluid transport in plants to generate electric power. The battery was ecodesigned to meet a life cycle for precision agriculture (PA) applications; from raw material selection to disposability considerations, the battery is conceived to minimize its environmental impact while meeting PA power requirements. The paper-based fluidic system relies on evaporation as the main pumping force to pull the reactants through a pair of porous carbon electrodes where the electrochemical reaction takes place. This transpiration naturally occurring effect enables to significantly expand the operational lifespan of the battery, overcoming the time-limitation of current capillary-based power sources. Most relevant parameters affecting the battery performance, such as evaporation flow and redox species degradation, are thoroughly studied to carry out the device optimization. Flow rates and power outputs comparable to capillary-based power sources are achieved. The prototype practicality has been demonstrated by powering a wireless plant caring commercial device. Standardized biodegradability and phytotoxicity assessments show that the battery is harmless for the environment at the end of its operational lifetime. Placing sustainability as the main driver leads to the generation of a disruptive battery concept that aims to address societal needs within the planetary environmental boundaries.

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 will be developed and integrated in a variety of applications, including smart cities, smart interiors, industry 4.0 and wearables, among others.

TOWARDS NEXT-GENERATION MOBILE DIAGNOSTICS: NEAR FIELD COMMUNICATION-POWERED ELECTROCHEMILUMINESCENT DETECTION

Joseba Totoricaguena-Gorriño, Michele Dei, Alejandro Fidel Alba, Nikola Perinka, Leire-Ruiz Rubio, José Luis Vilas-Vilela, Francisco Javier del Campo, ACS Sensors. 2022, 7, 5, 1544–1554

This work demonstrates that smartphones can both power and analyze an electrochemiluminescence (ECL) signal by using Near Field Communication (NFC) as the power source, and the camera as the detector. The device consists of an electrochemical cell in series with a rectenna, and uses $Ru(bpy)_3^{2+}$/ tri-n-propylamine to generate ECL. Images are captured by the smartphone camera for analysis. An NFC signal provides the energy to generate ECL from $Ru(bpy)_3^{2+}$, which has been detected down to 0.64 μM and up to 1.0 mM.

Fig 1
A photorealistic render of the NFC electrochemical platform for electrogenerated chemiluminescence point of care devices.

Mobile phones have been used in combination with point of care (PoC) devices for over a decade now. However, their use seems restricted to the detection of sensing events using the video and camera functions. In contrast, the complementary ability to use mobile phones to power such PoC devices has been largely unexplored.

This work demonstrates proof of principle that a smartphone can be used to both power and analyze an electrochemiluminescence (ECL) detection system. A printed device is presented featuring an electrochemical cell connected in series to a rectenna that is able to use the Near Field Communication (NFC, 13.56 MHz) signal to provide the energy needed to generate ECL from $Ru(bpy)_3^{2+}$ / tri-n-propylamine. The emitted light, which intensity is directly proportional to the concentration of the ruthenium complex, can then be captured by the mobile phone camera, and analyzed. This work presents the fabrication, and the electrical and electrochemical characterization of the device.

Effective voltages ranging from 0.90 to 4.50 V have been recorded, depending on the coupling between emitter and receiver, which translate into working electrode potentials ranging from 0.76 up to 1.79 V vs Ag. Detection and quantification limits of 0.64 μM and 1.52 μM, respectively have been achieved for $Ru(bpy)_3^{2+}$, and linear ranges up to 0.1 mM (red channel) and no less than 1.0 mM (green channel) have been found.

One major advantage of this technology is its portability and ease of use. By utilizing a smartphone as both the power source and the detection system, the device can be easily used in remote or resource-limited areas. Additionally, the device is relatively inexpensive to fabricate, which makes it even more attractive.

Furthermore, this work is significant as it can open new possibilities in the field of ECL and bio-sensing, bringing a new generation of portable and low-cost diagnostic devices for clinical and environmental testing. This proof of principle opens the door for further research and development in this field, and for the creation of new applications utilizing this technology.

In conclusion, this work shows a practical and a cost-effective solution to power and analyze diagnostic device by using a smartphone, which is a readily available device. This technology could lead to a new generation of portable and low-cost diagnostic devices for clinical and environmental testing, especially in resource-limited settings.

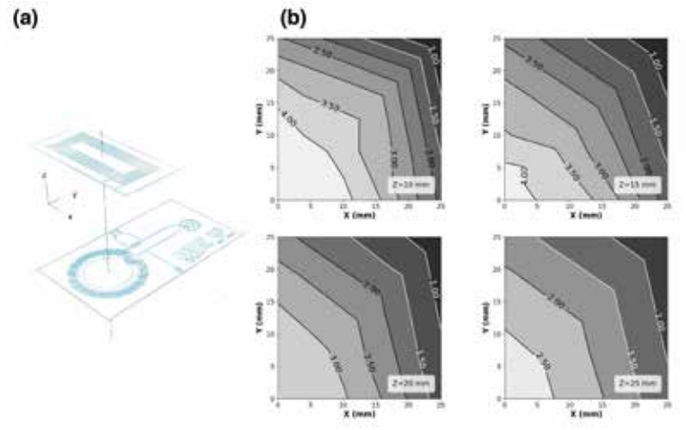


Fig 2
(a) Diagrammatic representation of the experimental setup, where a movable square emitter antenna is placed on top of a fixed printed device round antenna. (b) The resulting DC voltage X, Y maps, measured as potential difference between auxiliary and working electrodes, are shown for different antenna separations (Z).

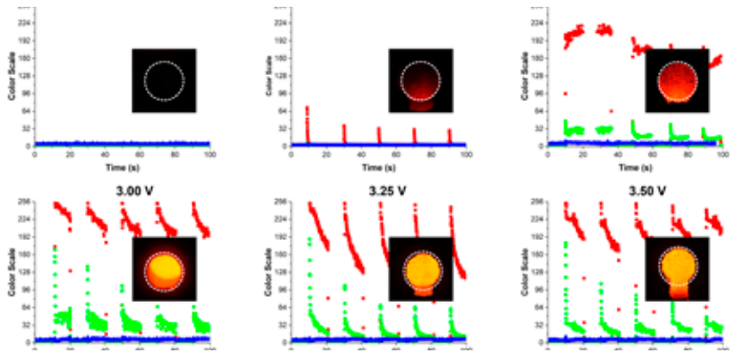


Fig 3
Potential steps generated by a sequence of 10s on/off NFC cycles in the presence of 0.5mM $Ru(bpy)_3^{2+}$ in 25mM TPrA. The total voltage between auxiliary and working electrode was determined by the potentiostat, and controlled through the separation distance between emitter and receiver antennas. The red squares correspond to the Red channel, the green dots correspond to the Green channel, and the blue traces correspond to the Blue channel. Inset images show the electrode during the first NFC-on cycle.

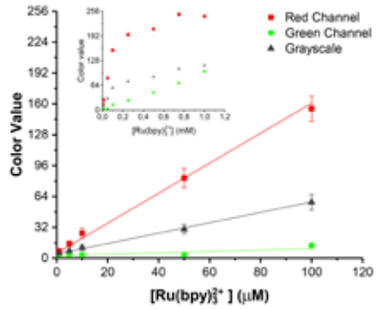


Fig 4
Calibration plots for the detection of $Ru(bpy)_3^{2+}$ electrochemiluminescence produced by NFC at 2.5 V cell polarization. Both red and green channels respond, providing a wide detection range starting at 15 μM and 120 μM, respectively. In both cases the regression coefficient, R, was greater than 0.98 in the ranges shown. Grayscale analysis (middle data set) leads to poorer limits of detection than Red channel analysis, but the same linear range.

MULTIFUNCTIONAL TERNARY COMPOSITES WITH SILVER NANOWIRES AND TITANIUM DIOXIDE NANOPARTICLES FOR CAPACITIVE SENSING AND PHOTOCATALYTIC SELF-CLEANING APPLICATIONS

Carmen R. Tubio, Nelson Pereira, Lia Campos-Arias, Pedro Manuel Martins, Jose Luis Vilas-Vilela, Carlos M. Costa, and Senentxu Lanceros-Méndez. ACS Applied Electrononic Materials. 2022, 4, 8, 3815–3824

Fig 1
Cover art for this paper on ACS Applied Electronics. August 2022

> The combination of self-cleaning and self-sensing capabilities is relevant in the scope of hygienic surfaces due to the sensing performance for capacitive response in clean environments without dirt and bacteria. Detection and cleaning performance are essential for the next-generation smart composites. Here, novel ternary composite material are presented, and they were characterized in terms of microstructure, polymer phase, and thermal, optical, mechanical, and dielectric properties. Further, the applicability of these composites for photocatalytic self-cleaning and capacitive sensing has been demonstrated.

Hybrid materials with both self-cleaning and capacitive sensing capabilities have been developed. The ternary composites were produced by solvent casting technique based on titanium dioxide nanoparticles (TiO_2) and silver nanowires (AgNWs) in a poly(vinylidene fluoride) (PVDF) matrix varying the contents of the filler up to 10 wt%. Mainly, TiO2 particles are chosen due to their photocatalytic properties, with well kown potential for environmental remediation and energy applications. While, AgNWs are selected based on their catalytic, optical, and antimicrobial properties. The experimental results prove that the morphology of the composites is compact, and the fillers are well dispersed. The filler type and its content does not affect the polymer phase and the thermal properties. The optical properties are determined by TiO_2 filler versus AgNW filler with higher absorbance. Furthermore, the Young's Modulus of the composites increases with increasing TiO_2content and decreases with the inclusion of AgNW content (7.5 and 10 wt.%). Dielectric constants up to 14 at 1 kHz have been obtained for the 7.5%AgNWs/2.5%TiO_2/PVDF sample. Finally, the photocatalytic self-cleaning and capacitive sensing functional response are testing. The photocatalytic activity was proved for sample 5%AgNWs/5%TiO_2/PVDF by removing ≈ 70% of methylene blue (MB) molecules in solution under 360 min of UVA irradiation; additionally, the reactive oxygen species (ROS) generation necessary for the photocatalytic process allows to foresee a self-cleaning ability. Additionally, the capacitive sensing capability has been demonstrated with excellent functional response for the same sample. The response of the capacitive sensor does not show clamping effects, hysteresis, or degradation over time, demonstrating adequate mechanical stability. This work demonstrates that it is possible to develop multifunctional materials based on two different fillers with tailored functional responses (photocatalytic self-cleaning and capacitive behaviour) for the next generation of smart materials.

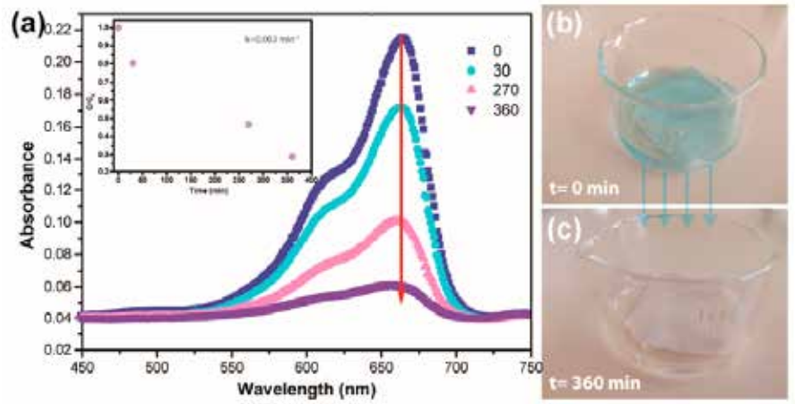


Fig 2
Photocatalytic degradation of MB in solution (1×10^{-5} M and pH=6.5) using the 5%AgNWs/5%TiO_2/PVDF sample, under 360 min of UVA radiation – inset presents the photocatalytic degradation kinetic and the apparent reaction rate (k). (a). Pictures of the 5%AgNWs/5%TiO_2/PVDF sample in contact with the MB aqueous solution before (b) and after (c) 360 min of UVA irradiation.

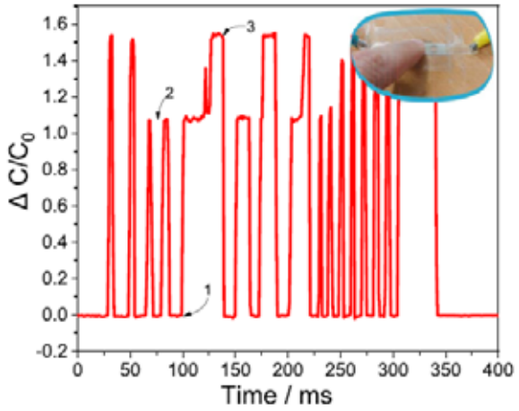


Fig 3
Demonstration of the capacitive sensor response upon repeated finger touch.

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.

CORE-SHELL Fe_3O_4@Au NANOROD-LOADED GELS FOR TUNABLE AND ANISOTROPIC MAGNETO- AND PHOTO-THERMIA

Mikel Rincón-Iglesias, Irati Rodrigo, Leixuri B. Berganza, Esraa Samy Abu Serea, Fernando Plazaola, Senentxu Lanceros-Méndez, Erlantz Lizundia, Javier Reguera.
ACS Applied Materials & Interfaces 2022, 14, 5, 7130−7140

Advanced hyperthermia treatments require the creation of multifunctional materials that offer synergetic properties. Here we report on the tunable synthesis of Fe_3O_4@Au core-shell nanorods through a multistep method. Anisotropic hydrogels were produced with these nanoparticles by gelation under an external magnetic field. The generated hydrogels presented an enhancement of the magnetothermal specific absorption rate (SAR) in the direction of the orientation of the nanorods. On the other side, a reduction was produced in the parallel direction, offering a tunability tool to fine-control the amount of produced hyperthermia. Moreover, photothermia in the near IR was also generated due to the rod-shell hybrid plasmonic modes, converting this material into a multifunctional system for enhanced and synergistic properties, and opening the door to many advanced nanobiomedical applications.

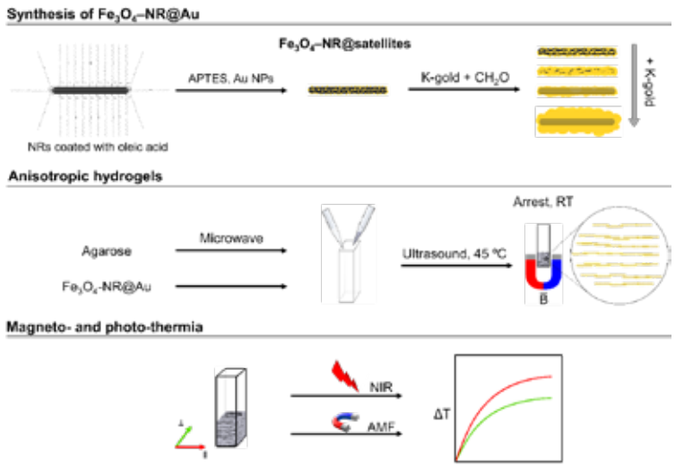


Fig 1
Representation of the different steps followed to achieve the anisotropic gel and its use in magnetothermia. From top to down: Synthesis of the hybrid nanoparticles Fe_3O_4-NR@Au. Preparation of the nanoparticle-loaded anisotropic agarose hydrogel. Use of the loaded hydrogel in magneto- and photothermia with directional characteristics.

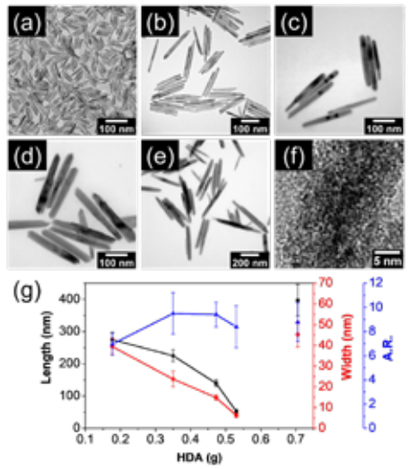


Fig 2
TEM images of the synthesized NRs at different amounts of the capping ligand HDA: (a) 0.53 g, (b) 0.47 g, (c) 0.35 g (d) 0.18 g (e) 0.70 g. Error bars correspond to the standard deviation of an average of 50 measured nanoparticles. (f) HRTEM of a NR from Figure 1(b). (g) Average sizes of the NRs in a-e (black squares: length, red circles: width, and blue triangles: aspect ratio (A.R.)) representing their evolution with the HDA and maintaining the rest of the parameters constant.

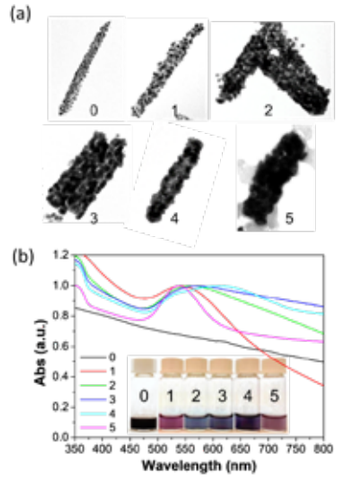


Fig 3
a) TEM image of the rods at different growth conditions. Sample 0 corresponds to Fe_3O_4-NR-satellites structure, and the subsequent samples (1-5) were prepared increasing the amount of the ratio [K-gold]/[NR-satellite seeds], generating different degrees of core-satellites until a complete core-shell is obtained. b) UV-Vis spectra of the solution of the different nanoparticles and their pictures showing the differences in the optical properties (a).

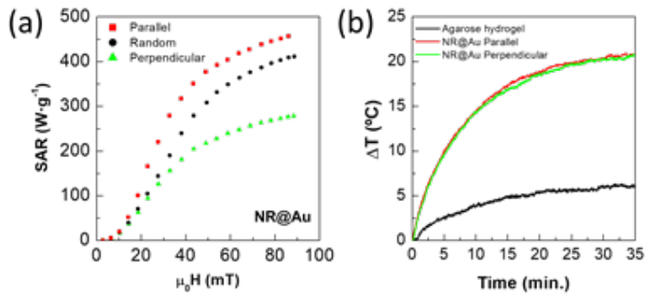


Fig 4
a) Specific absorption rate (SAR) measured by AC magnetometry of Fe_3O_4-NR@Au in parallel, random, and perpendicular orientations with the magnetic field. b) Photothermia Fe_3O_4-NR@Au under near IR illumination at different orientations.

Hyperthermia therapeutic treatments are those that use local heat, which is triggered externally, to produce a therapeutic effect. Tissue regeneration, drug delivery, or thermal ablation of cancer tumours are some prominent examples. The most important requirement for their development is the creation of efficient nanoheaters that produce an increase in temperature where the therapeutic effect is required. Multifunctional materials with tunable synergetic properties can offer a high advantage due to synergistic hyperthermal effects while offering additional functionalities. Here we report on the tunable synthesis of Fe_3O_4@Au core-shell nanorods through a multistep method and their subsequent incorporation into an agarose hydrogel to obtain anisotropic magnetic and optical properties for magneto- and photo-thermal anisotropic transductions. To obtain those multicomponent nanoparticles, highly monodisperse ferrimagnetic Fe_3O_4 nanorods with tunable sizes between 50 and 300 nm were synthesized by a solvothermal method by varying the amount of hexadecylamine capping ligand. A gold shell was coated onto Fe_3O_4 nanorods by the intermediate formation of core-satellite structures. The shell was produced in a subsequent controlled growth process where each individual satellite grew until, due to the surface confinement, they merged to form a continuous shell. This tunable growth led to an optical response variation from the visible to the near IR region. The nanorods were oriented within an agarose hydrogel to fabricate free-standing anisotropic materials, providing a proof of concept for the applicability of these materials for anisotropic magneto- and photo-thermia applications. The generated gels presented an enhancement of the specific absorption rate (SAR) of magnetothermia in the direction of the orientation of the nanorods. On the other side, a reduction was produced in the parallel direction, offering a tunability tool to fine-control the amount of produced hyperthermia. Finally, the strong gelling upon cooling and shear-thinning behavior of agarose enabled the fabrication of magnetically active continuous hydrogel filaments upon injection. These developed multifunctional nanohybrid materials represent a base for advanced sensing, biomedical, or actuator applications with an anisotropic response.

PRINTED MULTIFUNCTIONAL MAGNETICALLY ACTIVATED ENERGY HARVESTER WITH SENSING CAPABILITIES

R. Brito-Pereira, C. Ribeiro, N. Pereira, S. Lanceros-Mendez and P.Martins. Nano Energy, Volume 94, 2022,106885

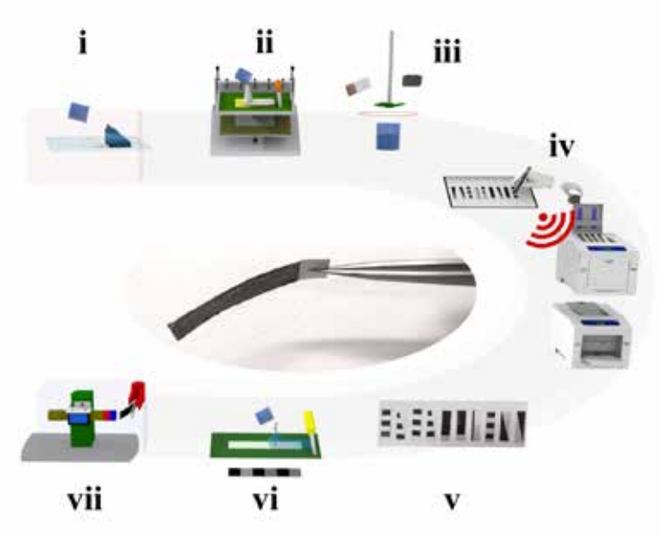


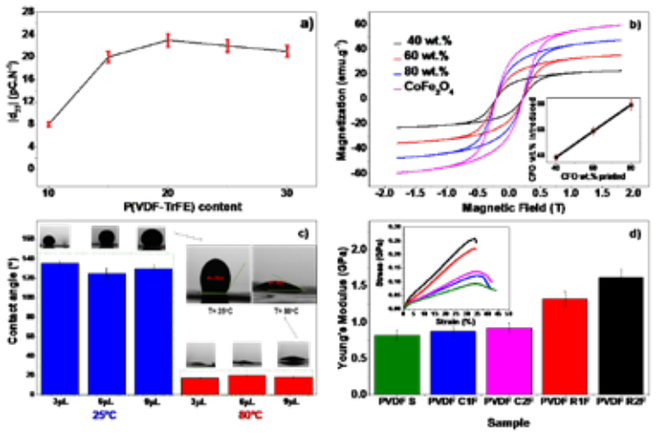
Fig 1
Printing procedure of the proposed sensing/harvesting platform.

The exponential growth and ubiquitous use of mobile electronics supported by the Internet of Things (IoT) is leading to an increasing need of self-powered wearable electronic devices. Magneto-mechano-electric energy conversion is an effective way to convert magnetic fields into electricity for low power applications. The successful printing of such materials allows the design of customized structures, improved integration into devices and reduced materials waste. Here, a self-powered printed sensing device is presented, by exploiting piezoelectric/magnetic composites in response to magnetic stimuli via magneto-mechano-electric energy conversion.

Fifteen years ago, the International Telecommunications Union (ITU) published its first report on the Internet of Things (IoT), introducing a new dimension on Information and Communication Technologies linked to the premises of connecting anyone, anything, anytime and anywhere.

Additive manufacturing, and particularly printing technologies offer not only the possibility to fulfil such needs but also to integrate those smart materials faster, easier, and more cost-effective. Additionally printing technologies are more versatile and environmentally-friendly, also allowing the design of customized structures (micro-, nano-, asymmetric, flexible, or stretchable) that are essential for an effective IoT environment.

A novel printed magnetic sensor/harvester based on a piezoelectric polymer and $CoFe_2O_4$ nanoparticles/wax composite is designed and fabricated by printing technologies. The self-powered magneto-mechano-electric printed device not only provides excellent harvesting capability, but also suitable self-powered magnetic sensing performance. The printed device can harvest magnetic energy with maximum output power densities of 4 and 10 $mW.cm^{-3}$, on magnetic and magnetic+mechanical solicitation conditions, respectively. Additionally, the device reveals a sensing performance characterized by r^2 of 0.9991 and a sensitivity of 30 $V.T^{-1}$. The presented sensing/harvesting principle, as well as the simple and cost-effective fabrication technology, will allow advances in self-powered wearable sensors and devices compatible with IoT-related systems.



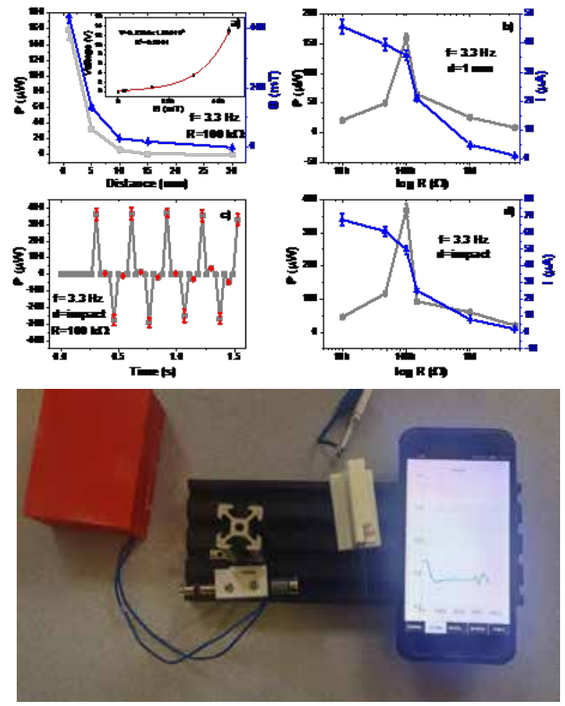


Fig 2
a) Relation between the |d33| piezoelectric coefficient and the P(VDF-TrFE) weight content in the printed polymer prepared with different P(VDF-TrFE)/ DMF ratios. b) Room-temperature magnetic hysteresis cycles for the printed wax-$CoFe_2O_4$ compositions with different $CoFe_2O_4$ wt.% content. The inset reveals the relation between the $CoFe_2O_4$ wt.% in solution and the CFO wt.% in the corresponding printed layers. c) Contact angle at room-temperature and at 80°C of different wax-$CoFe_2O_4$ (80 wt.% of $CoFe_2O_4$) drops on printed P(VDF-TrFE) with silver electrodes. d) Young's Modulus of the different samples. The inset shows a representative stress-strain curve for each sample. Representative e)-cross section and f)-surface SEM images of the P(VDF-TrFE)/silver//Wax-CFO/ Resin 3-layered composite.

Fig 3
a) Harvested power (P) and magnetic field (B) as a function of the distance to the magnet without the mechanical deformation resulting from the impact between the magnet and the printed composite. b) Relation between the measured power, load resistance (R) and current (I) without the mechanical impact between the magnet and the printed composite. c) Harvested power (P) as a function of the cycling solicitation (f=3.3 Hz). d) Relation between the measured power, load resistance (R) and current (I) with mechanical impact between the magnet and the printed composite. e) Data sent (through Bluetooth) by the microcontroller and received by a smartphone.

PHOTOCROSSLINKABLE AND SELF-HEALABLE HYDROGELS OF CHITOSAN AND HYALURONIC ACID

Sheila Maiz-Fernández, Leyre Pérez-Álvarez, Unai Silván, José Luis Vilas-Vilela, Senentxu Lanceros-Mendez.. International Journal of Biological Macromolecules.216 (2022) 291-302

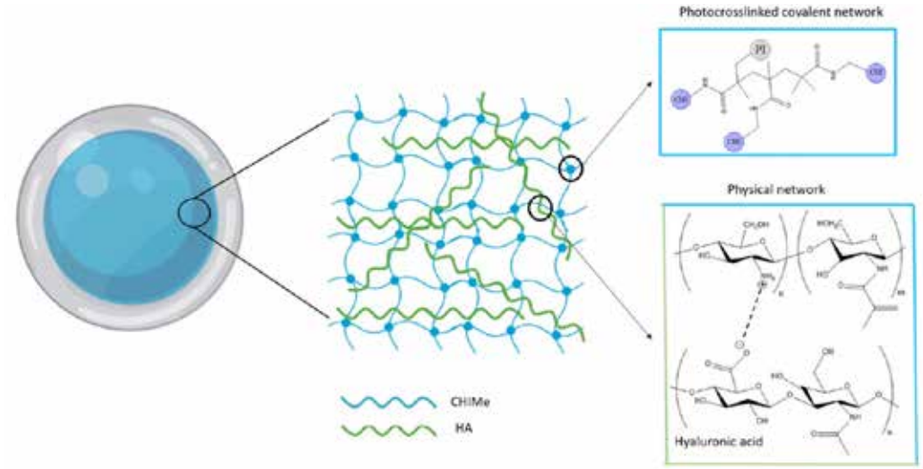


Fig 1
Schematic representation of the formation of a photocrosslinkable and self-healing hydrogel based on chitosan methacrylate and hyaluronic acid.

> In this work we describe a novel photocrosslinkable, injectable and self-healing hydrogel based on chitosan methacrylate and hyaluronic acid. The study of the physicochemical properties of the hydrogels revealed their capability of generating doubly crosslinked networks with similar Young's moduli, independent of the number of self-healing cycles, as well as tailored swelling, mechanical and rheological properties, depending on the relative polysaccharide content. Additionally, these hydrogels are highly biocompatible, biodegradable, and therefore suitable for advanced biomedical and tissue engineering applications.

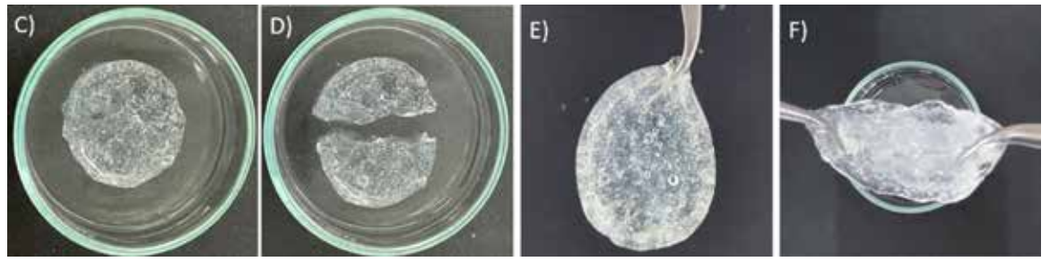
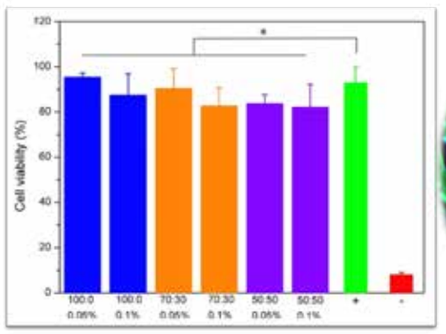


Fig 2
Demonstration of the self-healing ability of the chitosan and hyaluronic acid hydrogels.



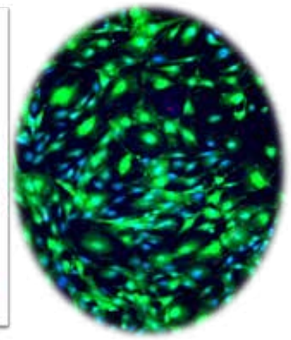


Fig 3
All produced hydrogels have excellent biocompatibility with a cell survival rate of over 80% (green cells).

Hydrogels have repeatedly been suggested as biomimetic three-dimensional scaffolds for tissue regeneration that offer structural support and deliver factors that promote tissue restoration. Their structural similarities to the extracellular matrix present in many tissues, mild processing techniques, and ability to be injected, make them ideal for a variety of biological applications. In this regard, a promising method for the creation of in situ gelling hydrogels for tissue engineering applications is the polymerization of monomers or polymers by illumination with ultraviolet and visible light. With this in mind, in this work we produced hydrogels based on chitosan methacrylate and hyaluronic acid and investigated the physicochemical characteristics and biocompatibility of the resulting materials. Our results show that lower content of photocrosslinkable chitosan increases the hydrophilicity of the resulting hydrogels, therefore supporting their swelling. In turn, mixtures with a high percentage of methacrylated chitosan generate hydrogels with improved mechanical and rheological properties. Therefore, it is possible to create hydrogels with tailored properties by adjusting the relative quantity of the primary components. In a hydrolytic medium, all hydrogels eventually degrade completely within 3 weeks, and in a medium containing lysozyme and hyaluronidase, this process takes about a week. All hydrogels also exhibit excellent biocompatibility and the capacity to recover their original shape after damage. These characteristics make them promising candidates for their application as scaffolds and drug or cell carriers.

RESEARCH **LINE 2**

MICRO & NANOSTRUCTURED 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.

FROM AN ANTIFERROMAGNETIC INSULATOR TO A STRONGLY CORRELATED METAL IN SQUARE-LATTICE $MCl_2(pyrazine)_2$ COORDINATION SOLIDS

Panagiota Perlepe, Itziar Oyarzabal, Laura Voigt, Mariusz Kubus, Daniel N. Woodruff, Sebastian E. Reyes-Lillo, Michael L. Aubrey, Philippe Négrier, Mathieu Rouzières, Fabrice Wilhelm, Andrei Rogalev, Jeffrey B. Neaton, Jeffrey R. Long, Corine Mathonière, Baptiste Vignolle, Kasper S. Pedersen, and Rodolphe Clérac.
Nat. Commun. 2022, 13, 5766.

In molecule-based materials, the electronic synergy between metal ions and organic linkers is essential to chemically engineer desired conductive and magnetic properties and ultimately, to find applications in spintronic devices. This work demonstrates how the choice of the metal ion in a series of isostructural materials ($MCl_2(pyz)_2$; M = Cr, Ti, V; pyz = pyrazine) allows precise control of their physical properties, converting a ferrimagnetic semiconductor (M = Cr) into an antiferromagnetic insulator (M = V) or a strongly correlated Fermi liquid (M = Ti).

The ability of coordination polymers (CPs) to be insulators, semiconductors, or even metals, while displaying remarkable magnetic properties, makes them attractive candidates for next-generation spintronic devices. For such purpose, CPs must have perfectly controlled magnetic and conductive properties, which is why chemists and physicists strive to understand the precise role of physical-chemical parameters in the origin of these physical properties.

Take for example the two-dimensional CPs $MCl_2(pyz)_2$ (M = Cr, Ti, V; pyz = pyrazine; Figure 1). Why does the ferrimagnetic and semiconducting chromium-based compound (Nat. Chem. 2018) become an insulator when this ion is replaced by vanadium and a conductor when titanium is chosen, even though they all have the same structure? In the case of vanadium, the pyrazine ligands simply serve as mediators for interactions between the electrons of the vanadium ions, which remain localized on each metal center. Instead, during the synthesis of the chromium and titanium analogues, an electron is transferred from the metals to the pyrazine ligands, giving rise to CPs incorporating M(III) ions and singly reduced pyrazine scaffolds. Due to a good orbital overlap and electronic delocalization, $TiCl_2(pyz)_2$ displays a room temperature conductivity value of 5 S/cm, which is two orders of magnitude higher than that observed in the chromium analogue (σ_{RT} = 0.03 S/cm) and the highest value observed for any CP based on octahedrally coordinated metal ions. Despite the apparent semiconducting behaviour of $TiCl_2(pyz)_2$ (Figure 2a), the combined and consistent analysis of the electrical conductivity, the large and positive magnetoresistance (Figure 2b), the specific heat (Figure 2c), the magnetisation data and DFT calculations demonstrate the presence of a correlated Fermi liquid state in this metal-organic material. These complementary theoretical and experimental techniques unambiguously prove the existence of metallic conductivity in $TiCl_2(pyz)_2$, providing a general methodology to study conducting CPs.

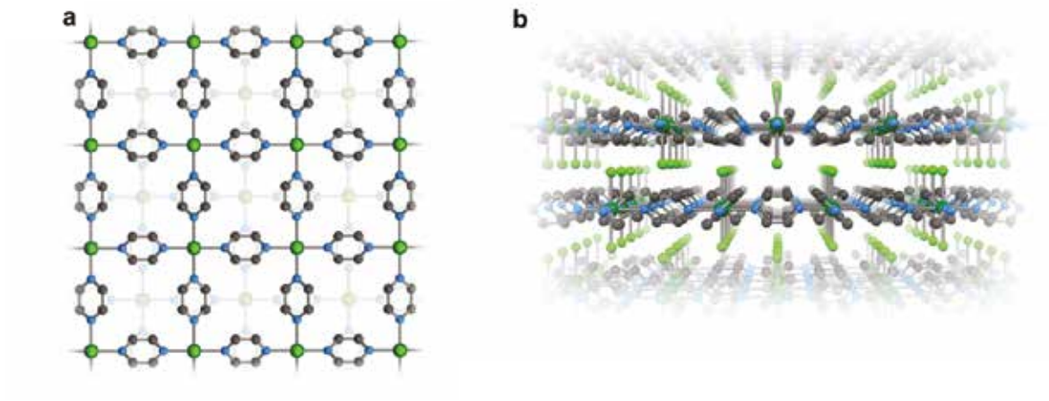


Fig 1
Structure of $MCl_2(pyz)_2$ (M = Cr, V, Ti) shown (a) perpendicular and (b) parallel to the two-dimensional lattice. Colour code: M, dark green; Cl, light green; C, dark grey; N, blue; H, omitted for clarity.

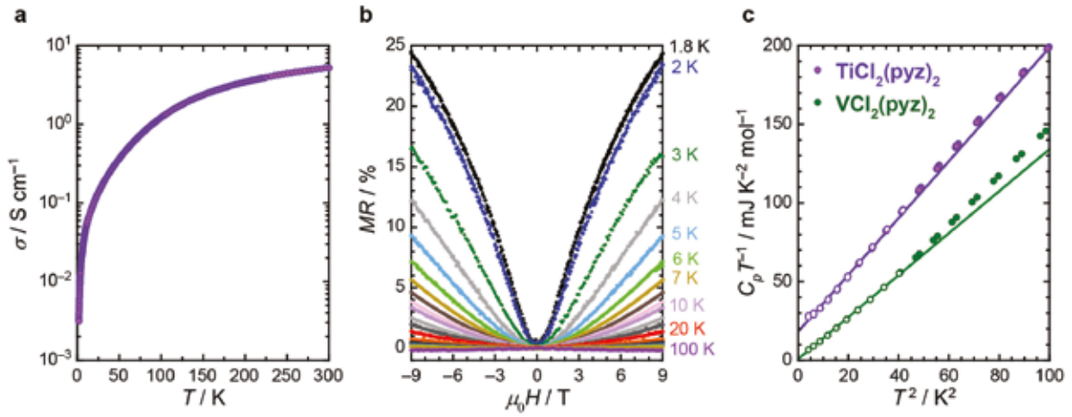


Fig 2
a Temperature dependence of the pressed-pellet conductivity of $TiCl_2(pyz)_2$. b Magnetoresistance vs magnetic field at selected temperatures for $TiCl_2(pyz)_2$. c Specific heat capacity, C_p, shown as C_pT^{-1} vs T^2 (all symbols) for $TiCl_2(pyz)_2$ (purple) and $VCl_2(pyz)_2$ (green). Solid lines are best fits to the data (shown in open circles).

MOF SYNTHESIS PREDICTION ENABLED BY AUTOMATIC DATA MINING AND MACHINE LEARNING

Yi Luo, Saientan Bag, Orysia Zaremba, Adrian Cierpka, Jacopo Andreo, Stefan Wuttke, Pascal Friederich, Manuel Tsotsalas. Angewandte Chemie International. Ed.2022,61,e202200242

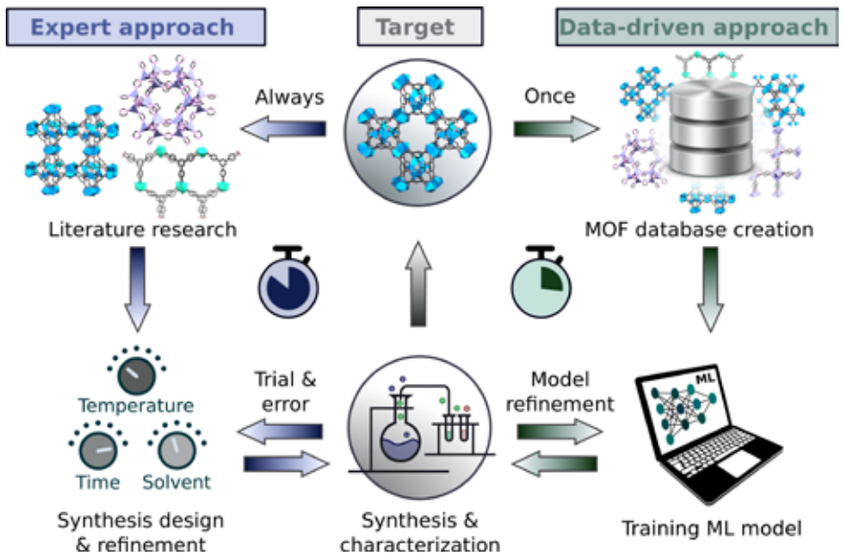


Fig 1
A new approach to MOF synthesis.

> We show how machine learning (ML) can be used for rationalization and acceleration of the MOF discovery process by directly predicting the synthesis conditions of a MOF based on its crystal structure. Our approach is based on: i) establishing the first MOF synthesis database via automatic extraction of synthesis parameters from the literature, ii) training and optimizing ML models by employing the MOF database, and iii) predicting the synthesis conditions for new MOF structures. The automated synthesis prediction is available via a web-tool on https://mof-synthesis.aimat.science.

This work represents a first step towards predicting synthesis conditions for an arbitrary MOF. We show a complete ML workflow for the inverse synthesis design of MOFs. First, we developed an automatic process to extract information on MOF synthesis for all publicly available MOF structures in the CoRE MOF database. The six relevant parameters that were extracted are metal source(s), linker(s), solvent(s), additive, synthesis time, and temperature. Ultimately, we combined the extracted synthesis details into the SynMOF database consisting of 983 MOF structures. Our central assumption in this work is that the established SynMOF database can be used to train ML models to facilitate the discovery of similarity patterns in the synthesis conditions to reach the final goal of predicting synthesis protocols for new MOF structures. In the next step, we set up and trained ML models. The prediction of synthesis time and temperature was achieved via regression models, such as random forests or neural networks. Furthermore, we developed a ML model which predicts solvent properties, such as partition coefficients, boiling point, rather than the specific solvent. In the case of additives, we found that the main parameter that distinguishes different additives is their acidity/basicity strength. Thus, we split the dataset into three groups (acidic, basic, or no additive) and used a classification model for additive prediction. Finally, we compared ML predicted synthesis conditions for new MOF structures with human experts' predictions. The ML models, even at an initial stage, exhibit a good prediction performance, outperforming human expert predictions, obtained through a synthesis survey. Our approach marks the starting point for the transition from a trial-and-error approach that is based on experience and heuristics, towards an inverse synthesis design approach in the MOF synthesis, ultimately enabling fully autonomous MOF discovery in automated labs.

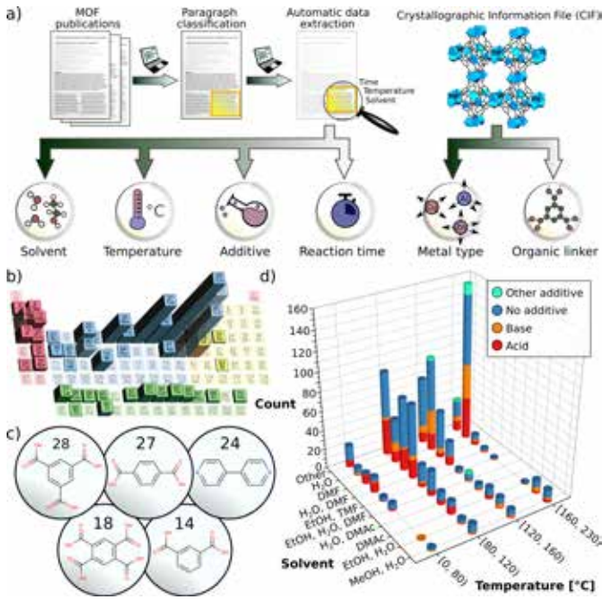


Fig 2
SynMOF database. a) Data mining pipeline and content of the SynMOF database; b) the statistics on the most common metal source and c) structures and occurrences of the most common linkers in the SynMOF database; d) 3D graph exhibiting correlation between solvent type, additive, and temperature.

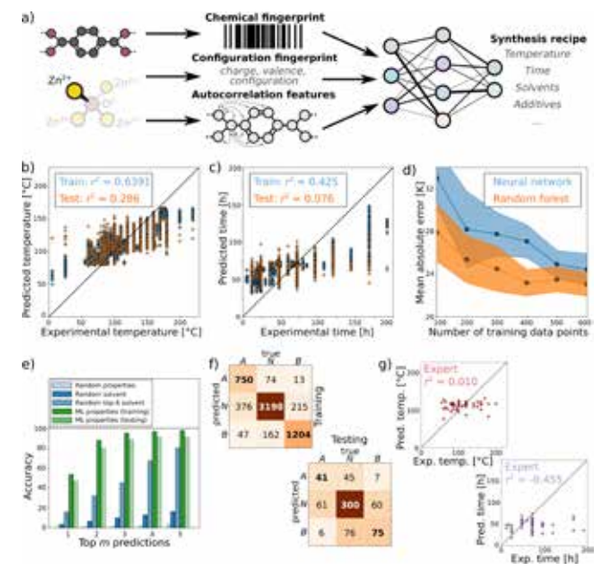


Fig 3
Machine learning models trained on the SynMOF-A database. a) ML workflow, including fingerprint representation of the linkers and the feature representation of the metal type and oxidation state; b) and c) comparison of ML predictions of temperature and time for training and test sets with the initial data extracted from literature; d) learning curve of temperature predictions, i.e. mean absolute error as a function of the training set size, for neural network and random forest regression models; e) ML solvent prediction accuracy for a subset of single-solvent MOFs, compared to different methods of random predictions; f) training and test set performance of additive classification where A, B, and N correspond to acid, base, and no additive respectively and g) average of eleven human expert predictions of temperature and time for 50 MOFs to evaluate the complexity of the problem.

A METAL-ORGANIC FRAMEWORK BASED ON CO(II) AND 3-AMINOISONICOTINATE SHOWING SPECIFIC AND REVERSIBLE COLOURIMETRIC RESPONSE TO SOLVENT EXCHANGE WITH VARIABLE MAGNET BEHAVIOUR

O. Pajuelo-Corral, S. Pérez-Yánez, I.J. Vitorica-Yrezabal, G. Beobide, A. Zabala-Lekuona, A. Rodríguez-Diéguez, J.M. Seco, J. Cepeda. Materials Today Chemistry 24 (2022) 100794

A versatile metal-organic system consisting of Co-based compounds that show reversible transformations between a 3D metal-organic framework (MOF, 1) and a 0D monomeric (2) complex is reported. The 1 ↔ 2 transformation, triggered by the exposure of compounds to H_2O and DMF, involves colour changes from purple (in 1) to light brown (in 2), promoting a colorimetric sensing capacity. The MOF presents good thermal stability and permanent porosity with high CO_2 capture capacity, further analysed by in situ SCXRD. 3D and 0D compounds present distinct SMM behaviour.

In this article we present the synthesis and physico-chemical, structural characterization as well as the analysis of the porous structure and magnetic properties of two cobalt(II) and 3-aminoisonicotinate based compounds synthetized following different synthetic routes. Compound 1 shows an open 3D metal-organic framework of {[Co(μ-3isoani)$_2$]·DMF}n (1) formula (where 3isoani = 3-aminoisonicotinato and DMF = dimethylformamide) with channels occupied by solvent molecules. On its part, compound 2 consists of 0D monomeric complex with [Co(3isoani)$_2$(H$_2$O)$_4$] formula (2) that crystallizes into a hydrogen-bonded structure. The compounds present different colours due to their distinct octahedral coordination environments around Co(II), in such a way that N_2O_4 and O_6 donor sets provide 1 and 2 with reddish purple and light brown colours, respectively. Both compounds are purely obtained by different synthetic routes using different solvents (DMF for 1 and H_2O for 2). Interestingly, the exposure of solid compounds to the other solvent, that is, sample of 1 H_2O and sample of 2 to DMF, promotes the mutual interconversion of the compounds. Therefore, the system acts as a smart colorimetric sensor of the mentioned solvents by reversibly changing the colour of the sample when exposed to saturated atmosphere of (or in direct contact with) the solvents. Despite the high reactivity of the MOF in contact with water, it presents good thermal stability and permanent porosity with a remarkably high CO_2 capture capacity at room temperature (3.35 mmol g^{-1}), which is further analysed by in situ determination of the gas at variable pressures into the pores of the MOF by single-crystal X-ray diffraction. Experimental magnetic measurements and CASSCF/NEVPT2 calculations reveal that both cobalt(II) compounds present field induced SMM behaviour at low temperature derived from easy-plane magnetic anisotropy with considerable SOC, although the magnetic relaxation processes differ due to their distinct coordination environment. On the one hand, the orbital splitting in 1 is best described as a distorted tetrahedral $CoN_2(CO_2)_2$ environment, in such a way that slow magnetic relaxation proceeds through Raman and QTM mechanisms. On the other hand, the almost perfect octahedral environment of 2 gives rise to the increase of zfs parameters, making the magnetic relaxation to proceed at a higher temperature by means of Raman and direct mechanisms.

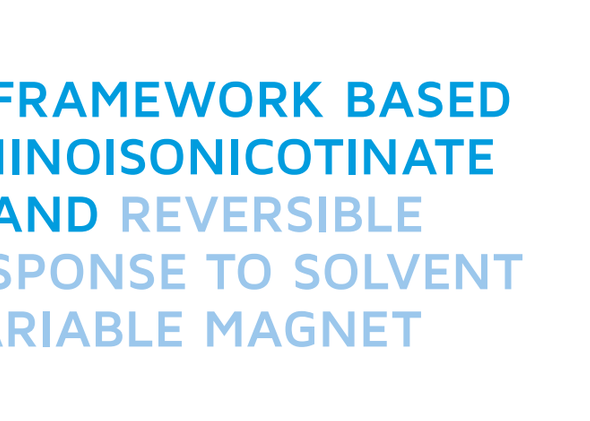


Fig 1
Summary of the reversible solvent-triggered transformations between compounds 1 (left) ↔ 2 (right). Photographs of the compounds are shown at the top of the figure, whereas the central images show their X-ray structures and coordination shells.

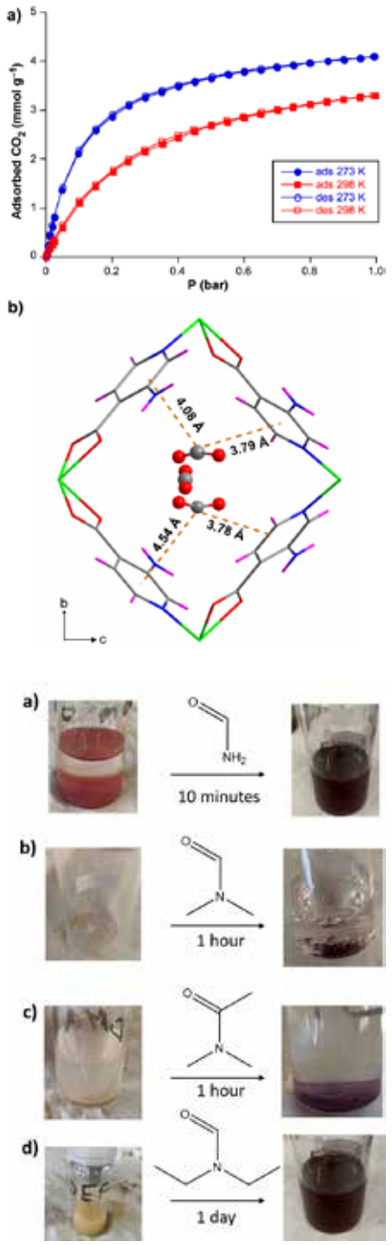


Fig 2
a) Adsorption and desorption isotherms of compound 1 recorded at 298 and 273 K. b) Crystal structure of MOF loaded with CO_2 at 298 K and 1 bar showing the interactions between guest molecules and the framework.

Fig 3
Solvent exchange experiments conducted starting from compound 2 to obtain 1. Photographs show how the colour changes from compound 2 in the initial stage (solid sample or in contact with the formamide derivative, time 0). Note that the first exchange (with formamide) is so rapid that the transformation is almost completed in the photograph shown at the left.

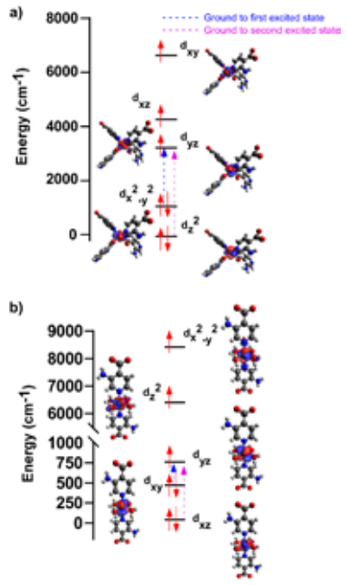
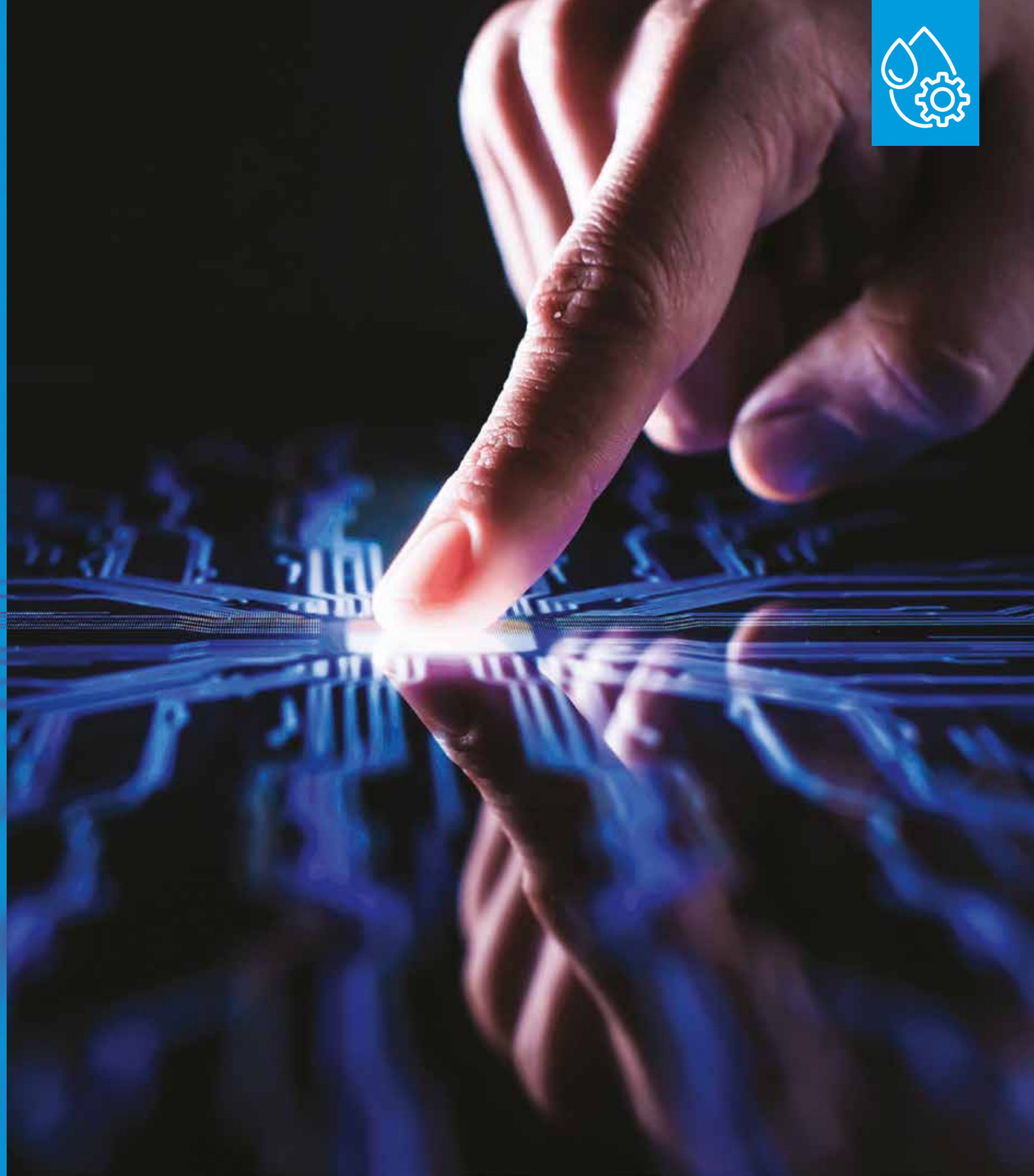


Fig 4
NEVPT2 computed d-orbital splitting for compounds a) 1 and b) 2. Brick lines represent dominant electronic transitions from ground to first and ground to second excited states, respectively.

RESEARCH **LINE 3**

ADVANCED FUNCTIONAL MATERIALS & SURFACES

This research line concerns mainly the implementation through deep fundamental understanding of functional materials for advanced 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.



LEVERAGE OF PYRIDINE ISOMER ON PHENOTHIAZINE CORE: ORGANIC SEMICONDUCTORS AS SELECTIVE LAYERS IN PEROVSKITE SOLAR CELLS

Peng Huang, Manju, Samrana Kazim, Luis Lezama, Rajneesh Misra and Shahzada Ahmad
ACS Appl. Mater. Interfaces 2022, 14, 5729-5739.

The development of organic semiconductors as hole-transporting materials is imperative. We developed pyridine derivatives as small molecules-based hole-transporting materials due to their Lewis base and electron-deficient unit. Where the pyridine nitrogen heteroatom is located at the 2, 3, and 4 positions, termed as 2PyPTPDAn, 3PyPTPDAn, and 4PyPTPDAn, respectively, and unravel the structure–properties–device performance relationship impacted by the different N-atom positions in pyridine. We suggested guidelines to develop small molecules for organic solar cells, organic light-emitting diodes, and thermally activated delayed fluorescence.

Fig 1
Graphical abstract of the impact of pyridine Isomer on phenothiazine core as organic semiconductors. Reproduced from ACS Appl. Mater. Interfaces 2022, 14, 729–5739.

The hole-selective layers (HSLs) are substantial to expedite photogenerated hole extraction and transport and hinder the degradation of the perovskite layers and are of paramount interest for other organic semiconductors based devices. 2,2′ 7,7′ -tetrakis-(N,N-di-p-methoxyphenylamine)-9,9′ -spirobifluorene (Spiro-OMeTAD) is the most studied HSLs for perovskite solar cells. However, its demanding synthesis process, expensive cost of the spirobifluorene core, and poor transportability in its pristine state hamper the upscaling. Small molecules are considered to be attractive alternatives for Spiro-OMeTAD, and are being designed and synthesized owing to their important merits i.e. tuneable properties via molecular engineering, cost efficiency, and simplified purification process. We investigated pyridine isomer molecules 4,4′ -(10-(pyridin-x-yl)-10H-phenothiazine-3,7-diyl) bis(N,N-bis(4-methoxyphenyl)aniline) (x = 2, 3, or 4), in which the pyridine nitrogen heteroatom is located at the 2, 3, and 4 positions, as 2PyPTPDAn, 3PyPTPDAn, and 4PyPTPDAn, respectively. In the case of 3PyPTPDAn, the partial orbital overlap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) favors the generation of neutral excitons and hole transport, and this induces efficient hole extraction as compared to their 2,4 analogs.

The developed molecules consisting of the pyridine (Py) unit either in the core or in the arms have been investigated as HSLs. The pyridine unit, by virtue of its being a Lewis base, can also passivate the lead ion (Pb^{2+}) defects at the surface and grain boundaries. More importantly, it was considered as an electron-deficient unit to construct D–A-type HSLs. Our report suggests guidelines to develop small molecules based on innovative pyridine derivatives with linking topology as effective HSLs. The solar cells fabricated with 3PyPTPDAn gave an on-par photovoltaic performance as that of typical Spiro-OMeTAD, and higher performance than those of 2PyPTPDAn and 4PyPTPDAn.

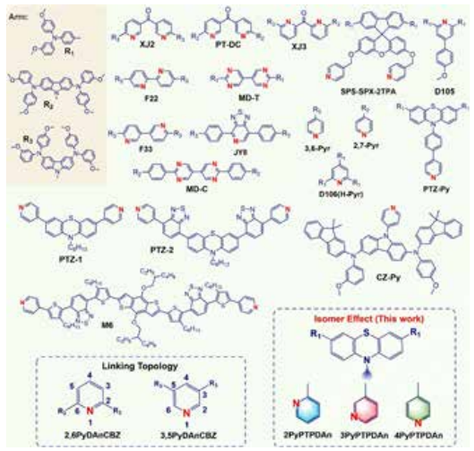


Fig 2
Molecular structure of the various pyridine-based hole selective layer reported in the state of the art. and the isomer effects of pyridine-based as HSLs highlighted in 2PyPTPDAn, 3PyPTPDAn, and 4PyPTPDAn.

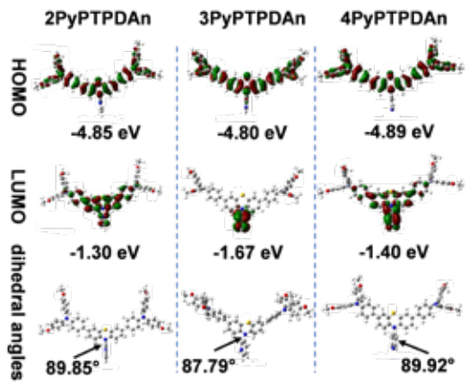


Fig 3
Energy level diagram showing the E_{HOMO} and E_{LUMO} levels of 2PyPTPDAn, 3PyPTPDAn, and 4PyPTPDAn and their dihedral angles.

Table
Photophysical and electrochemical properties of developed HSLs.

HSL	$\lambda_{max}/\lambda_{onset}$(nm)	E_g^{opt}/E_g	E_{HOMO} (eV)	E_{LUMO} (eV)	T_d(°C)	T_g(°C)	Conductivity (μS cm^{-1})	Mobility (10^{-4} cm^{2}V^{-1}s^{-1})
2PyPTPDAn	305/349	3.09/3.48	-5.64[a]/-4.85[b]	-2.55[a]/-1.30[b]	206	109	0.28	3.0
3PyPTPDAn	309/334	2.85/3.13	-5.60[a]/-4.80[b]	-2.75[a]/-1.67[b]	223	120	0.46	5.4
4PyPTPDAn	310/348	2.79/3.35	-5.71[a]/-4.89[b]	-2.79[a]/-1.40[b]	265	128	0.02	0.3

LARGE ELECTROCALORIC EFFECT IN TWO-STEP-SPS PROCESSED PB $(Sc_{0.25}In_{0.25}Nb_{0.25}Ta_{0.25})O_3$ MEDIUM-ENTROPY CERAMICS

Siyue Wei, Xue Chen, Guangzhi Dong, Laijun Liu, Qi Zhang, Biaolin Peng. Ceramics International, Volume 48, Issue 11, 2022,Pages 15640-15646,

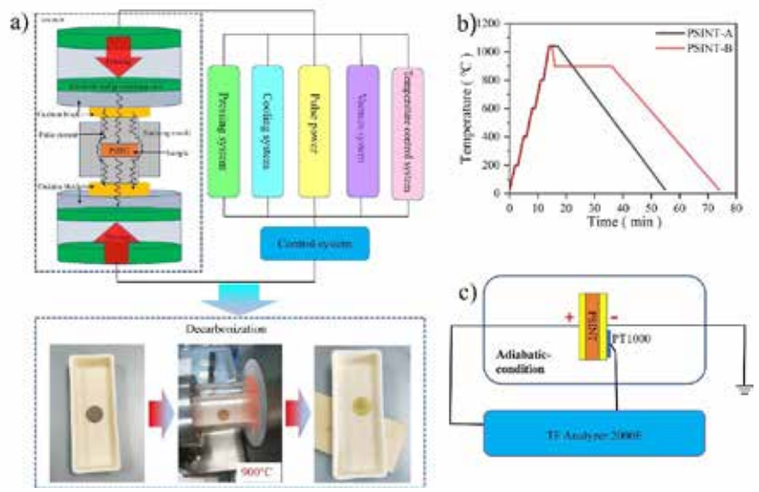


Fig 1
a) The flow chart of PSINT ceramic process. b) Sintering process of PSINT ceramic. c) The measurement setup of electrocaloric effect.

Eco-friendly solid-state refrigeration based on the electrocaloric effect (ECE) is attracting much attention for communications, medica and modern electronics, etc. There is almost no breakthrough since ECE was found in 1930s. ECE is closely related to the entropy change before and after the application of an electric field to the ECE material. In this work, two PSINT medium entropy ceramics were designed and synthesized. It is found that a large ΔT (~0.85 K) with a high EC strength (~0.021 K cm/kV) at a low electric field (~40 kV/cm) within a wide temperature range (~120 K) can be achieved.

High-entropy ceramics (HECs) have found many potential promising applications, such as energy storage, ionic conductors, catalyst carrier, and magneto resistance, etc. The high disorder of the lattice of HECs is mainly responsible for the excellent performance. It has been well known that high entropy materials are intentionally designed by controlling configurational entropy that is defined as the following equation:

$$\Delta S_{config} = R \sum_{i=1}^{N} X_i \, lnX_i$$

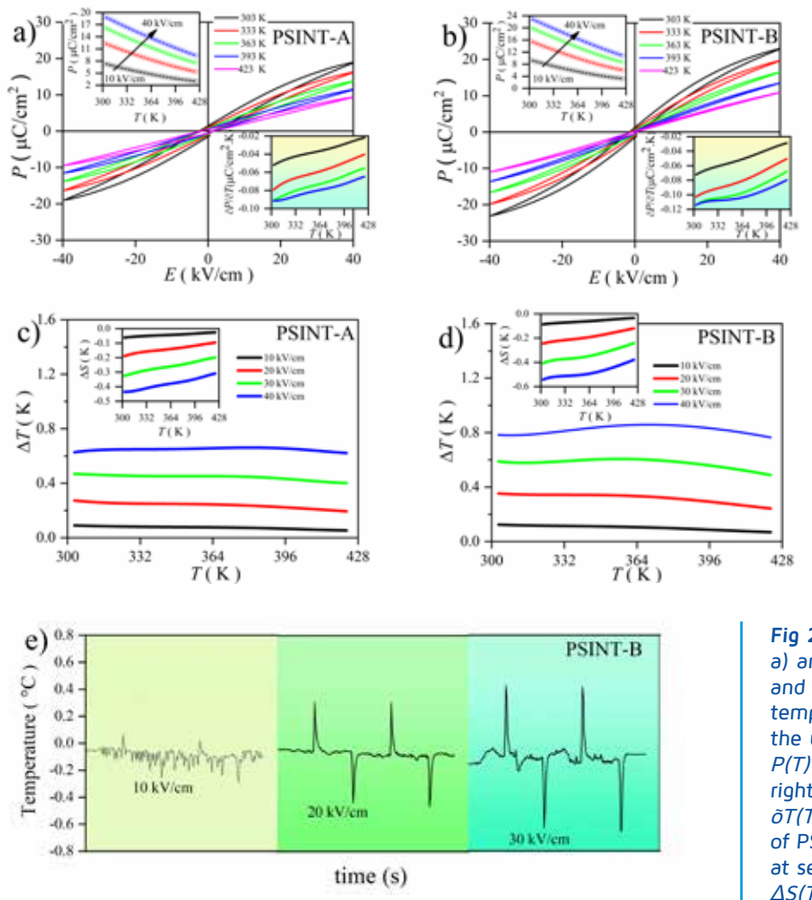


Fig 2
a) and b) the P-E loops of PSINT-A and PSINT-B ceramics at selected temperature at 10 Hz, insets in the upper-left corners of a) and b): P(T) curves, insets in the lower-right corners of a) and b): the õP/õT(T) curves. c) and d): The ΔT(T) of PSINT-A and PSINT-B ceramics at selected electric fields, insets: ΔS(T). e) The EC effect change of PSINT-B ceramic as a function of time by the direct measurement method at three different electric field at room temperature

where R is gas constant and the X_i is the molar content of each element. Obviously, it is easy to obtain a large ΔS_{config} by multiplying more components and adjusting their relative ratio. A large electrocaloric effect is caused by the isothermal entropy change (S) in a polarizable dielectric material when applying or withdrawing the external electric field in an adiabatic environment. A universal strategy or method to improve the electrocaloric effect is enhancing the dipolar entropy (number and disorder dipoles).

In this work, two Pb $(Sc_{0.25}In_{0.25}Nb_{0.25}Ta_{0.25})O3$ (PSINT) medium-entropy ceramics including the one-step-SPS processed and the two-step-SPS processed samples were synthesized by using the SPS technology, as shown in Fig. 1, that is regarded as a powerful method to consolidate ceramic powder. The electrocaloric effect of these samples are evaluated by using the indirect method based on the Maxwell relation (Fig.2 a-d) and the direct method (Fig.2 e). The results for the electrocaloric effect from two evaluation methods are quite conformed. The large electrocaloric effect (~0.85 K at 40 kV/cm) with a high EC strength (~0.021 K cm/kV) around room temperature in the two-step processed PSINT ceramic has been confirmed by the direct measurement. The high-entropy strategy not only enhances configurational entropy but also increases polarization entropy of perovskite ferroelectric ceramics, then improves the electrocaloric effect. It is a simple method to design high performance EC materials for next-generation solid state refrigerators.

INFLUENCE OF W DOPING ON THE STRUCTURE, MAGNETISM AND EXCHANGE BIAS IN $NI_{47}MN_{40}SN_{13-X}W_X$ HEUSLER ALLOYS

M Norouzi-Inallu, P Kameli , A Ghotbi Varzaneh, I Abdolhosseini Sarsari , M Abbasi Eskandari, I Orue, B Rodríguez-Crespo and V Chernenko. J. Phys.: Condens. Matter 34 (2022) 225803 (9pp)

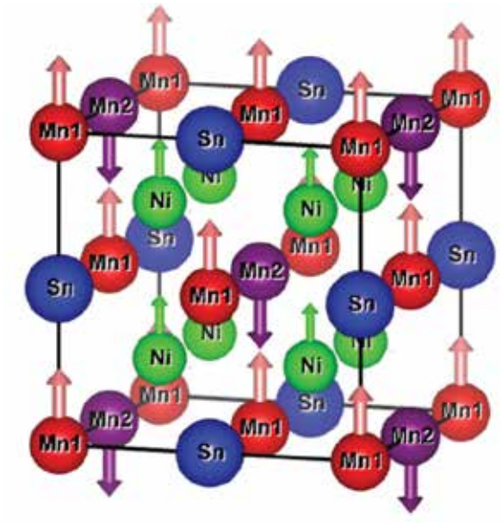


Fig 1
$L2_1$ structure of the off-stoichiometric Ni–Mn–Sn Heusler-type alloy (Ni8Mn6Sn2). Mn1 atoms occupy the regular Mn sites, whereas Mn2 atoms (excess Mn) are located at Sn sites. Arrows show the orientation of magnetic moments: 3.8μ_B are located on Mn atoms, 0.3μ_B on Ni.

Previously we found that doping of Heusler type $Ni_{47}Mn_{40}Sn_{13}$ magnetic shape memory alloy (MSMA) by 1at.% of W essentially enhanced its magnetocaloric properties. In present work a systematic influence of W-doping of 0, 0.5, 1, 1.25at.% instead of Sn on martensitic transformation (MT), magnetic properties and exchange bias (EB) effect was studied, whereby phase diagram of structural and magnetic states as a function of W concentration was determined. Magnetic memory measurements revealed the presence of a glassy magnetic ground state, which significantly impacted the reduction of magnetization and enhancement of EB in the studied bulk alloys. It was concluded that these alloys are promising for spintronic applications.

Owing to strong dependence of exchange interactions on the interatomic distance in Heusler-type MSMA, ferromagnetic coupling (FM) occurs in Mn1-Mn1 long-distanced pairs, whereas antiferromagnetic one (AFM) is in much shorter Mn1-Mn2 pairs (Fig. 1). Magnetically frustrated state appears when unit cell exhibits spontaneous distortion and volume

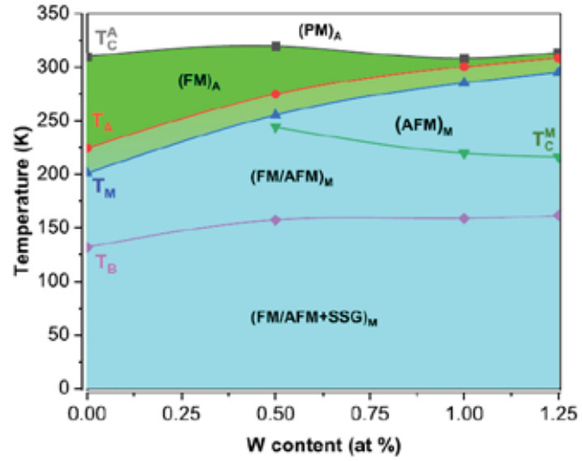


Fig 2
The structural and magnetic phase diagram of studied alloys. White and green regions correspond to the austenitic phase, blue area represents martensitic phase. T_A and T_M are MT characteristic temperatures; T_{AC} and T_{MC} are Curie temperatures of austenite and martensite, respectively; T_B is the blocking temperature. PM, FM and AFM stand for paramagnetic, FM, and AFM phases; glassy magnetic ground state results from cooperative freezing of individual spins or spin clusters (SSG).

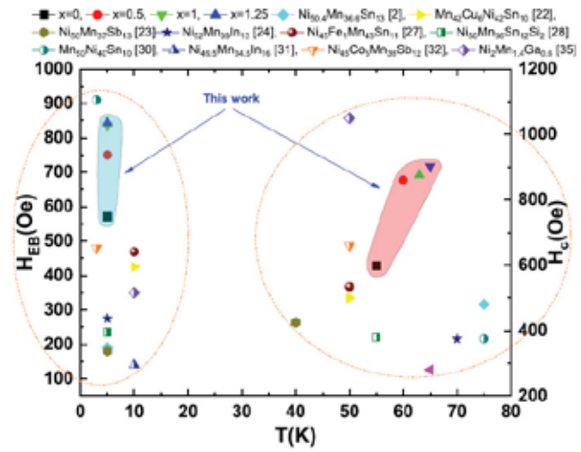


Fig 3
Comparison of exchange bias HEB and coercive field H_c values at different temperatures obtained in present work with the literature data for Ni–Mn-based MSMAs.

reduction, both as a result of MT. Doping by smaller W atoms reinforce the frustration by introduction/intensifying AFM coupling as Fig. 2 demonstrates. Phase diagram shown in Fig. 2 also reveals the formation of spin-glass-like state at low temperatures which favours one of the largest around Heusler-type MSMAs EB effect as depicted in Fig. 3.

RESEARCH **LINE 4**

MICRO & NANO-DEVICES

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 will be 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

Alaine Sánchez, Ahmed Esmail Shalan, Maibelín Rosales, Idoia Ruiz de Larramendia, Francisco Javier del Campo. Journal of Electroanalytical Chemistry, Volume 928, 2023, 117052

This work details a method for creating metal-oxide inks for screen-printing. Nickel hydroxide was grown on conducting microparticles and used to make screen-printing inks. The materials were characterized using SEM, TEM, electrochemistry, and spectroscopy. The screen-printed electrodes show potential for electrolysis and enzyme-less biosensing, as well as electrochromism and an optical bandgap of 4.06-4.15 eV. This approach can be applied to other metal oxides, expanding the range of screen-printable semiconductors and catalysts.

In this work, the authors report the first instance of an electrochromic, screen-printable nickel hydroxide paste. This material has potential applications in energy storage, electrocatalysis, and even in the creation of printed displays for disposable devices such as smart tags. The nickel hydroxide was grown by co-precipitation on conducting particles, and the SEM and TEM images reveal that the structure and thickness of the nickel hydroxide deposits vary based on the synthesis conditions. By using more conducting particles, a larger surface area can be achieved, resulting in thin coatings with better properties.

The electrochemical behaviour of the screen-printed ATO/$Ni(OH)_2$ electrodes was studied, and it was observed that when the ATO to nickel precursor ratio is low, the voltammetric response is sluggish and ill-defined. However, as the nickel layer becomes thinner, the voltammetric response improves and becomes better defined with higher currents. The electrocatalytic properties of the $Ni(OH)_2$ electrodes were also studied in terms of the oxygen evolution reaction and the direct oxidation of glucose, showing their suitability for use in electrolyzers and as potential enzyme-less glucose sensors.

The electrochromism of the materials was also studied and it was found that the best response was achieved for ATO to nickel precursor weight ratio-paste electrodes between 10:1 and 15:1. The materials displayed colour efficiencies of up to 50 $cm^2\ C^{-1}$, and although the contrast ratio was generally low, these materials enable the creation of printed displays for disposable devices. It was also determined that the bandgap of the printed structures can be adjusted by controlling the thickness of the semiconductor material on the supporting conducting particles, which could be useful for the development of printed electronics devices. This approach can also be extended to other metal oxides, greatly expanding the potential applications of these materials.

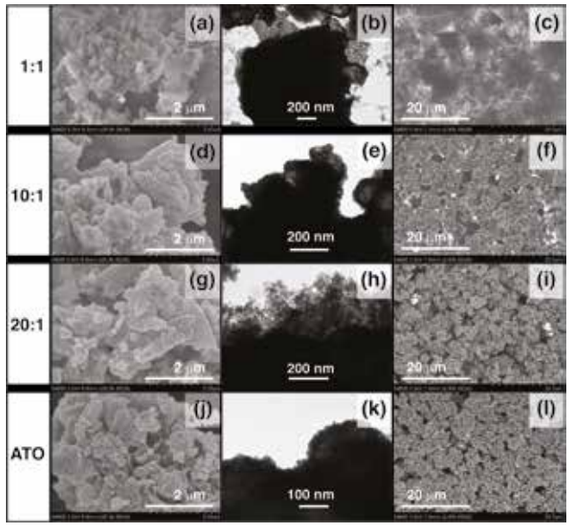


Fig 1
SEM and TEM images of ATO/$Ni(OH)_2$ particles and electrodes. (a). SiO_2/ATO/$Ni(OH)_2$ particles obtained from different ATO particle: Ni precursor mass ratios. (a-c) 1:1, (d-f) 10:1, (g-i) 20:1, (j-l) As-received SiO_2/ATO particles.

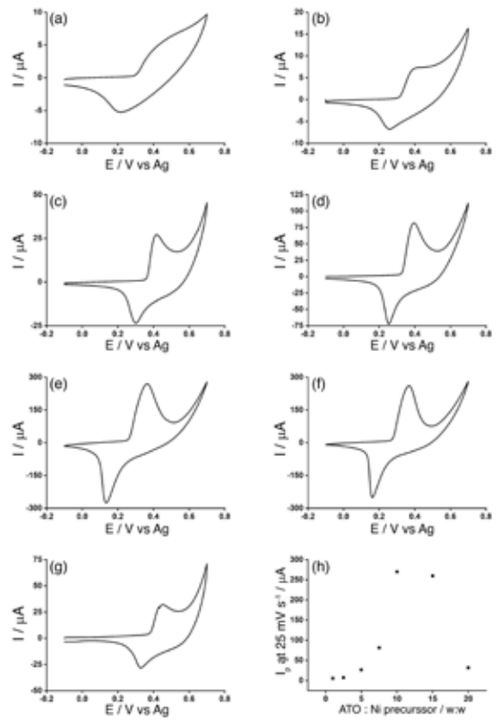


Fig 2
Cyclic voltammograms of various ATO/$Ni(OH)_2$ electrodes in 0.1 M KOH at 25 mV s 1. Different conducting particle to Ni precursor ratios: (a)1:1, (b)5:2, (c) 5:1, (d) 15:2, (e) 10:1, (f) 15:1, and (g) 20:1. (h) Voltammetric peak currents as a function of particle composition. Potential shifts were due to different degrees of Ag pseudo-reference electrode oxidation.

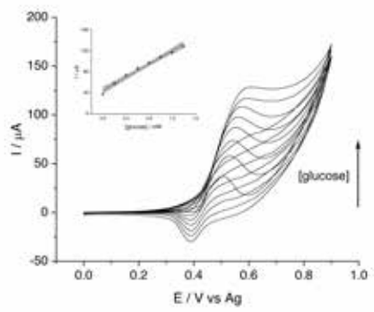


Fig 3
Cyclic voltammetry of a 20:1 ATO to Nickel particle screen printed electrode in the absence and in the presence of increasing glucose concentrations in 0.1 M KOH. Scan rate was 5 mV s^{-1}. The inset shows the peak current values as a function of glucose concentration.

DESIGN AND FABRICATION OF PRINTED HUMAN SKIN MODEL EQUIVALENT CIRCUIT: A TOOL FOR TESTING BIOMEDICAL ELECTRODES WITHOUT HUMAN TRIALS

Nikola Perinka, Matija Strbac, Milos Kostic, Jovana Malesevic, Nélson Castro, Vítor Correia, Senentxu Lanceros-Méndez. Advanced Engineering Materials, 24: 2100684.

The present work deals with development of a printed Human model equivalent circuit (HMEC), which, when connected to the functional electrical stimulation system, mirrors the electrical behavior of biomedical electrodes as if they are placed on a human subject. A simulation model of the electrical stimulation system was developed based on the experimental data, in order to optimize printed electronic components' characteristics and design. The fully printed flexible HMEC is a feasible approach to enabling the testing of transcutaneous electrical stimulation devices, reducing the need for tests on human subjects.

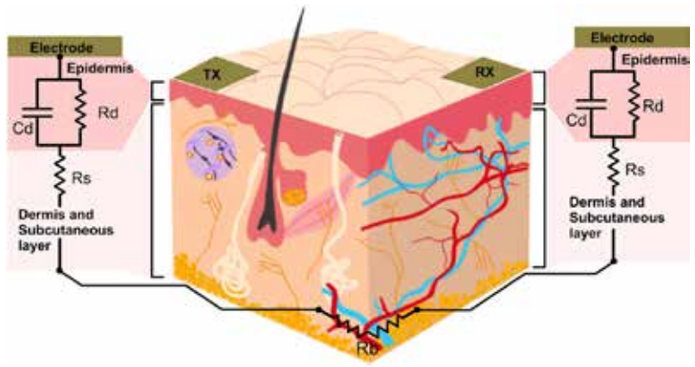


Fig 1
Human skin morphology and the Montague model.

The current smart devices have an ever-closer relationship with human beings, some of them exercising sustained contact with human beings through their skin, with the aim of physiological functions monitoring or by providing external electrical stimulation. Electrodes that allow controlled propagation and delivery of electrical pulses play a key role in a variety of applications such as neuromotor rehabilitation, electrotactile feedback, cosmetics, sports, wound healing, and drug delivery, etc. To define the HMEC parameters, the Montague model was applied. This model is widely used in the area of transcutaneous electrical stimulation due to its simplicity. It is composed of only three elements: two resistors and a capacitor (Figure 1). As depicted in Figure 1, the resistive and capacitive properties of the epidermis and the electrode–skin interface are represented by a parallel resistance Rd and a dielectric capacitance Cd. The deep layers of the skin (dermis) are represented by relatively low resistance R_s. The optimal electrode configuration for transcutaneous stimulation depends on the electrode–skin interface, skin impedance, and physical characteristics, and is therefore person-specific and changes on a daily basis. The proposed method enables initial assessment and direct estimation of how the overall system, including the electrode–skin interface material, will behave in different settings. For all components of the circuit, the characteristics of the materials and the conditions of the various layers and stages of printing by screen-printing are provided (Figure 2). For the printed components, capacitors were fabricated with a density of ≈0.804 nF cm^2, and resistances of 76 kΩ, 1.02 kΩ, and 852 Ω for different L/W ratios, with a resistive ink sheet resistance of ≈500 Ω sq^{-1}. The final circuit was tested electrically, having a response signature close to the simulations and in the range of the values present in the literature. The prototype was successfully tested with a stimulation device, where the signals obtained were analog to those recorded on humans. The presented fully functional flexible printed electronic circuit (Figure 3), is capable to electrically simulate human skin, which represents a starting point for the development of more realistic artificial skins, with the possibility of incorporating this solution in materials with mechanical and responsive skin-like characteristics.

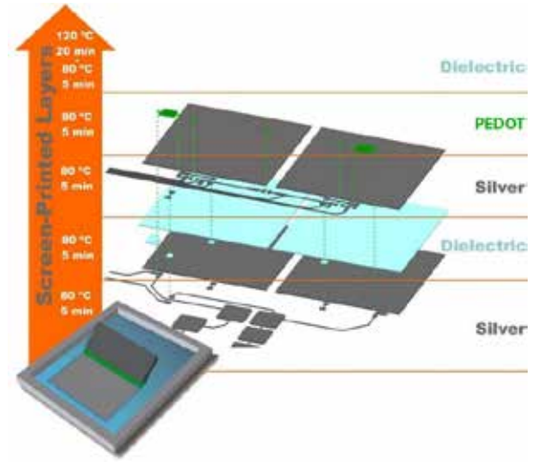


Fig 2
Schematic representation of the various printed layers according to corresponding printing order, from bottom to top. The curing conditions are also indicated for the different layers.

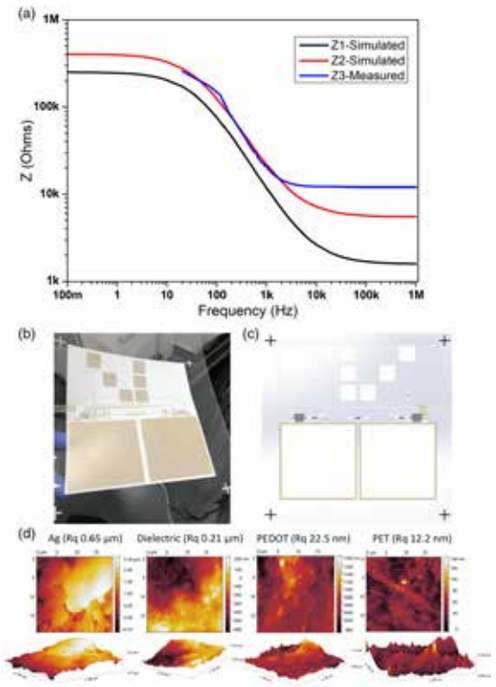


Fig 3
Model circuit: Graph of the simulation result and electrical response of the final circuit a), result of the printed circuit b), modeling of the various printed layers c), and AFM result of the various inks used in the manufacture of the printed skin d).

UNDERSTANDING ELECTROGENERATED CHEMILUMINESCENCE AT GRAPHITE SCREEN-PRINTED ELECTRODES

Alejandro Fidel Alba, Roberto Fernández-de Luis, Joseba Totoricaguena-Gorriño, Leire Ruiz-Rubio, Julia Sánchez, José Luis Vilas-Vilela, Senentxu Lanceros-Méndez, Francisco Javier del Campo.
Journal of Electroanalytical Chemistry 914 (2022) 116331

This work studies the use of screen-printed graphite electrodes in electrochemiluminescence (ECL) by analyzing four electrodes made from three types of graphite paste, including the Dropsens electrode. The electrodes were also treated with a laser to remove impurities and increase electrochemical activity. The results show that ECL intensity depends on both electrode kinetics and wettability, which are affected by the composition of the graphite paste and the polymer binder used. The research also introduces an affordable method to evaluate electrode quality using ECL and a mobile phone camera.

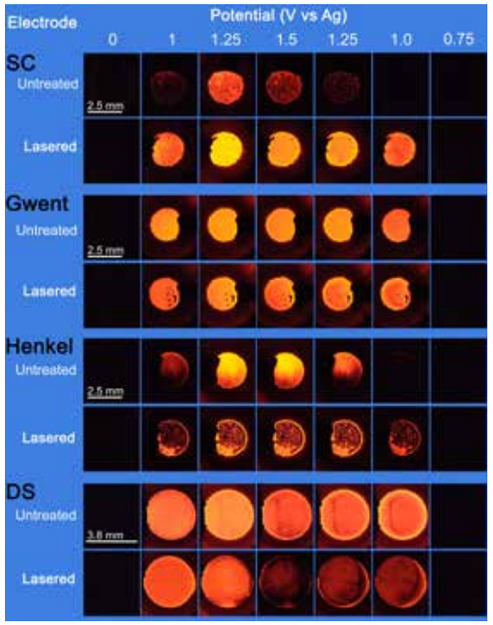


Fig 1
Working electrode surface pictures at different potentials during a cyclic voltammetry experiment at 25 mV s^{-1} (from left to right: 0, 1.0, 1.25, 1.5, 1.25, 1.0, 0.75 V vs Ag) for 1.59 mM $Ru(bpy)_3^{2+}$ and 27 mM TPrA at different electrodes. Switching potential is 1.5 V vs Ag.

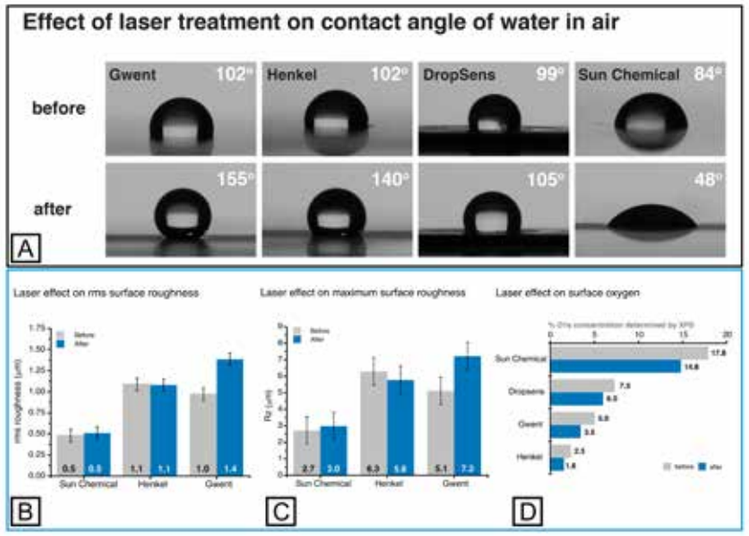


Fig 2
Contact angle measurements, surface roughness, height of profile and surface oxygen composition for SC, Gwent, Henkel and DropSens electrodes before and after laser treatment.

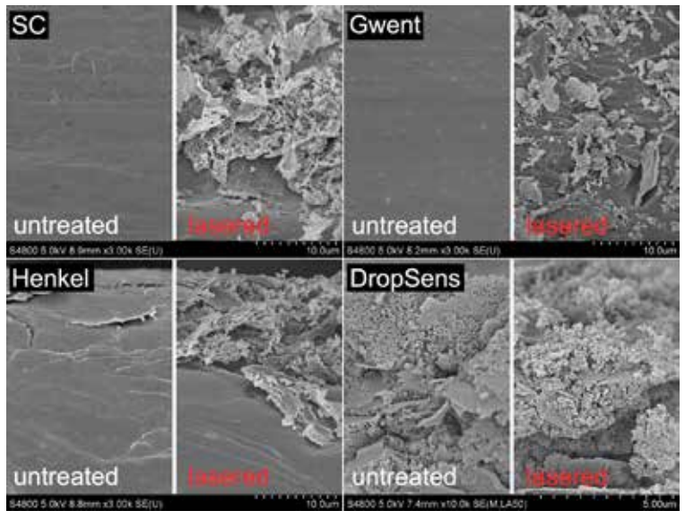


Fig 3
SEM electrode section micrographs of SC, Gwent, Henkel and DropSens electrodes before and after laser activation.

This work provides information on the development of printed detection systems using the $Ru(bpy)_3^{2+}$/TPrA electrochemiluminescence system. The study focuses on screen-printed graphite electrodes, which are commonly used in electroanalytical applications but have varying performance due to the materials selection and fabrication processes. The authors found that laser activation of these electrodes enhances their electrochemical properties by removing surface binder and low-quality amorphous carbon, and exposing highly crystalline graphite similar to highly oriented pyrolytic graphite (HOPG). However, laser activation also affects surface wettability, which is critical for the generation of strong ECL signals. The study also emphasizes the importance of paste composition in affecting both wettability and electron transfer. This is because faster electron transfer does not necessarily translate into brighter ECL signals. In addition, the study introduced an affordable method to evaluate electrode quality using ECL and a mobile phone camera. An important clonclusion is that when choosing a screen-printing paste for these applications, it's important to consider both binder hydrophilicity and paste composition to achieve the best ECL performance.

SPECIAL ACTIONS

NEUTRON & COMPUTATIONAL MATERIALS SCIENCES

As part of the actions foreseen in its 2022-2025 Strategic Plan and in line with the work promoted by the IKUR Strategy of the Basque Government for the international promotion of strategic areas of Basque research, BCMaterials launched in 2022 two new research lines: neutron science and computational materials science. These two lines are transversal in nature, and are intrinsically related to the development and advances of the rest of the main research lines: active and smart materials, micro and nano-devices, micro and nanostructured materials, and advanced functional materials and surfaces.

ikur estrategia

TRANSVERSE
RESEARCH **LINE 1**

NEUTRON SCIENCE

Neutron science has been used extensively in all BCMaterials activities since its inception as one of the cornerstone tools for advanced materials characterization. In 2022, this research line has been provided with its own structure with financial and human resources, putting special efforts to push its activities in the framework of the neutrionics pillar of the IKUR strategy of the department of education of the Basque Government.

In this transversal line we have continued to apply different neutron techniques, including SANS, single crystal and powder neutron diffraction, neutron reflectometry and inelastic neutron scattering, in diverse research areas that include magnetism, smart materials, MOFs, energy generation and storage, soft matter and nanoparticles. Our researchers have led experiments in neutron sources around the globe, including the ILL (Grenoble, France), ISIS (Oxfordshire, UK), BNC (Budapest, Hungary) and ANSTO (Sydney, Australia).

At the same time, we have reinforced synergies with academic institutions and the industrial sector related to neutron science at the Basque, national and international levels. A clear example of this was the organization of the IMOH'22 conference, the 1st International Meeting on Opportunities and Challenges for HICANS (High Intensity Compact Advanced Neutron Sources) conference in June, at our headquarters in Leioa. The event brought together close to a hundred international experts who analysed the potential and feasibility of HICANS, including world-renowned scientists in the field of compact neutron sources, researchers from technological centres and corporations, and attendees from industry companies.

The activities carried out by the group members of the neutron science research line have resulted not only into the publication of research articles in high impact journals; but also into the participation of the group leaders of this research line in scientific (evaluation of beamtime proposals) and user (support to user communities) committees at different neutron sources, as well as in the Board of Directors of the Spanish society of neutron scattering; Sociedad Española de Técnicas Neutrónicas (SETN).

HOW FULLERENES INHIBIT THE AMYLOID FIBRIL FORMATION OF HEN LYSOZYME

One-Sun Lee, Viktor Petrenko, Katarina ipo ová, Andrey Musatov, Heesoo Park, Senentxu Lanceros-Méndez.. Journal of Industrial and Engineering Chemistry 106 (2022) 168-176

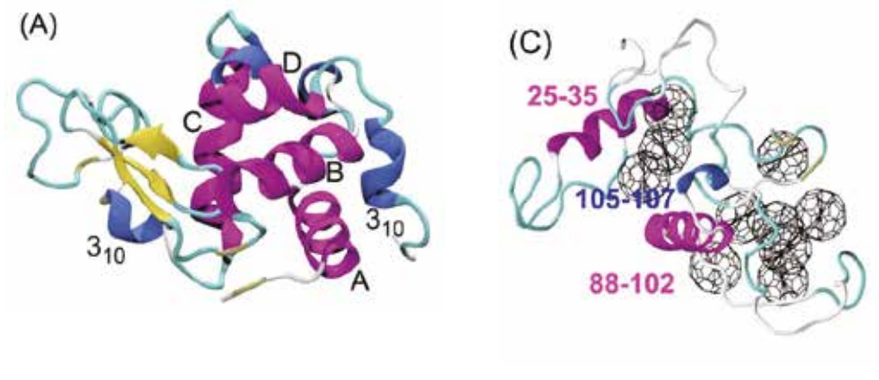


Fig 1
Schematic representation of HEWL protein structure and snapshot after MD modelling with fullerenes.

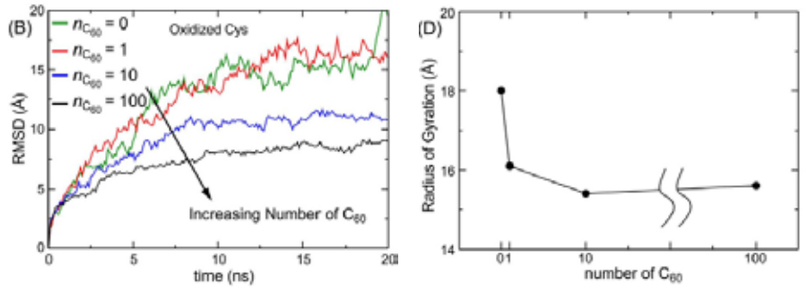


Fig 2
Fluctuation of HEWL backbone and changes of the radius of gyration of HEWL at different number of added C60 molecules.

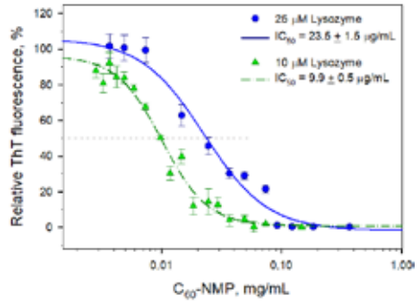


Fig 3
The dose-dependent inhibiting effect of C_{60}-NMP on HEWL amyloid aggregation and the determination of IC_{50} values by ThT fluorescence assays.

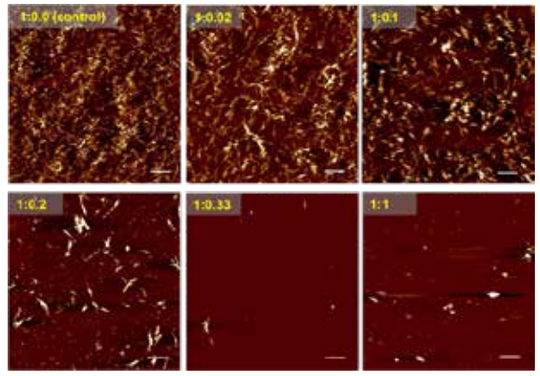


Fig 4
AFM visualization of the inhibiting effect of C60-NMP on HEWL amyloid aggregation at various protein to fullerene ratios.

Amyloids fibrils (specific protein aggregates) are related to various neuro-degenerative diseases. Inhibition of protein unfolding and self-assembly into fibrils using nanoparticles is a potential medicinal strategy to impede amyloid-related diseases. Among various nanoparticles, fullerenes have attracted great interest because of their inhibition effect on protein fibrillization, but this inhibition mechanism is still not properly understood. To explore the inhibition mechanisms, molecular dynamics simulations of HEWL protein have been performed in the presence of varied C60 concentrations.

Misfolded proteins and peptides can form insoluble and highly stable specific aggregates, called amyloid fibrils. Such aggregates are related to various neuro-degenerative diseases, and about fifty amyloid-related diseases have been identified. Lysozyme is one of the typical examples of fibril-forming proteins. Lysozyme is responsible for systemic amyloidosis and can form fibrils both in vivo and in vitro. With HEWL as a model protein, there have been a variety of studies aiming to understand the mechanism of amyloidosis and to develop detection methods at an early stage to prevent and destruct the amyloids.

The inhibition of protein unfolding and self-assembly into fibrils using nanoparticles (NPs) is a potential medicinal strategy to impede amyloid-related diseases. The large specific surface of NPs is one of the main features which facilitates their binding to fibrils and prevents further protein assembly into amyloid structures. At the same time, NPs can also inhibit conformational changes of monomers and thus inhibit aggregation and fibrillization processes. Among various nanoparticles and molecules, fullerenes are an excellent multifunctional platform for many biomedical applications due to their small size of 0.7 nm, unique caged structure, the capability to cross biological barriers, and surface functionalization. Recently, we have reported the disassembly activity of C60 and C70 on amyloid fibrils formed from insulin and lysozymes. Thus, it is tempting to speculate that fullerenes are also capable to inhibit insulin or lysozyme amyloid formation. The aim of this study is focused on fullerenes' ability to inhibit amyloid fibril formation experimentally and by simulation.

With MD simulations by varying the concentration of C60, we found that the structural fluctuation of HEWL decreases as the concentration of C60 increases. As the concentration of C60 increased they formed a clustered aggregation and the clustered aggregates were adsorbed on the surface of HEWL. It has been also experimentally confirmed that HEWL forms fewer fibrils with a higher concentration of C60 using ThT fluorescence assay and AFM experiments. These are the first simulations and experiments that show fullerenes' concentration effect on the inhibition of HEWL fibril formation, supporting the design of nanoparticles for inhibiting amyloidogenesis.

DESIGNING METAL-CHELATOR-LIKE TRAPS BY ENCODING AMINO ACIDS IN ZIRCONIUM-BASED METAL–ORGANIC FRAMEWORKS

Ainara Valverde, Gabriel I. Tovar, Natalia A. Rio-López, Dimas Torres, Maibelin Rosales, Stefan Wuttke, Arkaitz Fidalgo-Marijuan, José María Porro, Mónica Jiménez-Ruiz, Victoria García Sakai, Andreina García, José Manuel Laza, José Luis Vilas-Vilela, Luis Lezama, María I. Arriortua, Guillermo J. Copello, Roberto Fernández de Luis. Chemistry of Materials. 2022, 34, 21, 9666–9684

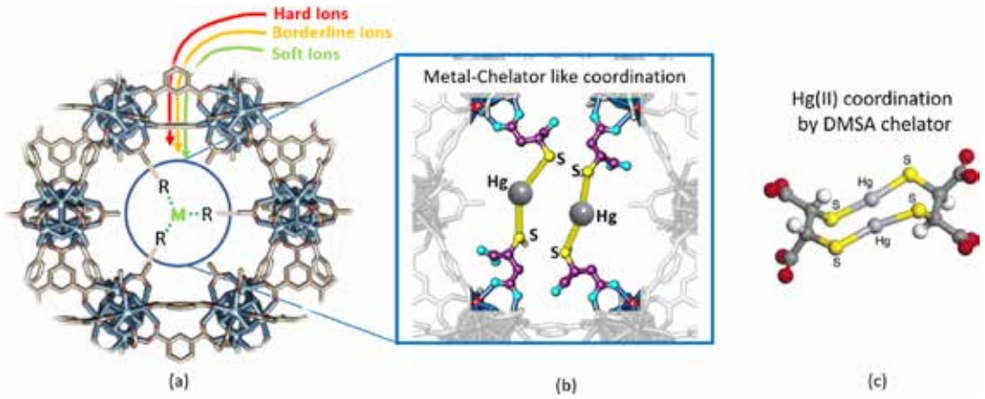


Fig 1
(a) Illustration of hard, borderline, and soft metal-chelator-like traps within the MOF-808 scaffold. (b) Illustration of tentative placement of the mercaptosuccinic molecules into the MOF-808 pore space and their coordination to Hg(II). (c) Coordination modes of dimercaptosuccinic acid chelators over Hg(II) ions.

Metal chelators and porous sorbents are two of the forefront technologies applied for the recovery and separation of metal ions from aqueous solutions. The transfer of the metal coordination functions of metal chelators to chemically stable host materials had only limited success so far. Here, we report the installation of amino acids within a porous zirconium-based trimesate metal–organic framework (MOF), namely, MOF-808. Applying this strategy, we were able to design a material able to separate different metals ions from complex mixtures in a continuous flow fashion when the material is packed as a column.

Metal chelators and porous sorbents are two of the forefront technologies applied for the recovery and separation of hazardous and/or valuable metal ions from aqueous solutions (i.e., polluted water sources, metal-rich mining wastewaters, acid leachates, and so forth) (Figure 1). The transfer of the metal coordination functions of metal chelators to chemically stable host materials had only limited success so far. Here, we report the installation of natural acids (i.e., malic acid, mercaptosuccinic acid, succinic acid, fumaric acid, and citric acid) and amino acids (i.e., histidine, cysteine, and asparagine) within a porous zirconium-based trimesate metal–organic framework (MOF), namely, MOF-808 (Figure 2). Applying this strategy, we were able to produce a pore environment spatially decorated with multiple functional groups usually found in commercial chelator molecules (Figure 2). The chemical stability of the amino acid molecules installed by the solvent-assisted ligand exchange has been studied to delimitate the applicability window of these materials. The adsorption affinity of MOF-808@(amino)acids in static and column-bed configurations can be fine-tuned as a function of the amino acid residues installed in the framework (Figure 3). MOF-808(amino) acid columns can be applied efficiently both for water remediation of heavy metals and for the separation of metal ions with different acidities. For instance, the initial trends for the dispersion of rare-earth elements have been identified. Electron paramagnetic resonance and inelastic neutron scattering spectroscopy reveal that MOF-808@(amino)acids stabilize metal centres as isolated and clustered species in a coordination fashion that involves both the amine and thiol functionals and that affects the vibrational freedom of some of the chemical groups of the amino acid molecules. The metal-ion stabilization within amino acid-decorated MOFs opens the avenue for application for pseudo biocatalysis purposes in the near future.

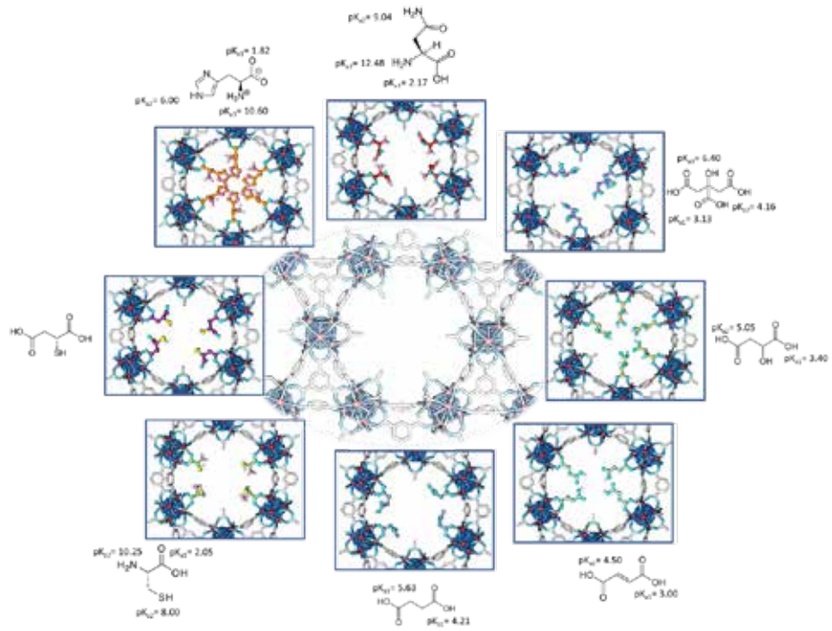


Fig 2
Illustration of the pore environment of MOF-808 after its decoration with l-asparagine (Asp), l-histidine (His), mercaptosuccinic acid (Msc), l-cysteine (Cys), succinic acid (Suc), fumaric acid (Fum), l-malic acid (Mal), and citric acid (Cit). Atom labeling scheme of the MOF structure: C, gray; O, red, Zr, blue; N pink; and S yellow. H atoms are omitted for clarity. Amino acid functionality has been drawn with different colors to highlight their possible spatial disposition within the MOF-808 scaffold.

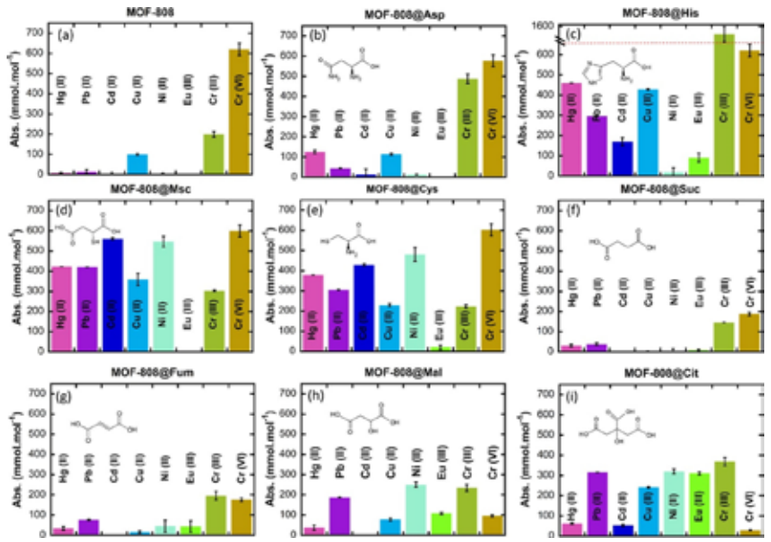


Fig 3
Adsorption capacity (mmol mol^{-1}) of different MOF-808@(amino)acid samples over Hg(II), Pb(II), Cd(II), Cu(II), Ni(II), Eu(III), Cr(III), and Cr(VI). Experiments were performed with an initial metal-ion concentration of 100 ppm, using 2 mg MOF/mL.

TRANSVERSE
RESEARCH **LINE 2**

COMPUTATIONAL MATERIALS SCIENCE

The creation of this transversal line aims at integrating the most important competences in BCMaterials with the area of advanced computing to coordinate the design of novel materials, the understanding and modulation of physicochemical interactions at the atomistic scale and the implementation of devices.

Computational methods have reached a high level of maturity, enabling the simulation of complex systems, such as biological systems, with large size and long-time scales. These simulations offer a highly detailed description, similar to that of an atomic microscope, and bridge the gap between traditionally disparate fields like biology and materials science. By reducing complex systems to their common features, such as modeling proteins as polymers, computational approaches simplify the design of bio-inspired materials and improve our control over their interactions.

Collaboration with computational groups has been key over the years in BCMaterials research, with support from density functional theory to molecular dynamics, from finite element simulation to artificial intelligence. However, the implementation of this new line of research in-situ is a fundamental step given the relevance of advanced computing in the design and understanding of new materials.

This new step is addressed by integrating two new Ikerbasque Research Professors, as well as post and pre-doctoral staff whose work is beginning to bear fruit both through academic publications and by increasing the influence of advanced computational tools in a significant portion of the experimental activities carried out in the center.

CLASSICAL FORCE-FIELD PARAMETERS FOR $CsPbBr_3$ PEROVSKITE NANOCRYSTALS

Roberta Pascazio, Francesco Zaccaria, Bas van Beek, and Ivan Infante. The Journal of Physical Chemistry C 2022, 126, 23, 9898–9908

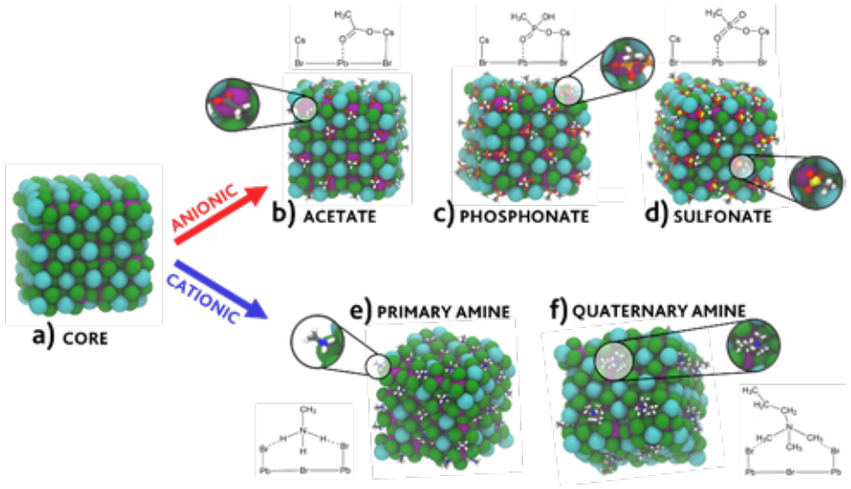


Fig 1
Snapshots of the NC models parametrized in this work: (a) inorganic $CsPbBr_3$ core and nanocrystal models capped with (b) acetate, (c) methylphosphonate, (d) methylsulfonate, (e) methylammonium (a primary amine), and (f) trimethyl propylammonium (a quaternary amine).

Understanding the chemico-physical properties of colloidal semiconductor NCs requires exploration of the dynamic processes occurring on their surface. Classical molecular dynamics (MD) simulations, based on available sets of force-field (FF) parameters are a powerful investigation tool because of their good accuracy and low computational cost. We employed a stochastic algorithm, the adaptive rate Monte Carlo method, to optimize and validate the FF parameters of ligand-capped CsPbBr3 perovskite NCs against reference trajectories. We then tested the transferability of the model on realistically sized structures.

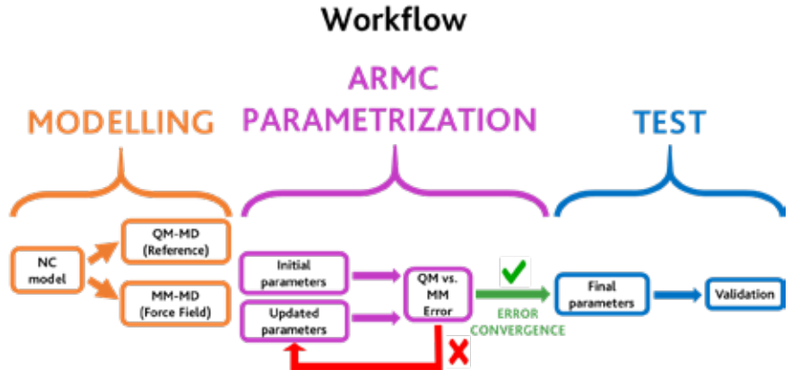


Fig 2
Adaptive Rate Monte Carlo Parametrization workflow.

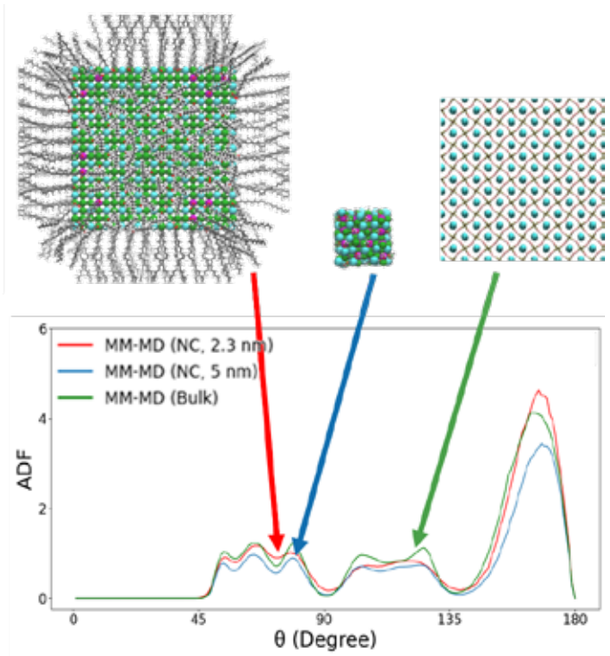


Fig 3
Comparison between the angular distribution functions (ADFs) of the Pb Br Pb angle obtained for the downscaled 2.3 nm NC model (red plot), for the upscaled 5.0 nm NC model in vacuum (blue plot), and for the bulk structure (green plot), plotted using the best set of ARMC-optimized FF parameters.

During the past two decades, research on colloidal semiconductor nanocrystals (NCs) has prompted a wide variety of novel applications thanks to their solution processability and remarkable versatility. These materials are composed of a semiconductive crystalline core, surrounded by organic ligands that maintain the NC colloidally stable. A comprehensive understanding of their optoelectronic characteristics should thus not neglect the atomistic processes occurring at their surfaces. Recent computational research endeavors in this field have gradually extended to larger-scale models, including the presence of ligands and solvents, and longer timescales. However, the high computational cost of density functional theory (DFT) sets an upper boundary to the feasibility of NC models, both in terms of their dimensions and simulation time spans. A computationally much cheaper alternative is currently based on classical MD simulations, which utilize classical potential energy functions (force fields, FF). Historically speaking, only minor endeavors have attempted to use FF for inorganic materials, leading to a limited availability of their FF parameters. Within this background, we optimized FF parameters for a class of highly promising materials, i.e. $CsPbBr_3$ perovskite NC models, including also the most common passivating ligands (Fig. 1). our procedure, the FF parameters are fitted against DFT references by means of a stochastic algorithm known as adaptive rate Monte Carlo (ARMC) (Fig. 2), which compares nonfitted properties to their DFT-computed equivalents and validates the robustness of the optimized set of parameters through the comparison of a range of structural properties available in the existing literature from both theoretical and experimental standpoints. We then demonstrated the scalability of the newly developed FF model on upscaled sized systems, mirroring those used in experiments (an example is shown in Fig. 3). The classical force fields obtained with the newly developed parameters provide an efficient, computationally feasible methodology for the description of the structure and dynamics of perovskite NCs, paving the way toward long timescale simulations of more realistically sized systems and processes.

KEY ASPECTS OF THE PAST 30 YEARS OF PROTEIN DESIGN

Giulia Magi Meconi, Ivan R. Sasselli, Valentino Bianco, Jose Onuchic and Ivan Coluzza.
Reports on Progress in Physics 2022, 85 086601

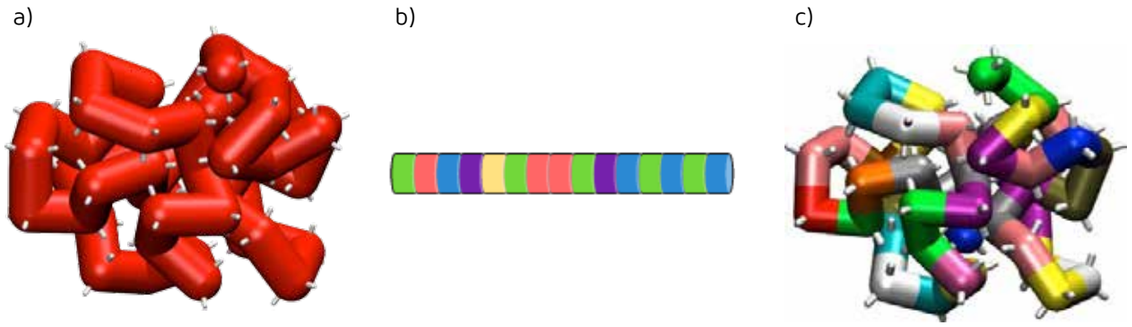


Fig 1
Structure and sequences are the fundamental elements of proteins. a) Space conformation of a chain that defines a target function. b) the sequence of monomers that encode such function. c) Assembled structure. The White sticks direct the interactions between the monomers towards preferential geometry. That is the key features that allows the encoding to be done with few monomers' types

Proteins are the workhorse of life. They are the building infrastructure of living systems; they are the most efficient molecular machines known, and their enzymatic activity is still unmatched in versatility by any artificial system. Perhaps proteins' most remarkable feature is their modularity. The large amount of information required to specify each protein's function is analogically encoded with an alphabet of just 20 letters. The protein folding problem is how to encode all such information in a sequence of 20 letters. In this review, we go through the last 30 years of research to summarize the state of the art and highlight some applications related to fundamental problems of protein evolution.

The ability of Biodegradable materials to be broken down into modular units is crucial for sustainability and is why it is essential to look to nature when designing biodegradable materials.
Among the various materials found in nature, proteins are one of the most remarkable. They are the building blocks of life, the most efficient molecular machines, and their versatility and modularity are unmatched by any artificial system.
Proteins are made up of a simple string of amino acids assembled into a chain and connected by peptide bonds. A large amount of information required to specify each protein's function is encoded with an alphabet of just 20 letters, which is the same for all species.
The correct sequence for assembling the proteins is written in the DNA and is the result of millions of years of evolution through natural selection. This relationship between the DNA code and the function allows for evolution to create new solutions. Hence, life could only emerge from a chaotic mixture of chemicals when a necessary function could be encoded into a string of monomers.
Based on these considerations, a material industry based on modular strings would have the potential to exploit the benefits of natural materials and evolve towards higher versatility and sustainability.
Understanding how to convert a string into a function is a crucial problem in material science and is central to understanding life's emergence.
The study of how a function is encoded in a protein string is called protein design, while the prediction of the function of a given string is called protein folding. In this review, we show how our discovery that directional interactions is enough for a material to allow for encoding a function into a string using a limited set of monomers is critical. Proteins use 20 amino acids, but it is known that proteins can be built using only 4 or 5 monomers. If such directional interactions are present in artificial polymers, they can be designed or evolved like proteins to have desired target functions, which are called "bionic proteins".
This result has benefits not only for designing new modular materials but also for searching for life on other planets. The information encoding is the first step in Darwinian evolution to emerge, and if the encoding is possible, it is not inconceivable that life could start from different materials and solvents other than protein in water, as it did on Earth.

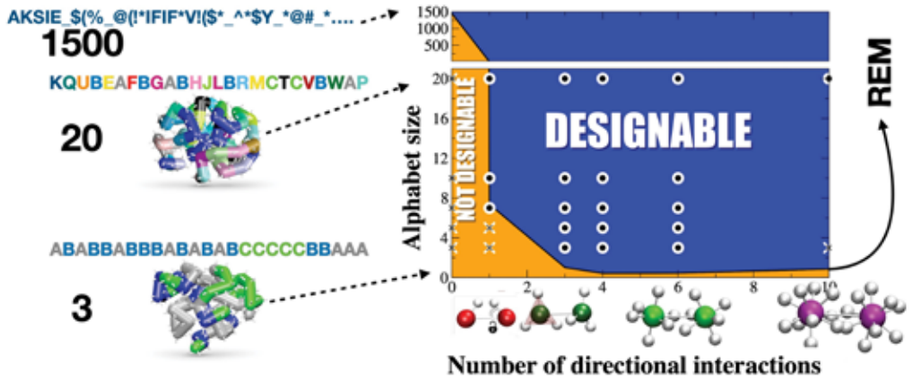
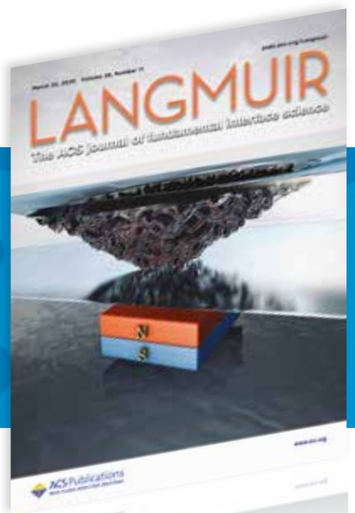


Fig 2
This graph shows the relationship between compact protein structures and the ability to design them. The broken line represents the point at which a protein structure becomes "designable." The yellow area shows structures that are not designable, while the blue area shows structures that are. The circles represent structures that have been verified as designable, and the crosses represent those that have not. According to our theory, proteins can be designed using only 4 unique building blocks, which we have verified through independent research. However, to design a chain of 50 monomers without directional interactions, an alphabet of 1500 letters would be required, making it highly unlikely to occur naturally. Therefore, directional interactions play a crucial role in enabling design and, as a result, life itself.

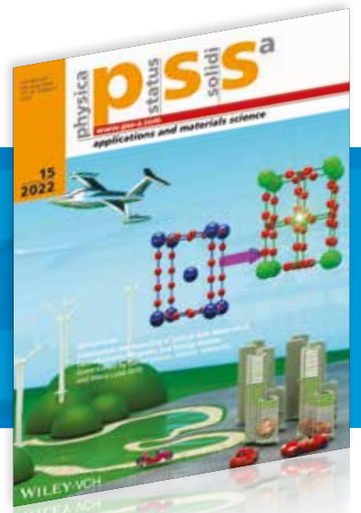
JOURNAL **COVERS SELECTION**



Langmuir

Magneto Twister: Magneto Deformation of the Water–Air Interface by a Superhydrophobic Magnetic Nanoparticle Layer. *Udara Bimendra Gunatilake, Rafael Morales, Lourdes Basabe-Desmonts and Fernando Benito-Lopez.*

Remote manipulation of superhydrophobic surfaces provides fascinating features in water interface-related applications. A superhydrophobic magnetic nanoparticle colloid layer is able to float on the water–air interface and form a stable water–solid–air interface due to its inherent water repulsion, buoyancy, and lateral capillarity properties. Moreover, it easily bends downward under an externally applied gradient magnetic field. Thanks to that, the layer creates a stable twister-like structure with a flipped conical shape, under controlled water levels, behaving as a soft and elastic material that proportionally deforms with the applied magnetic field and then goes back to its initial state in the absence of an external force. When the tip of the twister structure touches the bottom of the water container, it provides a stable magneto movable system, which has many applications in the microfluidic field. We introduce, as a proof-of-principle, three possible implementations of this structure in real scenarios, the cargo and transport of water droplets in aqueous media, the generation of magneto controllable plugs in open surface channels, and the removal of floating microplastics from the air–water interface.



Physica Status Solidi A

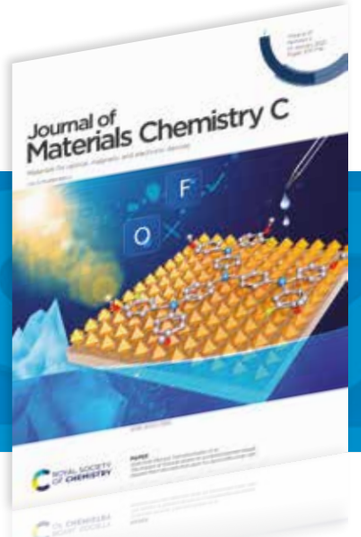
Magnetic Properties of Tetragonal SmFe12-xMox Alloys in Bulk and Melt-Spun Ribbons. *Bosco Rodríguez-Crespo, Andrés Garcia-Franco, James Janderson Rosero-Romo, Cristina Echevarria-Bonet, Jose Maria Porro, Paula G. Saiz, Daniel Salazar.*

Currently, electric motors and generators use high-energy permanent magnets based on RE2Fe14B phases (RE: rare earth) with high amounts of RE often including heavy-RE metals (Dy, Tb), the most critical group of the raw materials. REFe12 alloys are seen as potential alternatives to RE2Fe14B because they contain a significantly lower amount of RE metals with similar or better values of remanent magnetization (MR) and high magnetocrystalline anisotropy, which can give rise to a large energy product (BH)max. Herein, the effect of heat treatments on the coercivity and magnetic properties on melt-spun ribbons of SmFe12 xMox (x = 0.5, 1) alloys with wheel speeds of 15 and 35 m s 1 is studied. The maximum coercivity after heat treatments is obtained in as-spun ribbons at a speed of 35 m s 1. For the x = 0.5 ribbons, μ0Hc increases from 0.06 to 0.36 T, while for the x = 1.0 ones μ0Hc is enhanced from 0.02 to 0.34 T. The highest values of saturation magnetization are obtained for the x = 0.5 ribbons (≈145 A m2 kg 1).

Applied Electronic Materials

Multifunctional Ternary Composites with Silver Nanowires and Titanium Dioxide Nanoparticles for Capacitive Sensing and Photocatalytic Self-Cleaning Applications. *Carmen R. Tubio, Nelson Pereira, Lia Campos-Arias, Pedro Manuel Martins, Jose Luis Vilas-Vilela, Carlos M. Costa, and Senentxu Lanceros-Méndez*

Multifunctional polymer composites are of increasing interest as they allow tuning of physical–chemical properties for specific applications. A ternary composite material is presented based on the incorporation of titanium dioxide (TiO2) nanoparticles and conductive silver nanowires (AgNWs) into a poly(vinylidene fluoride) (PVDF) polymer matrix. The films were prepared by solvent casting, varying the contents of the filler up to 10 wt %, and showed improved mechanical and dielectric responses and tailorable optical properties. In contrast, the morphology, polymer phase, and thermal stability are nearly independent of the filler type and content within the composite. A dielectric constant of up to 14 at 1 kHz was obtained for the 7.5%AgNWs/2.5%TiO2/PVDF sample. The (multi)functionality of the developed materials is demonstrated for photocatalytic self-cleaning and capacitive sensing applications, indicating the suitability of the approach for next-generation hybrid multifunctional materials.

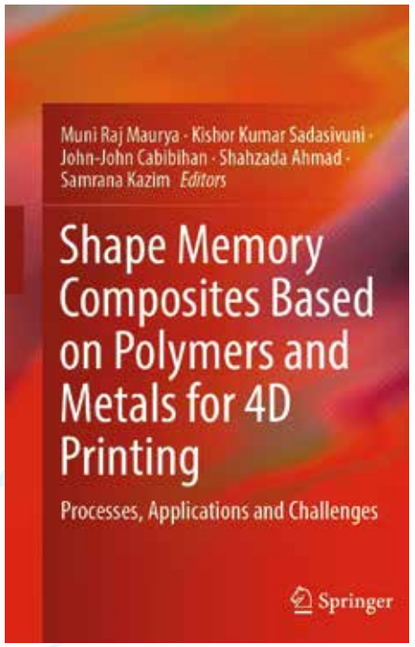


Journal of Materials Chemistry C

The impact of fluorine atoms on a triphenylamine-based dopant-free hole-selective layer for perovskite solar cells. *Abolfazl Ghaderian, Meenakshi Pegu, Naveen Harindu Hemasiri, Peng Huang, Shahzada Ahmad and Samrana Kazim.*

For industrial use, perovskite solar cells (PSCs) require long-term stability and a cost-effective hole-transport layer (HTL). The PSC stability can be substantially improved via the rational design of a dopant-free HTL that possesses inherent electrical merits. Further, through molecular engineering, via placing fluorinated arms on an established triphenylamine core, superior stability can be achieved using cost-effective precursors and easy synthesis routes. Here we developed a fluorinated triphenylamine-based HTL, probed its structural and electro-optical properties, and demonstrated the practical utility of the HTL in a PSC in its pristine form. The designed fluorinated HTL, called tri(3-fluoro-4-methoxy-N-(4-methoxyphenyl)aniline) triphenylamine (FOMePh), gave a high power conversion efficiency (PCE) of 17.08%, which exceeded that of doped Spiro-OMeTAD (16.9%) while consuming 2.3-times less material than Spiro-OMeTAD during PSC fabrication.

BOOKS & REVIEW PAPERS



SHAPE MEMORY COMPOSITES BASED ON POLYMERS AND METALS FOR 4D PRINTING

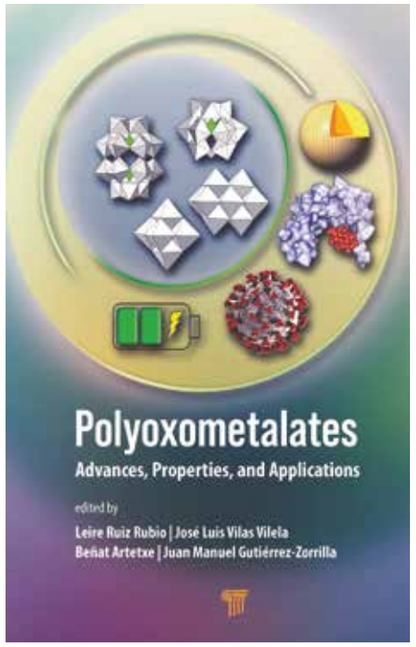
M. R. Maurya, K. K. Sadasivuni, S. Kazim, J. V. S. K. V. Kalyani, J.-J. Cabibihan, S. Ahmad

Shape Memory Composites Based on Polymers and Metals for 4D Printing is a thorough discussion of the physics and chemistry behind this developing area of materials science. It provides readers with a clear exposition of shape-memory-composite (SMC) preparation techniques for 3D and 4D printing processes and explains how intelligent manufacturing technology may be applied in fields such as robotics, construction, medical science, and smart sensors. This book provides practitioners, industrial researchers, and scholars with a state-of-the-art overview of shape memory polymers (SMP) and shape memory alloys (SMA) synthesis, additive manufacturing, modification in synthesis of SMCs for 4D printing, and their likely future applications.

POLYOXOMETALATES ADVANCES, PROPERTIES, AND APPLICATIONS

Leire Ruiz Rubio, José Luis Vilas Vilela, Beñat Artetxe, Juan Manuel Gutiérrez-Zorrilla

Polyoxometalates are anionic metal-oxo nanoclusters, which constitute a unique class of compounds owing to their rich solution equilibria and their unique compositional, electronic, reactive, and structural diversity. This book reviews metal-oxide cluster chemistry by covering topics ranging from fundamental aspects (i.e., structure, properties, self-assembly processes, derivatization) to functional materials that incorporate these molecular units, as well as their applications in the fields of current socioeconomic interest, such as energy storage systems, catalysis, molecular electronics, and biomedicine. Edited by prominent researchers in the field of polymer and polyoxometalate chemistries, the book compiles contributions from some of the most distinguished and promising scientists worldwide in such a way that it will appeal to a general readership involved in research areas related to chemistry and materials science.



Multicomponent magnetic nanoparticle engineering: the role of structure-property relationship in advanced applications

Díez, A.G., Rincón-Iglesias, M., Lanceros-Méndez, S., Reguera, J., Lizundia, E
Materials Today Chemistry 26,101220

Microfluidics for Electrochemical Energy Conversion

Ibrahim, O.A., Navarro-Segarra, M., Sadeghi, P., (...), Esquivel, J.P., Kjeang, E.
Chemical Reviews 122(7), pp. 7236-7266

Toxicity of metal-organic framework nanoparticles: From essential analyses to potential applications

Ettlinger, R., Lächelt, U., Gref, R., (...), Morris, R.E., Wuttke, S.
Chemical Society Reviews 51(2), pp. 464-484

Strategic factors to design the next generation of molecular water oxidation catalysts: Lesson learned from ruthenium complexes

Ghaderian, A., Kazim, S., Khaja Nazeeruddin, M., Ahmad, S
Coordination Chemistry Reviews 450,214256

State of the art and current trends on layered inorganic-polymer nanocomposite coatings for anticorrosion and multi-functional applications

Teijido, R., Ruiz-Rubio, L., Echaide, A.G., (...), Lanceros-Mendez, S., Zhang, Q.
Progress in Organic Coatings 163,106684

Recycling methods for different cathode chemistries – A critical review

Wang, Y., Goikolea, E., de Larramendi, I.R., Lanceros-Méndez, S., Zhang, Q.
Journal of Energy Storage 56,106053

PRICES & ACKNOWLEDGEMENTS

Award from Board of Governors of Acta & Scripta Materialia Inc. for excellent reviewing

Volodymyr Chernenko

Best poster at IMOH 2022 international conference (Leioa)

"Direct post-synthetic encoding of Metal-Organic Framework/PVDF composites for enzymatic-like capture and degradation of inorganic and organic pollutants".

Ainara Valverde

3rd Price in the project contest of the EU TALENTON event Leiden (Netherlands)

"Detecting and monitoring microplastics in surface waters using a combination of machine learning and citizen science" won this price in the category named. 'Recover our oceans and waters'.

Fangyuan Zheng

World's top 2% most influential scientists*

Senentxu Lanceros-Méndez

Koro de la Caba

Shahzada Ahmad

Stefan Wuttke

Volodymyr Chernenko

Qi Zhang

Pedro Guerrero

Erlantz Lizundia

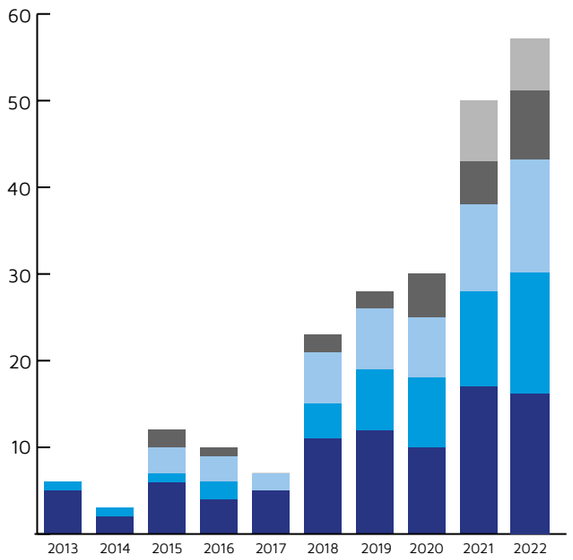
8 BCMaterials researchers in this annual list published by the Standford University (USA).

FOUNDING SOURCES & RESEARCH **PROJECTS**

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

3%	invoicing
33%	Private
22%	BERC
18%	Basque Government
7%	National funding
17%	International



- Regional projects
- Spanish projects
- International projects
- Private projects
- Other projects

81

SUBMITTED PROPOSALS

20%	Accepted
38%	Pending
42%	Rejected

FINANCIAL BODIES

BASQUE
RESEARCH PROJECTS

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

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

ALOPRP 3D III Creación de apósitos con plasma rico en plaquetas alogénicos para la curación de heridas crónicas
EJ/GV Ayudas a Proyectos de Investigación y Desarrollo en Salud Dep. Salud 2022_333047 2022

BIOBASED Investigación en materiales y procesos biobasados para la estrategia de bioeconomía de Euskadi
EJ/GV, ELKARTEK Tipo 1 KK-2021/00131 2021-2022

BISUM Bio-inspired SUrfaces for Machine elements (BISUM)
EJ/GV, ELKARTEK Tipo 1 KK-2021/00089 2021-2022

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

Ensol3 Investigación en tecnologías avanzadas para el liderazgo de la energía solar fotovoltaica
EJ/GV, ELKARTEK Tipo 1 KK-2022/00067 2021-2022

FRONT21 FRONTIERS 2021 - Superficies multifuncionales en la frontera del conocimiento
EJ/GV, ELKARTEK Tipo 1 KK-2021/00124 2021-2022

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

IDEA2 Investigación y Desarrollo en Electrónica Aditiva 3D Impresión e Integración
EJ/GV, ELKARTEK Tipo 1 KK-2021/00040 2021-2022

IMOH 2022 1st International Meeting on challenges and Opportunities for Hicans
EJ/GV, IKERBILERAK RC_2022_1_0030 2022

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

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

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

UIIOT Microtecnologías como motor de desarrollo de Microsistemasavanzados integrados en la Fábrica Inteligente y Digital en el marco de la IIoT4.0, Industrial Internet of Things
EJ/GV, ELKARTEK Tipo 1 KK-2021/00082 2021-2022

SPANISH 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

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

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

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

PINCHE Promoting INternational Collaboration for Horizon Europe framework programme
Europa Investigacion EIN2020-112406 2020-2022

RAMÓN Y CAJAL Ignacio Minguez Bacho
FJC2021-048154-I RYC2021-032931-I 2023-2027

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

EUROPEAN & OTHER INTERNATIONAL PROJECTS

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

ANIMOC Directional Assembly of Emergent Luminescent and Anisotropic d10 Coinage Metal Organic Chalcogenolate Nanomaterials for Fabrication of Pressure Sensitive Devices
H2020-MSCA-IF-2020 2021-2022

ECLICARE Bioensayos Electroquemiluminiscentes para Diagnóstico Personalizado
Euroregion 21 EUREG_2021 2021-2023

EUTOPIA European Topology Interdisciplinary Action
COST ACTION CA17139 2018-2023

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

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

SMILIES Two-dimensional Transition Metal Dichalcogenides as Charge Transporting Layers for High Efficient Perovskite Solar Cells
H2020-MSCA-IF-2019 2020-2022

TailingR32Green Mine tailings Reprocessing, Revalorization and Risk reduction connecting innovations in metal recovery, geopolymerization, ceramics & sealing layers
ERAMIN3 PCI2022-132969 2022-2024

PRIVATE PROJECTS

CURVE Desarrollo de decoraciones funcionalizadas por tintas transparentes para displays curvos basados en OLCDs
WALTER PACK 2020/2022

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

E-POLYMER Nuevos grados de abs sus copolímeros y blends termoplasticos con funcionalidades avanzadas para automocion e-mobility
ELIX POLYMERS 2020-2022

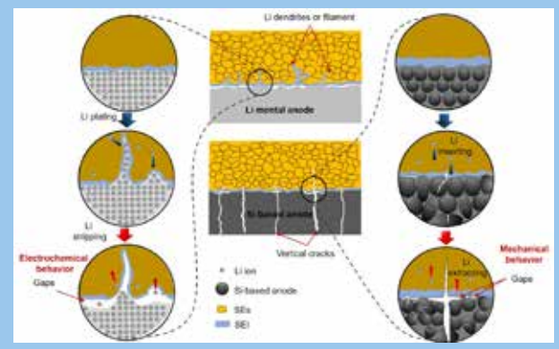
MELEXIS Verifying the feasibility of GMI sensor based on Melexis IMC soft magnetic materials
MELEXIS 2022-2023

TOUCHSENSOR Nuevos productos de inyección con superficies con capacidad sensorial táctil
GAIKER 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

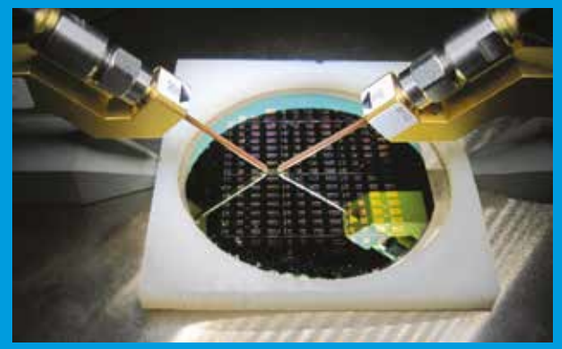
VIUDA DE SAINZ Protoptipo de deformaciones con cementos piezoresistivos
VIUDA DE SAINZ 2022

E-ONTECH
Development towards to next generation lithium batteries



E-Ontech is famous for its high quality Si-related products, such as, nano-sized Si spheres, C-coated Si nanoparticles, etc. These products are important anode components in lithium batteries. However, due to a large volume change of Si material during charging/discharging of the lithium batteries, a rapid decrease of energy density is unavoidable. The most of researches on the solid-state batteries are focused on the Li metal anode, as shown in the Figure. Li metal exists two big issues, the formation of Li dendrites and gap between Li metal and solid electrolyte, which is a electrochemical behaviour and unavoidable. However, the use of Si as anode can solve these two problems through the designs of ceramic/polymer composite electrolytes and Si composites because the formation of the gaps is a mechanical behaviour.
In this project, BCMaterials and E-Ontech would develop an all solid-state battery, in particular, a ceramic/polymer composite electrolyte, and pair with the Si anode developed by E-Ontech, in the hope that a high energy density, safe, all-solid-state batteries will eventually be viable for the applications, such as, electric vehicles, power tools, etc.
To achieve the ceramic/polymer composite electrolyte, high temperature sintering (>300 °C) is not viable due to the burn-off of organics. BCMaterials has a special technology that can sinter ceramic/polymer composites at very low temperatures (< 200 °C). To understand the mechanism of the ionic transport in the electrolytes, the Neutron team in BCMaterials are able to analyse the micro-structures of the electrolytes and interfaces between the Si anode and the electrolyte. The cold sintering technique and Neutron technique in BCMaterials can make a big contribution to the project.

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



Melexis is a company that creates microelectronic solutions. These solutions facilitate the work of their customers. By means of simple integration. By taking innovation to the next level, you can gain a competitive advantage. Their technology makes automobiles and other products smarter, safer, and more environmentally friendly. They sensors collect data from the analog world and process it digitally. Melexis primarily manufactures semiconductors for the automotive industry. Melexis is energizing the transition to electric vehicles (EVs). They increase ICE vehicle efficiency. In addition to the automotive market, they serve markets such as alternative mobility, smart appliances, smart buildings, robotics, energy management, and digital health. BCMaterials is assisting Melexis on the characterization of the soft materials used in their ICs magnetic sensors to push further the current capabilities of their sensors.

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.

18
PhD Defended

1. Adrian Angulo Ibáñez
Desarrollo de materiales fotocatalíticos mediante formulaciones sol-gel y estructuras metal-orgánicas de Ti(IV) para su aplicación en la degradación de materia orgánica y reducción de CO2.

2. Andrea Ochoa
Diseño de un biosensor para la detección de anticuerpos relacionados a alergias alimenticias

3. Bruno Filipe da Costa Hermenegildo
Electro and Magnetically Active Polymer-based Hybrid Microenvironments for Muscle Tissue Engineering

4. David Payno
Improving Kesterite for its use in low-cost superstrate solar cells

5. Iratxe Zarandona
Design of chitosan-based materials for food applications

6. Jon Andrade Del Olmo
Hyaluronic acid- and chitosan-based antibacterial coatings on ti6al4v for biomedical implant applications

7. Jon Pascual Colino
Merging porosity with magnetism and fluorescence in metal-organic materials for sensing purposes

8. Leire Etxeberria
Different approaches for mass production of thermoplastic microfluidic devices

9. Meenakshi Pegu
Developing Hole Selective Layers and Implementing Large-size Organic cations for Perovskite Solar Cells

10. Mikel Rincón Iglesias
Sustainable multifunctional materials with tailored magnetic and electrical properties for electronics applications

11. Mireia Andonegi
Valorization of agro-industrial wastes for the production of biodegradable products based on collagen / Nekazal eta industria hondakinen balorizazioa kolagenoan oinarrituriko produktu biodegradagarriak ekoizteko

12. Maria Teresa Guillot Ferriols
Electroactive environments for mesenchymal stem cells osteogenic Differentiation

13. Marina Navarro
Primary Batteries Paradigm Redefinition within the Environmental Planetary Boundaries

14. Ana Catarina Branco Lima
Magnetically responsive inks for printed electronics components and devices: integration into a fully printed magnetic sensor

15. Artykulnyi Oleksandr
Complexation of anionic surfactants with polyethylene glycol in the liquid systems of water solutions

16. Hugo Higino de Barros Machado Martins Salazar
New generation of polymer composite membranes for water purification

17. Nelson Miguel Macedo da Silva Pereira
Development of multifunctional inks for the implementation of interactive applications

18. Sérgio Abílio Pereira Gonçalves
New generation of interactive platforms based on novel printed smart materials

22
Master Theses

24
Undergraduated

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

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**

In 2022 BCMaterials undertook a major expansion of its research facilities with the implementation of new laboratories.
This substantial increase is consistent with the growth experienced by the center. With the implementation of these new laboratories, BCMaterials fulfils two important objectives: on the one hand, to have complete and high-level facilities to carry out its research and, on the other, to increase its catalogue of laboratory services to external agents, offering advanced equipments and high-level support.

LABS SERVING RESEARCH **AREAS**

Biomaterials and Biomedicine

Environmental Materials and Processes

Materials for Energy

Advanced Materials and Thin Films

Additive Manufacturing

LABS SERVING RESEARCH **TECHNIQUES**

Multifunctional Nanochemistry

Multifunctional Materials Synthesis

Metallurgy and Ceramics

Optics and Optoelectronics

Electricity and Electronics

MATERIALS **SYNTHESIS**

Synthesis of advanced and multifunctional materials is one of the cornerstones of materials innovations. State of 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 tailor made 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:

- 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.

04

OUTREACH ACTIVITIES

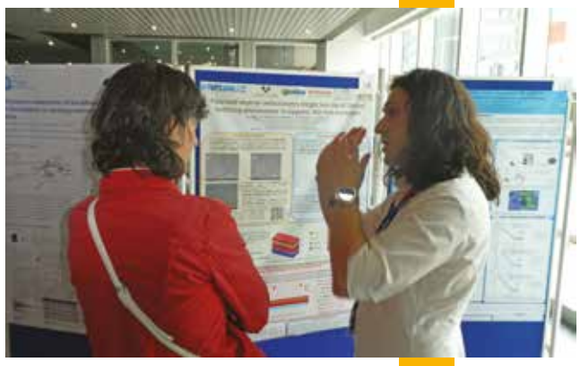
Working for the benefit of society. Society and fellow scientist must know our motivation, our aims, our way of facing science and technology and our results. Thus, communication activities, from the general to specialized public, represent one of the most rewarding of our activities.

AT
BCMATERIALS

IMOH 2022

1st International Meeting on Opportunities and Challanges for HICANS

Del 20 al 22 de junio, BCMaterials organizó, en colaboración con ESS Bilbao, CFM-MPC e Ineustar, el primer del primer encuentro en España dedicado monográficamente a los HICANS, instalaciones científicas compactas que facilitan el acceso a la experimentación con neutrones a científicos y estudiantes. La cita reunió a algunos de los mayores expertos europeos en ciencia de neutrones, que trataron el estado del arte y el desarrollo de las fuentes compactas de neutrones de alta intensidad, así como la posibilidad de que Euskadi acoja en un futuro cercano una de estas instalaciones. La organización de este encuentro fue, asismismo, una constatación en la práctica de la apuesta decidida de BCMaterials por una de las áreas clave en la investigación de futuro señalada por la Estrategia IKUR, del Gobierno Vasco, como es la neutrónica.



- 5 PLENARY SESSIONS
- 7 INVITED TALKS
- 13 ORAL PRE-SENTATIONS
- 16 POSTERS PRESENTED

- AVS
- BCMaterials
- Btesa
- Cadinox
- Centre for Energy Research (Hungary)
- CFM/MPC
- CINC
- Comenius University Bratislava (Slovakia)
- INFN and University of Milano Bicocca (Italy)
- Instituto de Ciencia de Materiales de Barcelona CSIC
- Paris-Saclay University, CNRS, CEA, Léon Brillouin Laboratory (France)
- Elytt Energy
- ENUSA
- ESS Bilbao
- Jülich Centre for Neutron Science (Germany)
- ILL- Institut Laue-Langevin (France)
- Ineustar
- ISIS Neutron and Muon Source (UK)
- JEMA
- University of Lund (Sweden)
- Mirrotron (Hungary)
- Nortemecánica
- NRC Soreq (Israel)
- Orolia
- Reuter-Stokes (USA)
- Science Engineering Associates S.L.
- Scientifica
- STFC Rutherford Appleton Laboratory (UK)
- Tekniker
- Thune Eureka
- Universidad de Cantabria
- Unviersidad de Granada
- Universidad de Navarra
- Uppsala University (Sweden)

- 80 ATTENDEES
- FROM 10 COUNTRIES

AT
BCMATERIALS

SEMINARS & TALKS

2022 was an intense year in terms of invited talks and seminars at the BCMaterials headquarters.With a total of 27 events, our center's researcher staff and visiting scientists, as well as our research associates and attendees coming from other institutions, received a complete view of different scientific disciplines and areas of interest, helping them to be aware of some interesting works led by international scientists. As for the fortnightly seminars presented by our researchers, they kept offering the oppotunity to see in depth what is going on in our four research lines. Our pre-doctoral researchers, especially, found in these seminars a way to show their current work and also train something so necessary like talking in front of the public.

27 EVENTS

17 SEMINARS

10 INVITED TALKS

OUT

BCMATERIALS

EXTERNAL DISEMINATION

One ob the best indicators of BCMaterials researchers work's quality is the number of external disemination activities in which they take part along the year. From poster contributions to oral presentations and talks in congresses and conferences, all these activities continue to increase at the same path the Center itself grows.

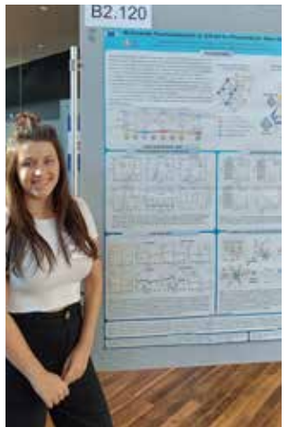
> **We choose to go to the Moon and do the other things, not because they are easy, but because they are hard**
>
> **John F. Kennedy (1917 – 1963)**

49 INVITED TALKS

59 ORAL PRESENTATIONS

49 POSTER CONTRIBUTIONS

Senentxu Lanceros-Méndez
Invited talk at the Tokyo Institute of Technology (Japan)
Oct. 2022



Sara Martín
Termis conference
Krakow (Poland)
June 2022

Ainara Valverde
Mof 2022 Conference.
Dresden (Germany)
Sept. 2022

Corina Rodríguez
Conference of the Association Française de Magnétisme Moléculaire (France)
Nov. 2022

BCMaterials representation at TMS Annual Meeting (USA)
Feb.- March 2022

Juan Pablo Esquivel
Naukas Bilbao
Sept. 2022

SCIENCE
FOR SOCIETY

12
EVENTS

As part of our agreement with the Elhuyar Fundazioa to promote scientific dissemination and vocations, BCMaterials participated in the 10th edition of **ZIENTZIA AZOKA** *(Science Fair). We evaluated the scientific projects of the students who participated in this contest, we held scientific workshops in downtown Bilbao for all kinds of public, and we showed our facilities to some of the groups awarded in the project contest.*

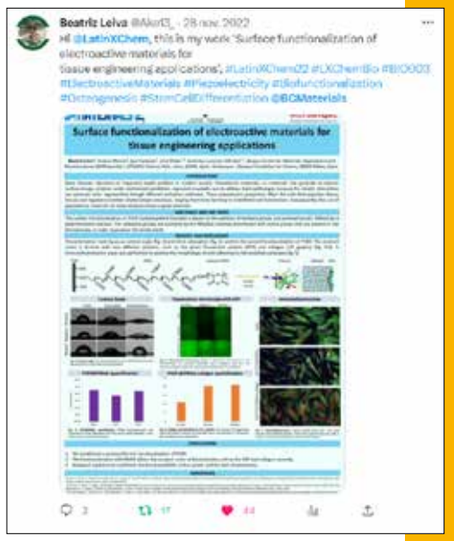
From November 9 to 12, BCMaterials participated in a new edition of the **ZIENTZIA ASTEA'** *(Science, Technology and Innovation Week), organized by the UPV/EHU. Some twenty researchers from the center explained to the hundreds of people who visited our stand how new materials can help create smart and climate-neutral cities. Likewise, the researchers Karla Merazzo and Beatriz Leiva collaborated with the 'She Mentoring' stand, an initiative to claim the role of women scientists and promote the female scientific vocation.*

SCIENCE **FOR SOCIETY**

*On September 30, we took part in the **EUROPEAN NIGHT OF RESEARCHERS** with the stand called "Future City". In this event organized by the UPV/EHU in Bilbao downtown, we showed different applications of new materials science to smart cities, environmental remediation, the generation of clean energy....*

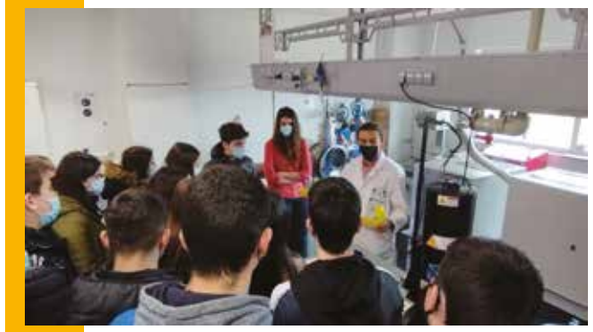
*Ikerbasque Research Professor Ivan Coluzza during his talk at the **PINT OF SCIENCE** scientific outreach festival in Donostia-San Sebastian in May 2022.*

Latin XChem



egin & ekin

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.



WOMEN IN SCIENCE DAY

On February 10 and 11, on the occasion of the Week of Women and Girls in Science, BCMaterials organized the activity called 'Woman+Science= a journey through time'. One hundred secondary school students participated in this event. The goal was 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. This STEM activity was a resounding success in terms of attendance, participation and involvement from the schools and the students who took part in it.

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PARTICIPANT STUDENTS

1. *Presentation*
The students were received at the Martina Casiano Auditorium where they learned about the difficulties that women have had through History to receive the same recognition as their male fellows.

2. *Exhibition*
After the presentation, the participants visited a poster exhibition with the achievements of great female scientists and with the experience and advices from BCMaterials researchers.

3. *My first scientific poster*
The students, divided in groups, were asked to create their first scientific posters by imagining the future of different scientifical and technological disciplines, and the role that women will play in them.

4. *Electronic poster session*
The electronic posters created by the students were exhibited at the BCMaterials display screen at the building's lobby during the two days in which the event took place.

MEDIA IMPACT

TV

Itziar Oyarzabal was interviewed for a TVE Report on Ikerbasque Researchers
Mar, 21 2022

Senentxu Lanceros-Méndez
Nov, 18 2022

Javier del Campo
Oct, 6 2022

Beatriz Leiva
Sept, 19 2022

Juan Pablo Esquivel & Marina Navarro
Jul, 22 2022

José María Porro
Jun, 22 2022

NEWS

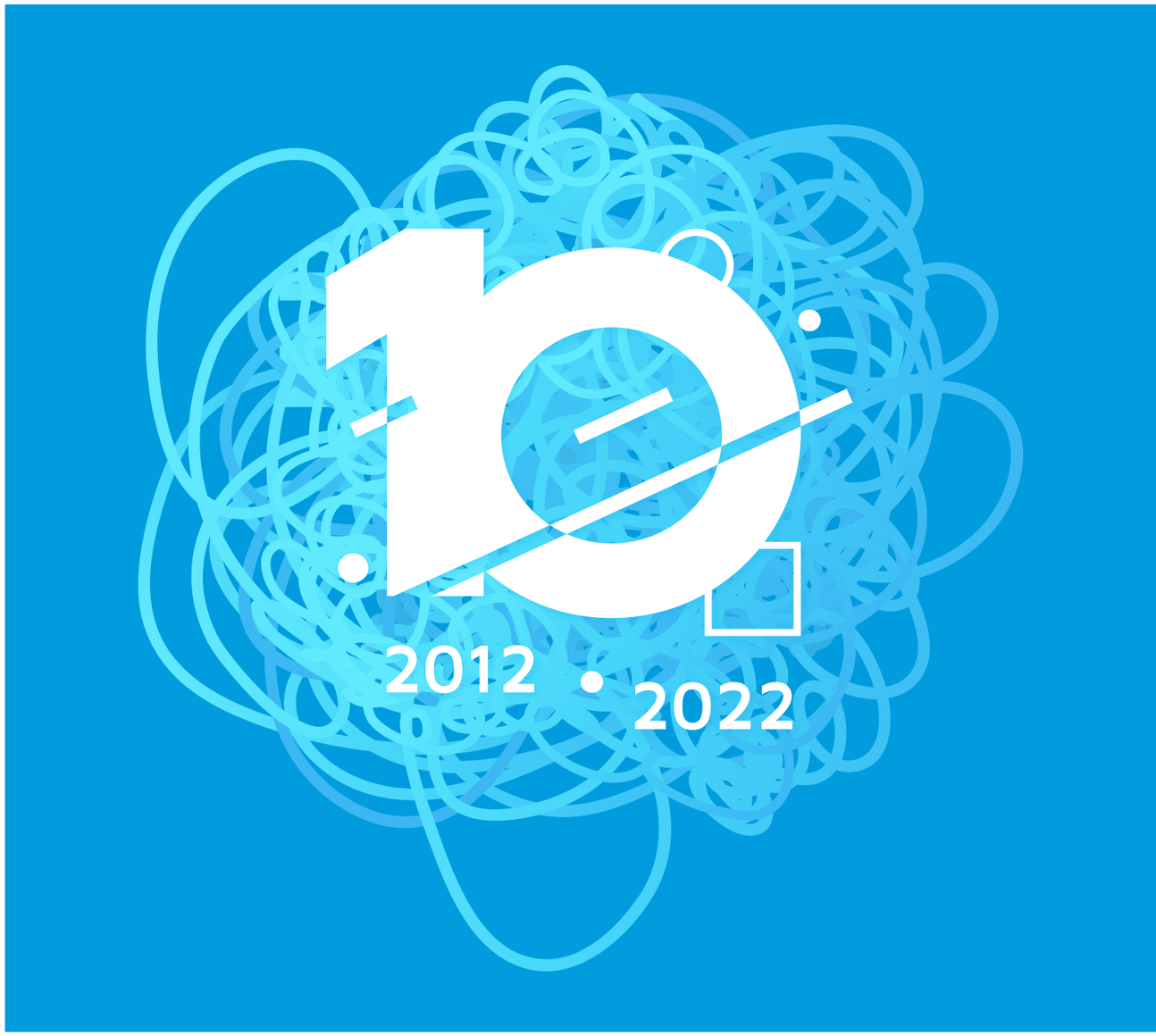
El Correo, report on women and Science (Itziar Oyarzabal)
Feb, 10 2022

BCMaterials 10th anniversary 'Empresa XXI'
Dec, 15 2022

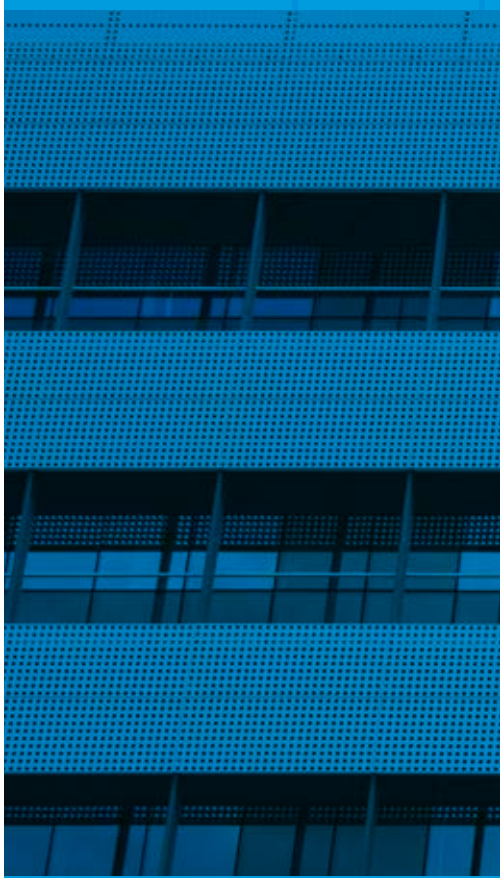
WWW

Contributions to Mapping Ignorance science blog

Articles in Zientzia Kaiera Basque spoken science blog


2012 • 2022

ANNUAL REPORT 2022



BCMATERIALS
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ehu group

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