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Since 2011 **ImagineNano** has strengthened its position as one of the main events dedicated to Nanoscience and Nanotechnology (N&N) in Europe. The outstanding results of participation that have been reached and the interest created by the discussions, have laid the foundations for the upcoming edition.

ImagineNano 2021 is now an established event and is an excellent platform for communication between science and business, bringing together Nanoscience and Nanotechnology in the same place.

Internationally renowned speakers will be presenting the latest trends and discoveries in Nanoscience and Nanotechnology.

Under the same roof will be held 6 International Conferences (QUANTUM, Graphene & 2DM, NanoSpain, IC2, 3DPrinting and 3PM), an exhibition showcasing cutting-edge advances in nanotechnology research and development and a brokerage event (one-to-one meetings).

ImagineNano will gather the global nanotechnology community, including researchers, industry, policymakers and investors. The latest trends and discoveries in N&N from some of the world's leading players in the field will be discussed.

We would like to thank all participants, sponsors and exhibitors that joined us this year.

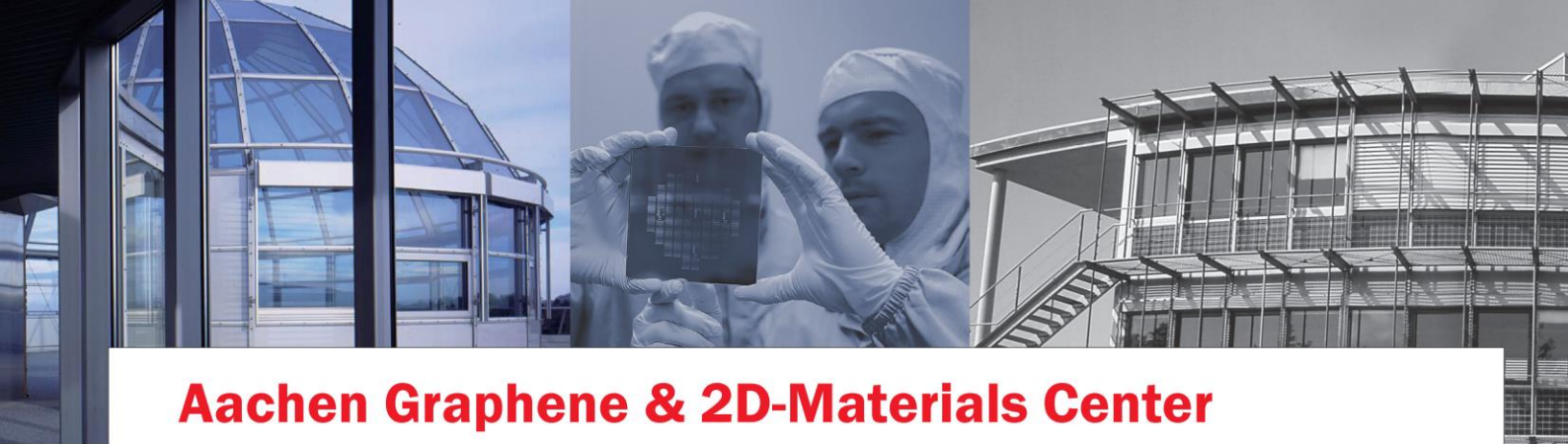
The Basque Country demonstrates its strengths in nanoscience, micro and nanotechnology, and positions itself as a major player in the "nano" world, reason why **ImagineNano** is organized for the 5th time in Bilbao.

There's no doubt that **ImagineNano 2021** is the right place to see and be seen.

Hope to see you again in the next edition of **ImagineNano** (2023) in Bilbao.

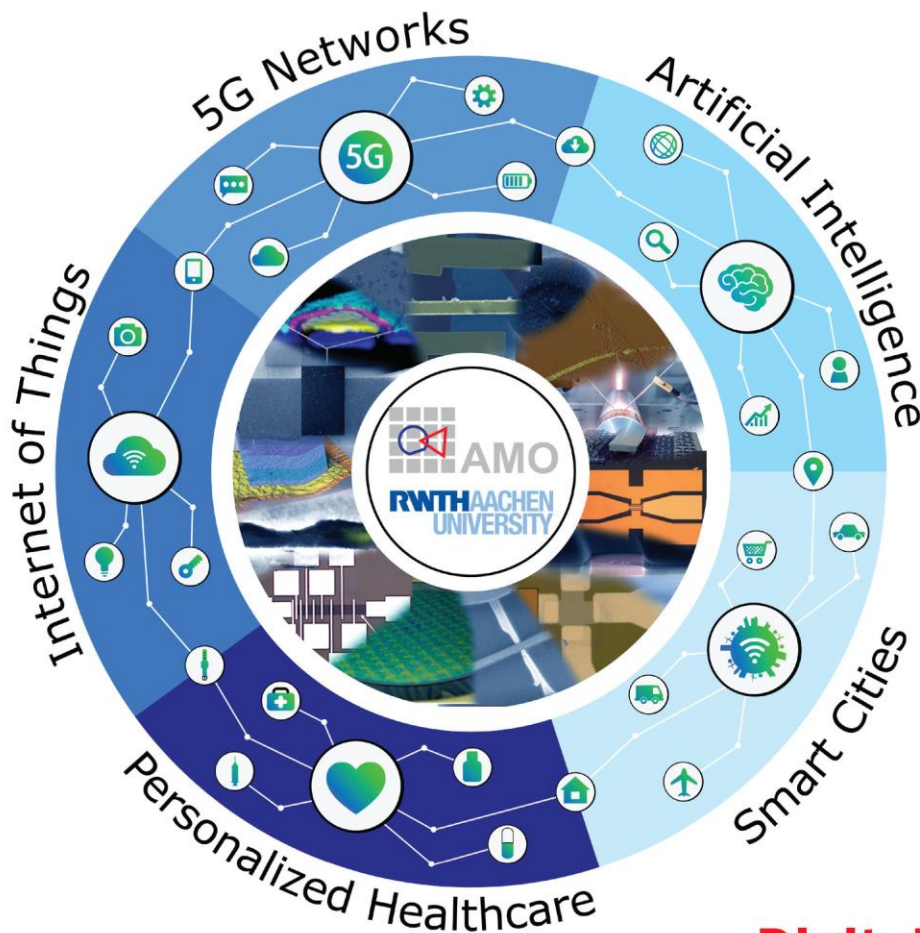
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● INDEX

Committees Page 6

Sponsors Page 8

Exhibitors Page 15

Speakers list Page 17

Abstracts Page 18

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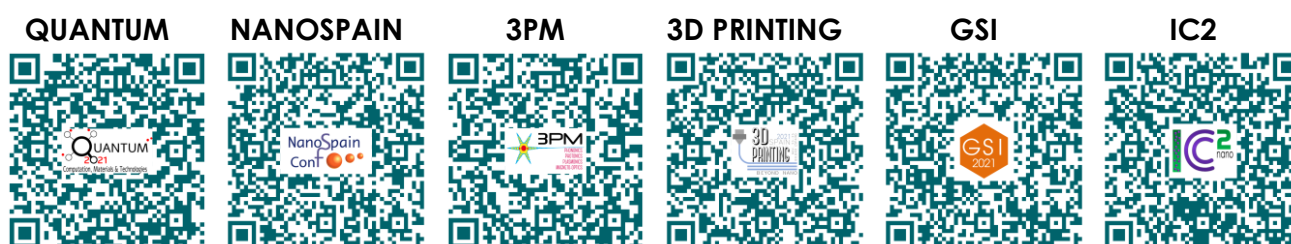
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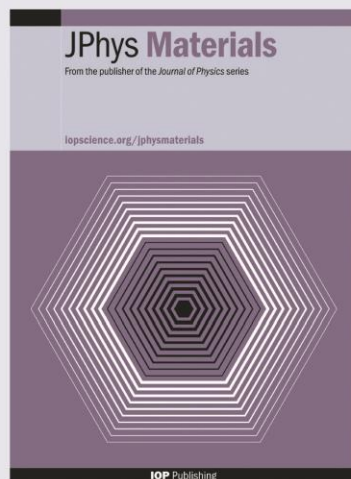
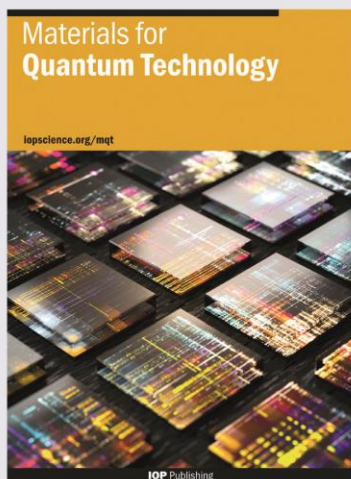
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Pilar Aranda (ICMM-CSIC, Spain)	Invited	23
Use of Clay-Based Bionanocomposites as Drug Delivery Systems		
Yehonadav Bekenstein (Technion, Israel)	Keynote	18
Nanoengineering next-generation energy materials the case of CsPbBr ₃ perovskite nanocrystals		
Miren Blanco (Tekniker, Spain)	Oral	28
Biobased epoxy vitrimer for reprocessable composites		
Nerea Casado (University of the Basque Country / POLYMAT, Spain)	Invited	24
Mixed Ionic-Electronic Composites based on Poly(3,4-ethylenedioxythiophene) and Organic Ionic Plastic Crystals		
Ander Garcia Díez (BCMaterials, Spain)	Poster	34
Magnetorheological elastomers as multifunctional materials for smart devices and applications		
Arrate Huegun (CIDETEC, Spain)	Invited	25
Nanomodified reshapeable, repairable and recyclable epoxy resin for conducting composite materials		
Ian Kinloch (The University of Manchester, UK)	Keynote	19
Graphene and other 2D Material Multifunctional Composites		
Anna Laromaine (ICMAB-CSIC, Spain)	Keynote	20
Cellulose responsive composites: control at the nanoscale		
María Adelia López Pérez (Applynano Solutions, S.L., Spain)	Poster	35
Carbon based materials in epoxy resin composites for self-heating applications		
Cristina Matos (ISQ, Portugal)	Oral	29
Challenges to the evaluation of the emerging risks concerning Nanocomposites - LightMe case study		
Daniil Nosov (Luxembourg Institute of Science and Technology, Luxembourg)	Oral	30
New trends in development of highly conductive poly(ionic liquid)s		
Ander Reizabal (BCMaterials, Spain)	Oral	31
Silk Fibroin composites for next generation of sustainable smart materials development		
Eva Rodil (Universidade de Santiago, Spain)	Poster	36
Green synthesis of gold nanoparticles supported in nanocrystalline cellulose (AuNPs@CNCs) with catalytic activity		
Eduardo Ruiz-Hitzky (ICMM-CSIC, Spain)	Keynote	21
Advances in Clay-Based Bionanocomposite Functional Materials		
Sarah Scheffler (Centre de recherche Paul Pascal, France)	Oral	32
Nanocomposite piezoelectric fibers		
Alexander S. Shaplov (LIST, Luxembourg)	Keynote	22
Five approaches towards design of single-ion conducting poly(ionic liquid)s for safe all-solid-state Li batteries		
Liliana C. Tomé (Universidade NOVA de Lisboa, Portugal)	Invited	26
Two and Three-component longel Membranes for CO ₂ Separation Applications		
Cristina Vallés (National Graphene Institute, UK)	Invited	27
Mechanical reinforcement and multifunctionality in graphene/polymer nanocomposites		
Fangyuan Zheng (BCMaterials, Spain)	Oral	33
Photocatalytic PVDF/TiO ₂ :Au nanostars membranes for ciprofloxacin degradation in water remediation		

Nanoengineering next-generation energy materials, the case of CsPbBr₃ perovskite nanocrystals

Yehonadav Bekenstein

Emma Massasa, Sasha Khalfin, Noam Veber

Technion, Department of Materials Science and Engineering & The Solid-State Institute, Israel Institute of Technology

Bekenstein@technion.ac.il

New energy materials promise advantages in the fight for a greener future. New optoelectronic materials, Lead-halide perovskites present excellent efficiencies in photovoltaic and light-emitting applications. The physical properties contrast with recent experimental observations of high dynamic disorder, room temperature structural transformation, and questionable material stability. We study cesium lead halide compositions at the limit of the smallest crystals we can make to understand and better control them. Through synthetic engineering of nanocrystal's shape, we control quantum confinement of excitons with atomic precision (in 2D nanoplates) and achieve anisotropic emission (in 1D nanowires). We discovered a typical strain build-up in two-dimensional CsPbBr₃ perovskite nanobelts that results in a structural deformation when adsorbed on carbon substrates. The microstructure is indicative of buckled nanobelts and determined using orientation dark-field imaging (SODFI) technique developed for this project. This method enabled the collection of scattered electrons from solid angles and traced them back to the specific orientation of the crystal. Apparent emission was measured from the buckled nanobelt using cathodoluminescence, signifying tolerance to mechanical deformations of the electronic properties. If time permits, I will discuss new compositions within a double perovskites structure engineered to improve perovskites' infamous toxic-instable reputation.

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Figures

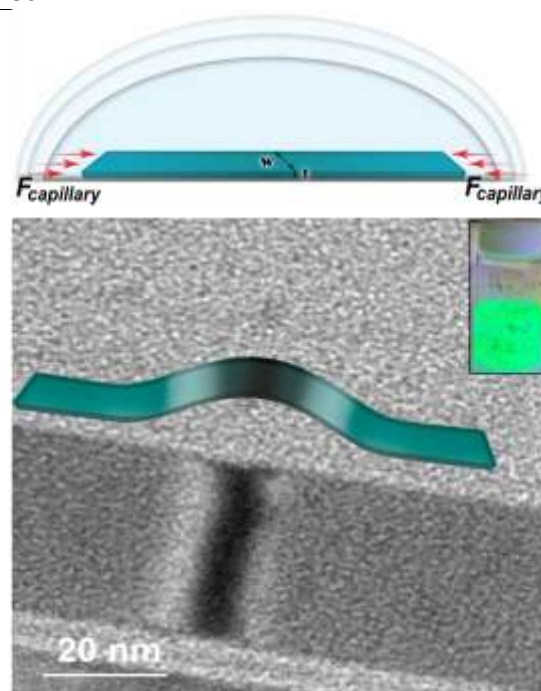


Figure 1: CsPbBr₃ colloidal nanobelts present bright emission. Adsorption on carbon substrates results in contrasts bands. Electron and force microscopy tools unravel a typical buckling structural deformation. Advancing perovskites into working technology warrant rational strain engineering.

Graphene and other 2D Material Multifunctional Composites

Ian Kinloch

University of Manchester, Manchester, UK
ian.kinloch@manchester.ac.uk

The intriguing physical properties of graphene and related materials make them ideal fillers in composites [1]. In particular, such 2D materials could enable multifunctional composites, where one obtains simultaneous benefits in mechanical reinforcement, electrical and thermal conductivity, gas barrier performance, corrosion control, anti-static properties, EMI shielding and/or structural health sensing.

Herein, we use model experimental systems to establish the design rules for atomically thin fillers with regard to the role of their diameter, thickness, chemical structure and interface [2,3,4]. We show these broad rules can apply to graphene, GNPS and TMDs. We also show that the ideal composite microstructure is highly dependent on the property being optimized, thus forcing compromises to be made in order to achievement multifunctionality.

We then transfer these rules to produce bulk composites using a range of matrices including thermoset, thermoplastic [6], elastomer [7] and inorganic [8] matrices. Particular promise is shown in hybrid composite systems where graphene is used in combination with conventional fillers.

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Cellulose responsive composites: control at the nanoscale

Anna Laromaine Sagué

Soledad Roig, Irene Antón-Sales, Anna Roig

*Institut Ciència de Materials de Barcelona,
Campus UAB, 08193 Bellaterra, Spain.)*

alaromaine@icmab.es

The need to provide eco-friendly materials to reduce costs and risks associated to waste echoes in many fields. In this context, raw materials of natural origin and in particular natural biopolymers like cellulose play an important role. Cellulose and nanocellulose-based materials have emerged as interesting candidates to industries, governments and consumers as green, sustainable and natural materials for the fabrication of advanced complex composites.

Additionally nanoparticles (NPs) offer the possibility to chemically and structurally tune their properties influencing how they interact with different materials.

The possibility to combine materials of raw origin, like cellulose, with nanoparticles open new avenues in the development of novel materials, which harness nanotechnology and nature.

In this context, we will present our latest development on novel stimuli responsive materials for a variety of applications based on bacterial cellulose, we will show a strategy to create multifunctional bacterial cellulose laminate material with topographic confinement of several types of nanoparticles using microwave-assisted synthesis routes and taking advantage of the self-adhesion of the BC fibers upon drying. This approach allowed us to create new functional materials on demand.

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Figures



Figure 1: Bacterial cellulose films and its responsive nanocomposites.

Advances in Clay-Based Bionanocomposite Functional Materials

Eduardo Ruiz-Hitzky

M. Mar González del Campo, Bernd Wicklein, Raquel Martín Sampedro, Cristina Ruiz-García¹, Margarita Darder & Pilar Aranda

Materials Science Institute of Madrid, CSIC, c/Sor Juana Inés de la Cruz 3, 28049 Madrid (Spain)

¹Present address: POR2E Group, CEMHTI (UPR 3079) CNRS-Université d'Orléans (France)

eduardo@icmm.csic.es

Abstract

This communication will introduce an overview on recent works, mainly developed in our Group, concerning functional composites based on the assembly of clay minerals to biopolymers. Clay Minerals are natural or synthetic silicates showing structural arrangement and morphologies typically of 2D phyllosilicates, which can be present as nanoplatelets (e.g. montmorillonite), nanofibers (e.g. sepiolite, palygorskite) or nanotubes (e.g. imogolite, halloysite). They can act as reinforcing charges of the involved polymer matrices as well as nanoparticles affording functional properties to the resulting hybrid materials. Recent examples of clay-based bionanocomposites incorporating diverse polysaccharides, including nanocellulose, will be here introduced emphasizing on their properties as biocompatible and biodegradable materials, showing interest as bioplastics and as fire-resistant composites. These composites can be considered as advanced eco-materials including applications as diverse as the removal of pollutants from wastewater, electrode materials and sensing agents for electrochemical and electroanalytical devices and, viral particles immobilization for adjuvants of vaccines, etc. [1-3]. A paradigmatic example consists in the development of nanostructured clay-based

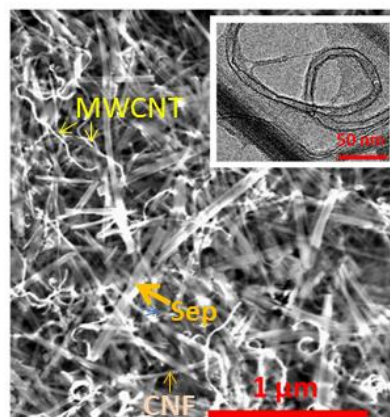


Figure 1: FE-SEM image of sepiolite (Sep), cellulose nanofibers (CNF) and MWCNT bionanocomposite [3]

carbonaceous materials containing carbon nanotubes and graphenes assembled to smectite and fibrous clay silicates, which appears of great interest for applications as improving components of electrochemical devices [4-5].

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Five approaches towards design of single-ion conducting poly(ionic liquid)s for safe all-solid-state Li batteries

A.S. Shaplov^a

E.I. Lozinskaya^b, G. Lingua^c and C. Gerbaldi^c

^aLuxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362 Esch-sur-Alzette, Luxembourg

^bA.N. Nesmeyanov Institute of Organoelement Compounds Russian Academy of Sciences (INEOS RAS), Vavilov str. 28, 119991, Moscow, Russia

^cGAME Lab, Department of Applied Science and Technology (DISAT), Politecnico di Torino, Torino 10129, Italy

alexander.shaplov@list.lu

The development of safe, efficient solid-state lithium batteries requires polymer electrolytes with high ionic conductivity ($>10^{-5}$ S cm⁻¹ at 25 °C) as well as good electrochemical and thermal stabilities. Among promising candidates, a new class of polyelectrolytes, namely poly(ionic liquid)s (PILs), has recently gained significant attention. PILs can be considered as the macromolecular analogs of ionic liquids (ILs), in the best cases combining the advantages of polymers (viscoelasticity, processability, film-forming properties, etc.) and ILs (high thermal and electrochemical stabilities, enhanced ionic conductivity, etc.). In this work, five approaches for the design and preparation of novel anionic PILs or "polymeric single-ion conductors" and their testing in Li batteries will be presented.

I. First approach consists in synthesis of **block copolymers** via RAFT polymerization. Such copolymers comprise poly(lithium 1-[3-(methacryloyloxy)propylsulfonyl]-1-(trifluoromethylsulfonyl)imide) (poly**LiM**) and poly(ethylene glycol) methyl ether methacrylate (poly**PEGM**) blocks. The "best" obtained PIL shows $T_g = -61^\circ\text{C}$, ionic conductivity of 2.3×10^{-6} (25°C) S/cm, electrochemical stability (ESW) of 4.5 V vs Li⁺/Li and lithium-ion transference number $t_{\text{Li}^+} = 0.83$.

II. Second approach deals with the synthesis of **triblock copolymers** by RAFT polymerization of **LiM** using PEG-based

macroRAFT agents. This method provided solid PILs as self-standing films with $T_g = -55 \pm 7^\circ\text{C}$, $\sigma = 4.4 \times 10^{-10} \div 3.4 \times 10^{-8}$ (25°C) and 10^{-4} (70°C) S/cm, $t_{\text{Li}^+} = 0.91$ and ESW = 4.0V vs Li⁺/Li.

III. Third method utilizes free radical copolymerization of anionic monomers with PEGM for the preparation of **random copolymers** showing $T_g = -56 \div -50^\circ\text{C}$, conductivity of 1.8×10^{-6} (25°C) S/cm, ESW = 4.2 V vs Li⁺/Li and $t_{\text{Li}^+} = 0.91$.

IV. Fourth approach involves **network formation** via copolymerization of **LiM**, PEGM and bifunctional dimethacrylate in the presence of propylene carbonate as plasticizer. This allows to achieve the formation of solid films demonstrating conductivity of 10^{-4} S/cm (25°C), ESW = 5.5 V vs Li⁺/Li and $t_{\text{Li}^+} = 0.86$.

V. Fifth approach applies combination of ring opening polymerization of trimethylene carbonate by RAFT-agent with terminal hydroxyl group and further utilization of such macro-RAFT in RAFT copolymerization of **LiM** and PEGM. In these **block copolymers** one block is responsible for ionic conductivity (2.9×10^{-7} (25°C)), while the second block - for improved mechanical properties and outstanding electrochemical stability (ESW > 4.8V vs Li⁺/Li) [1].

This work was in part supported by Russian Science Foundation (grant # 21-13-00173).

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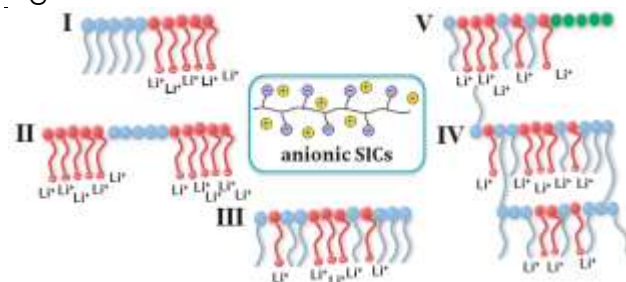


Figure 1: Five approaches for design of PILs.

Use of Clay-Based Bionanocomposites as Drug Delivery Systems

Pilar Aranda

Ediana P. Rebitski, Lorenzo Lisuzzo¹, Bernd Wicklein, Margarita Darder & Eduardo Ruiz-Hitzky

Materials Science Institute of Madrid, CSIC, c/Sor Juana Inés de la Cruz 3, 28049 Madrid (Spain)

Present address: ¹University of Palermo (Italy)

pilar.aranda@csic.es

Abstract

Clay-based bionanocomposite materials attract much research for numerous applications ranging from bioplastics in food-packaging to uses in biomedicine [1]. In this last research field, biopolymers are relevant components that combined with clays of diverse structure, in which bioactive species are previously incorporated, may produce materials of interest as drug delivery systems (DDS) [2]. In these DDS the clay component can be a layered (e.g. smectites) or a fibrous silicate (sepiolite & palygorskite), a tubular container, as it is in the case of halloysite, or layered double hydroxides (LDH), also known as anionic clays. The biopolymeric counterpart is frequently a polysaccharide, as for instance alginate, though proteins can also be used. The association of clays and biopolymers attempts to combine the advantages offered by each of them to produce more efficient and even targeted DDS. In this context, the present communication will introduce various examples of DDS based on the assembly of clay minerals to biopolymers, developed in our Group, addressed to illustrate the relevance and potential of bionanocomposites in biomedicine. For instance, the incorporation of gentamicin intercalated in montmorillonite into a hydrophilic biopolymer, e.g., hydroxypropylmethyl cellulose, may contribute to increase

mechanical and other properties of the polymer matrix. Similarly, the bioactive component can be incorporated in the lumen of halloysite nanotubes that can be further assembled to sepiolite and cellulose nanofibers to produce bionanocomposite films for wound dressing applications [3]. The combination of biopolymers of opposite wetting behaviour, for instance alginate and zein, allows the production of bionanocomposite beads with controllable speed of release for oral administration of ibuprofen intercalated into a LDH [4]. Moreover, the possibility to produce core-shell beads combining biopolymers has been applied to prepare bionanocomposite systems that combine pectin and chitosan biopolymers to target the oral administration of mesalazine or metformin drug in the intestinal tract [5,6].

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Mixed Ionic-Electronic Composites based on Poly(3,4-ethylenedioxythiophene) and Organic Ionic Plastic Crystals

Nerea Casado

S. Zendegi, R. del Olmo, M. Forsyth

POLYMAT, University of the Basque Country UPV/EHU, Joxe Mari Korta Center, Ave. Tolosa 72, 20018 Donostia-San Sebastián, Spain)

nerea.casado@ehu.eus

Mixed ionic and electronic conduction plays a key role in energy storage systems (ESS) such as fuel cells, batteries and supercapacitors [1]. The operating mechanism of these devices involves the concomitant processes of ion conduction along with the electron transfer, which determines the efficiency of the device. Mixed ionic-electronic conductors (MIECs) are potentially ideal additives for electrodes to provide that electron conduction together with the ionic conductivity, which makes possible the transport of the ions through the electrode.

In this presentation, we will present mixed ionic-electronic conducting materials based on the conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) and Organic Ionic Plastic Crystals. Nowadays, PEDOT is the most used conducting polymer due to its high electronic conductivity, stability and easy processing. On the other hand, OIPCs consist of an organic cation and anion pairs that have regular crystal structures in the solid state. One or both ions in the crystal can exhibit translational motions, which allow the material to flow under stress. These motions provide OIPCs of multiple solid-solid phase transitions and plastic mechanical properties, which are highly desirable in electrochemical devices to improve the poor contact between the electrode and electrolyte and facilitate ion diffusion [2].

In this talk, we will present the development of MIEC composites, together with their structural, and electrochemical characterization, as well as their application in energy storage systems. It will also be shown the synergy created in the composites to improve the intrinsic properties of the individual components [3,4].

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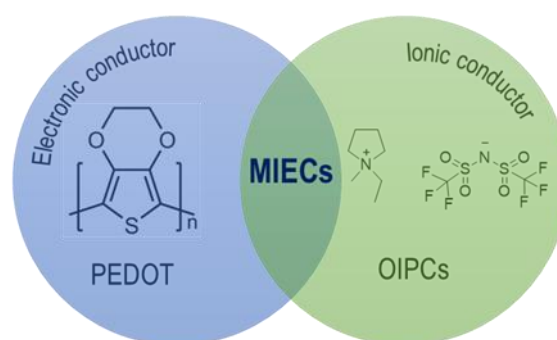


Figure 1: Representation of Mixed Ionic Electronic Conducting (MIEC) composite materials

Nanomodified reshapeable, repairable and recyclable epoxy resin for conducting composite materials

Alaitz Rekondo

Arrate Huegun

CIDETEC, Basque Research and Technology Alliance (BRTA), Po. Miramón 196, 20014 Donostia-San Sebastián, Spain

arekondo@cidetec.es

Thermoset resins due to their high thermal stability, good rigidity, hardness and resistance to creep and solvents are the most widely used resins in fibre reinforced composite manufacturing. In addition, epoxy resin systems provide strong adhesive properties, chemical resistance and toughness as well. But a traditional thermoset composite cannot be reshaped, repaired neither recycled due to its permanently cross-linked structure. To overcome such limitations, a novel 3R (Reshape-able, Repair-able and Recyclable) epoxy matrix was developed by Odriozola et al. which is based on dynamic covalent bonds (Figure 1)¹. The 3R epoxy resin offers mechanical properties equivalent to traditional epoxy counterpart, but additionally presents: (i) good reprocessability of postcured composites by thermoforming, (ii) reparability of delamination and micro-cracks by applying heat and pressure in the damaged part, and (iii) recyclability by matrix chemical dissolution with specific reagents or by grinding and mechanical processing into second generation composites.

The aim of this work is to develop a novel 3R epoxy resin with enhance thermal conductivity to be implemented in thermoelectric generation (TEG) enabled composites within HARVEST project (www.harvest-project.eu)². As any typically polymer resin, 3R system is a good thermal insulator and presents very low thermal conductivity. Therefore, here the addition of nanoparticles such as carbon nanotubes (CNT) and carbon black (CB) into the resin

has been explored in order to facilitate the heat transportation in the system.

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Figures

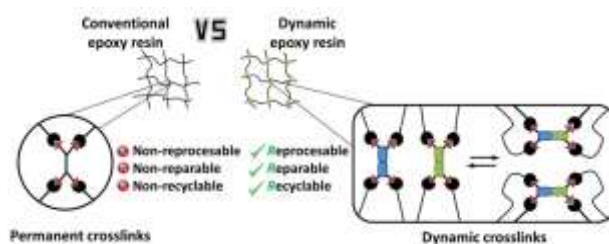


Figure 1: Schematic representation of a conventional thermoset resin network vs the dynamic thermoset network

Two and Three-component Iongel Membranes for CO₂ Separation Applications

Liliana C. Tomé

LAQV-REQUIMTE, Department of Chemistry,
NOVA School of Science and Technology,
Universidade NOVA de Lisboa, 2829-516
Caparica, Portugal.

liliana.tome@fct.unl.pt

Ionic liquids (ILs) have undoubtedly found their place as new functional materials. In particular, and due to their remarkable CO₂ affinity, as well as tuneable nature, there has been a growing interest in the exploitation of IL-based materials for CO₂ separation membranes [1]. In this context, the development of iongel membranes, with a high IL content (>60 wt%) is a promising strategy to obtain high gas separation performances, while at the same time overcome the stability issues reported for supported IL membranes or the limitation in the IL/polymer composition of poly(ionic liquid)-based membranes.

In this communication, two and three-component iongel membranes consisted of a cross-linked polymer network (PEGDA), ionic liquids (ILs), and azo-linked porous organic polymers (azo-POPs) will be presented [2-3]. The membranes were prepared by UV-initiated free radical polymerization. The compatibility and miscibility of the polymer network, different ILs and azo-POPs were evaluated. The obtained cross-linked iongel membranes were characterized in terms of structural, thermal, mechanical and morphological properties. Gas permeation experiments were also performed and the results were compared to the Robeson's upper bound limits.

The aim is to show the versatility of these materials, point up their easy preparation, and reveal insights into the relationships between gas transport properties, IL structures, diverse azo-POPs and iongel

compositions. Breakthroughs and key challenges will be discussed, as well as possible paths for future research.

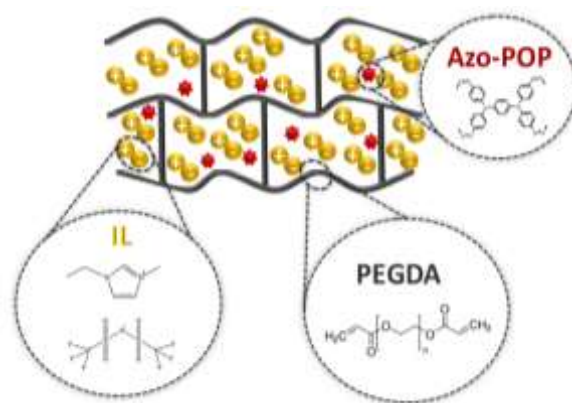


Figure 1 Schematic representation of a three-component mixed matrix membrane consisting of poly(ethylene glycol) diacrylate (PEGDA), ionic liquid (IL), and azo-linked porous organic polymer (azo-POP).

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Mechanical reinforcement and multifunctionality in graphene/polymer nanocomposites

Cristina Vallés

Ian Kinloch, Robert J. Young

Department of Materials and National Graphene Institute, University of Manchester, Oxford Road, Manchester M13 9PL, UK

cristina.valles@manchester.ac.uk

Graphene-related materials (GRMs) are of particular interest to the field of polymer composites due to GRMs' exceptional mechanical, electrical and thermal properties.

In order to achieve their potential as mechanical reinforcement, good dispersions of the flakes in the polymer matrix and strong interfaces between both components are required. Gong et al. [1] used Raman spectroscopy to monitor the stress transfer efficiency of the graphene/polymer interface, finding that this interface is weak, and the stress transfer between polymer and graphene depends on both the aspect ratio of the graphene flake and the interfacial stress transfer efficiency (i.e. the degree of interaction between graphene and polymer matrix). Relatively large graphene flakes (>20 μm) will be thus needed before efficient reinforcement can take place in an unfunctionalized graphene/polymer composite [2, 3]. Alternatively, chemical modification of the graphene flakes may significantly strengthen the interface between graphene and polymer, reducing the critical length and increasing the interfacial stress transfer efficiency [4, 5]. This paper will show how GRMs of different nature (which includes unfunctionalized graphene, graphene oxide and polymer grafted graphene) lead to different levels of dispersion and different filler/polymer interfaces, which will determine the final mechanical and thermal properties of the composites.

In addition to mechanical and thermal reinforcement, GRMs are recently raising an

enormous interest to provide a polymer with additional functionality, such as electrical conductivity or electromagnetic interference (EMI) shielding properties, leading to multifunctional polymer nanocomposites with great potential for a wider range of technological applications. For example, we have recently demonstrated that above the critical loading the electrically conducting networks of GNPs formed in an epoxy matrix shows the ability to act as integrated nanoheaters when an electric current is passed through them, successfully curing the composites by a simple Joule heating. This emerges as a promising route for Out-of-Autoclave in-situ thermoset curing method with promise to replace the conventional processing methods [6].

Furthermore, electrically conductive GRMs can also provide a composite structure with outstanding EMI shielding performances. We have recently found that the EMI shielding performance of graphene-based composite structures can be easily tuned by varying the nature and electrical properties of the graphene employed [7], opening the door to applications of composite materials in the communications, medical, aerospace and electronics sectors, where it is vital to isolate the electromagnetic radiation emitted from electronic equipment.

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Biobased epoxy vitrimer for reprocessable composites

Miren Blanco¹

Cristina Monteserin¹, Nerea Uranga¹, Jose Manuel Laza², Jose Luis Vilas²

¹Tekniker, Iñaki Goenaga nº5, Eibar, Spain

²UPV/EHU, B. Sarriena, s/n Leioa, Spain

miren.blanco@tekniker.es

Vitrimers are a class of plastics, which are derived from thermosetting polymers (thermosets), but can be reprocessed, or recycled via network topology rearrangement through exchange reaction of the dynamic covalent bonds under external stimulus such as heat, pH, and UV light. There are different types of dynamic bonds such as disulfide, imine, or urethanes [1-2].

Epoxy vitrimers are being widely analyzed for developing fiber reinforced composites, but most of the explored epoxy vitrimers were still prepared from non-renewable and toxic DGEBA. [3]

In this study, a biobased epoxy vitrimer with dynamic Schiff based groups (imine bond) has been synthesized by reacting epoxidized oils, with a dynamic hardener obtained by reacting biodegradable vanillin (VAN), with 4,4'-diaminediphenylmethane (DAM). Two different biobased biodegradable epoxidized oils, soybean, and rapeseed oil, have been tested, to relate their chemical structure with the final properties of the vitrimers.

The synthesis of the dynamic hardener (VSB) has been carried out by dissolving the starting compounds VAN and DAM in methanol (MeOH) and heating the mixture at 65°C for 7h. After the time elapsed, the mixture was filtered and dried in the oven. The successful synthesis of the dynamic hardener has been checked by Proton nuclear magnetic resonance (NMR), Fourier transform infrared (FTIR), Differential scanning calorimeter (DSC) and thermogravimetry (TGA). For the preparation of the epoxy-amine system,

the VSB was mixed with the epoxidized oils. The curing process was carried out at 190°C for 2h under 10MPa pressure. The characterization of the vitrimers has been carried out by DSC, TGA or Dynamic Mechanical Analysis (DMA). The soybean based vitrimer and the rapeseed oil based vitrimer presented a Tg around 50 and 90 °C, respectively and a degradation temperature higher than 350 °C in both cases. The reprocess ability and self-healing capacity of the vitrimers have been also tested in a hot plate press.

Obtained vitrimers presented good solvent stability and good reprocess ability until 20 cycles, making them very interesting compounds for composite preparation.

Once the vitrimer was synthesized, the preparation of the composite was carried out. Two different composites have been synthesized, one based on glass fibers and the other based on linen fibers.

The new vitrimer thermosets will allow not only reprocess the composites at high temperatures, but also, recycling the cured composites by a simple chemical treatment to separate fibers from vitrimer, thus allowing the recovery of fibers and resins of end-of-life composites.

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Challenges to the evaluation of the emerging risks concerning Nanocomposites – LightMe case study

Cristina Matos

Rita Alberto, Gabriel Carmona-Aparício

ISQ, Taguspark, Oeiras, Portugal

mcmatos@isq.pt

LightMe is a European research project that will aspire to be a point of reference for boosting innovation for the introduction of new functionalities, features and capabilities in the field of lightweight metal matrix nanocomposites. The results are innovative nano reinforced metal matrix composites, produced by Casting methods, Additive Manufacturing and Spark Plasma Sintering, exhibiting advance properties and/or multifunctionality.

The properties of nanomaterials (NMs) differ from those of their micro and macro homologous substances (bulk). These differences result from the specific physical and chemical characteristics of NMs, and which will lead to the uncertainties regarding their behaviour when interacting with the human body or the environment. Whilst NMs are becoming a promising application and has the potential to grow much more, their associated health and environmental risks still remain far from being known.

In this presentation, we will explore the latest developments in the field of risk assessment for nanocomposites, including the legal and standardisation frameworks linked to their production and use, with the aim to clarify the current knowledge on nanosafety aspects. Using the LightMe project as a case study, we also intend to highlight the challenges arising from the lack of data on hazards and the subsequent risks within the scope of this emerging technology and contribute to research and propose solutions to overcome them.

Whilst the fundamental approach to conducting risk assessment (RA) of emerging technologies, such as nanocomposites, is similar to that of existing technologies, the former pose additional challenges. For

example, NMs as any chemical, are regulated by the registration evaluation authorization and restriction of chemicals (REACH) which require a chemical safety assessment (CSA) [1]. However, key information required for this process, such as dose-response data for the hazard identification, is in many cases inexistent [2]. This is because, in most cases, existing test guidelines and guidance documents applied to bulk materials need to be adapted. Some international bodies (ISO, OECD, ECHA) are working on to provide more generalized guidance, but there are still issues related onto how to adapt standards and guidelines to the unique properties of NMs and their sectors of application [3].

Specifically, within the LightMe project will been carried out monitoring activities at distinct industrial scenarios (particle concentration and size distribution), exposure assessment analyses that will determine the release, and transfer to receptor of MNs, and analysis/application of RA tools in order to overcome the current lack of information for determining the hazards and levels of exposure to health and environment.

The LightMe project aim to produce recommendations to improve key guidance, regarding chemical safety and exposure assessment of NMs, applicable to the industrial sector and to comply with regulations (e.g. REACH).

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New trends in development of highly conductive poly(ionic liquid)s

D.R. Nosov^a

L.F. Lepre^b, A.S. Shaplov^a and E. Drockenmüller^b

^aLuxembourg Institute of Science and Technology (LIST), 5 avenue des Hauts-Fourneaux, L-4362 Esch-sur-Alzette, Luxembourg

^bUniv Lyon, Université Lyon 1, CNRS, Ingénierie des Matériaux Polymères, UMR 5223, F-69003, Lyon, France

daniil.nosov@list.lu

The achievement of high ionic conductivity in poly(ionic liquid)s (PILs) is of great interest as all-solid-state electrolytes are becoming increasingly popular due to their processability, viscoelasticity and extreme safety. Although attempts to enhance the ionic conductivity of PILs applying various approaches have been made previously, the influence of the repeat unit charge density (Fig.1, I) and the nature of the cation's substitutes (Fig.1, II) on the bulk conductivity of PILs has been scarcely addressed [1].

To date the maximum number of ion pairs per monomer unit reported to date is three and the structure/conductivity relationships remain sometimes contradictory [2]. To fill this gap eight poly(ionic liquids)s were synthesised and structure/property correlations were established. The different repeat units contain one to four ion pairs, with one to four bis(trifluorosulfonyl)imide (TFSI) anions and one or two types of ammonium, imidazolium or 1,2,3-triazolium counter-cation. Generally, the higher the repeat unit charge density of PILs the higher their T_g and the lower their ionic conductivity and thermal stability. The observed dependences passed through a maximum when PILs had two cations per monomer unit that were separated by alkyl or oxyethylene chains. The highest conductivity ($1.8 \times 10^{-5} \text{ S cm}^{-1}$ at 25°C) was reached when PILs contain two 1,2,3-triazolium cations that are separated by an oxyethylene spacer.

The presence of the oxyethylene fragments in the backbone or in the side chains of PILs significantly improves the solubility of ionic species, facilitates their

dissociation, and promotes an increase in the conductivity of PILs [1]. Thus, in the second approach (Fig. 1, II) the PEO based polymers were chosen to undergo quaternization reaction and to form novel class of cationic PILs [3]. Eight different substitutes were selected to form the side chain in PILs: from alkyl and silyl, to siloxane and perfluorinated groups. As a result, almost all PILs with alkyl side chains showed lower T_g values and higher ionic conductivities in comparison with PILs bearing silyl-containing and fluorinated chains. The highest conductivity ($7.3 \times 10^{-6} \text{ S cm}^{-1}$ at 25°C) was reached in PIL with ethyl side chain.

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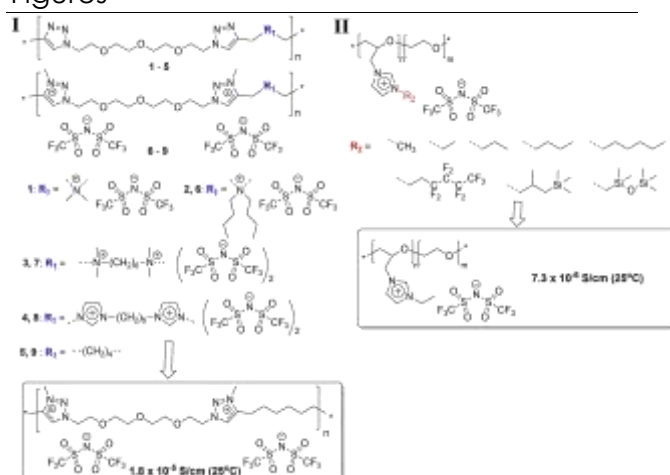


Figure 1: PILs prepared in this work.

Silk Fibroin composites for next generation of sustainable smart materials development

Ander Reizabal, C. M. Costa, Leyre Pérez, Jose-Luis Vilas, S. Lanceros-Mendez

- BCMaterials, s/n, Edif. Martina Casiano, Pl. 3
Parque Científico UPV/EHU Barrio Sarriena,
48940 Leioa, Bizkaia, España

- Departamento de Química Física, Facultad de
Ciencia y Tecnología, Universidad del País
Vasco/EHU, Apdo. 644, Bilbao, Spain

ander.reizabal@bcmaterials.net

Materials development supports the growth of new tools to meet social and technological challenges. Among the different materials, plastics are essential, and practically omnipresent because their properties, accessibility, and low cost. Unfortunately, plastics are synthesized from oil, and they tend to accumulate in nature, which represents a serious environmental impact. To minimize these injuries, replacing synthetic polymers (plastics) by bio-based materials is proposed. Unfortunately, the knowledge about these materials and how to modify them is still limited.

To boost the knowledge about bio-based materials and promote their use, the present work has focused on, the development of sustainable materials with advanced properties. In specific, Silk Fibroin (SF), a protein obtained from *Bombyx mori* (silkworm) cocoons has been selected as primary material. Mainly because its unique properties (such as piezoelectricity, mechanical resistance, and water processability) and accessibility. As a route for pushing the SF properties beyond its current limits, composite materials processing has been explored.

Based on SF potentiality, one main field of application has been selected: active composites for electronics. In this regard, SF has been combined with i) carbon nanotubes (CNT) to obtain force sensors with piezoresistive response (PR) of $\sim 4 \text{ MPa}^{-1}$ at pressures of 0.11 MPa ; ii) with silver nanowires (SNW) to obtain transparent sensors with a PR of 26 GPa^{-1} when the

pressure is between 0.2 and 0.4 MPa . A material also capable of producing energy; iii) with cobalt ferrite nanoparticles (CFO) to obtain magnetic actuators with a magnetization value of $\sim 10 \text{ emu g}^{-1}$ and coercivity of almost 4 kOe , (20 wt. \% CFO); iv) with ionic liquids (IL) to obtain bending actuators with bending responses of ~ 0.5 by applying low voltages ($3\text{--}5 \text{ V}$); and v) finally, with ceramic barium titanate (BaTiO_3) nanoparticles, to obtain capacitors with a dielectric constant up to 142 for the SF/BaTiO_3 composite with 40 wt \% .

The current work is presented as a general overview of different composites development to control the SF properties, and applicability. The developed different demonstrators representing a proof of concept about the bio-based materials and composites potentiality. This work, pretending to be a reference for future research.

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Figures



Figure 1: Scheme of SF nanocomposites for smart materials development.

Nanocomposite piezoelectric fibers

Scheffler Sarah

Wilfrid Neri, Jinkai Yuan, Philippe Poulin

*Centre de recherche Paul Pascal, 115 Avenue
Albert Schweitzer, 33600 Pessac, France*

sarah.scheffler@crpp.cnrs.fr

Piezoelectric conversion of mechanical vibrations into electrical energy is a promising approach to power embedded electronics and to develop new sensing technologies. Conventional piezoelectric materials are usually under the form of thin films or brittle crystals. Having piezoelectric materials under the form of flexible fibers would allow their implementation in smart textiles and new functional structures.

Inorganic fibers have good piezoelectric properties but are highly brittle. Organic polymer fibers are flexible but do not yet compete with inorganic materials in terms of piezoelectric efficiency. Here we present a new generation of nanocomposite fibers that combine the deformability and robustness of polymers and the high piezoelectric properties of inorganic nanoparticles. We use poly(vinyl alcohol) (PVA) as polymer because of its good mechanical properties and spinnability. The nanocomposite fibers are spun by a wet-spinning process and loaded with ZnO or BaTiO₃ piezoelectric nanorods. The anisotropic shape of the particles is used to promote the mechanical stress transfer from the PVA matrix to the piezoelectric particles.^[1] We present how the fibers can be assembled into flexible films and their first electromechanical characterizations.

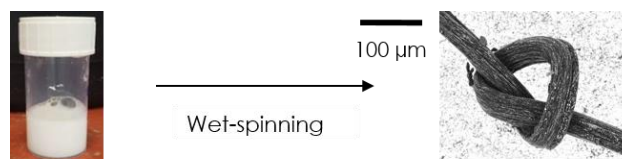


Figure 1: From nanoparticle suspensions to nanocomposite piezoelectric fibers (SEM photography).

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Figures

Photocatalytic PVDF/TiO₂:Au nanostars membranes for ciprofloxacin degradation in water remediation

Fangyuan Zheng¹

Pedro M. Martins^{2,3}, Senentxu Lanceros-Méndez^{1,4}, Javier Reguera¹

¹BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain

²Centre of Molecular and Environmental Biology (CBMA), Universidade do Minho, Braga 4710-057, Portugal

³IB-S e Institute for Research and Innovation on Bio-Sustainability, University of Minho, 4710-057, Braga, Portugal

⁴IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain

fangyuan.zheng@bcmaterials.net

Abstract

Photocatalysis has been considered as one of the most promising technologies for wastewater treatment because it is cost-less, eco-friendly and efficient in the removal of recalcitrant contaminants [1]. Titanium dioxide (TiO₂) is one of the most used photocatalysts due to its remarkable properties. However, its applicability is limited by its wide bandgap (3.0–3.2 eV) which results in poor efficiency upon visible light irradiation [1,2]. Although many works use the spherical Au nanoparticles to overcome this limitation, the absorption wavelength is still limited in the 500–550 nm [1]. On the other hand, the reuse and recovery of photocatalysts to avoid the possible secondary pollution coming from the nanoparticles are also a significant challenge [2]. Herein, we developed polymer (PVDF) highly porous membranes that incorporate nanocatalysts of TiO₂:Au with a branched morphology (TiO₂:Au-NSs) that make use of all the visible light spectrum to efficiently reuse for water treatment in the antibiotic ciprofloxacin degradation.

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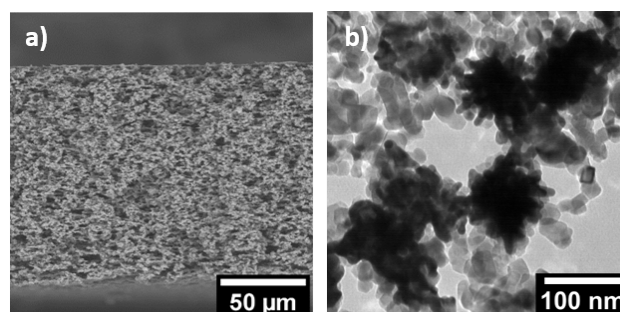


Figure 1: a) SEM image of PVDF-HFP membrane section. b) TEM image of TiO₂:Au-NSs

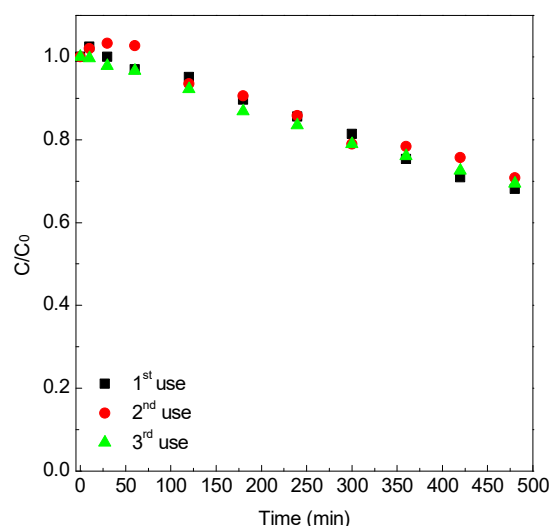


Figure 2: Reusability study of PVDF-HFP membrane containing 10% TiO₂:Au-NSs in ciprofloxacin degradation under visible light.

Magnetorheological elastomers as multifunctional materials for smart devices and applications

A. García Díez¹

C. Rial Tubio¹, A. Gómez², J. Berasategi², J. Gutiérrez Etxebarria^{1,3}, M. Mounir Bou-Ali², S. Lanceros-Méndez^{1,4}

¹ BCMaterials, UPV/EHU Science Park, Leioa, Spain

² Mondragon University, Loramendi 4, Arrasate-Mondragon, Spain

³ UPV/EHU, Barrio Sarriena s/n, Leioa, Spain

⁴ Ikerbasque, Bilbao, Spain

ander.garcia@bcmaterials.net

Abstract

Magnetorheological elastomers (MREs) are active materials composed of a polymeric matrix and an inorganic magnetic filler [1], with rheological and mechanical characteristics that can be actuated using a magnetic field. Typically, the inorganic component is a soft magnetic material with high saturation magnetization, so that switching between rheological states is achieved rapidly [2]. In this work, we explored the effect of different nanosized fillers (CoFe_2O_4 , Fe_3O_4 , Co, Ni and $\text{Ni}_{80}\text{Fe}_{17}\text{Mo}_3$) with distinct magnetic properties on the structural, magnetic, thermal, mechanical, and magnetorheological properties of MREs based on styrene-ethylene-butylene-styrene (SEBS) thermoplastic elastomer. The structure of the polymer does not significantly vary when the particles are included, and they distribute uniformly with the polymer matrix, showing an homogeneous distribution of small clusters (Figure 1a). A maximum saturation magnetization of $17.8 \text{ Am}^2/\text{kg}$ is achieved for magnetite (Fe_3O_4) based composite (Figure 1b). All samples retain the magnetic behaviour (in terms of magnetic hardness) of the pure nanofillers, indicating good compatibility with the matrix. The thermal properties of the polymer show a slight increase in the degradation temperature with the inclusion of the magnetic fillers (Figure 1c). The elastic modulus increases by at least a factor of 2,

from 0.7 MPa of the SEBS to a maximum of 1.8 MPa in the case of the sample with Fe_3O_4 nanoparticles (Figure 1d). Regarding the magnetorheology, the samples respond to the magnetic field by increasing their storage modulus, while the loss modulus remains almost unaltered. Further, it has been determined that the particles with higher saturation magnetization and lower coercivity are more appropriate in terms of enhancing the magnetorheological effect (Figure 1e). This study helps finding the most adequate nanofillers to fabricate MREs, with the advantage that these nanoparticles can be tuned with different sizes, shapes, orientations, differently from the traditionally used microparticles.

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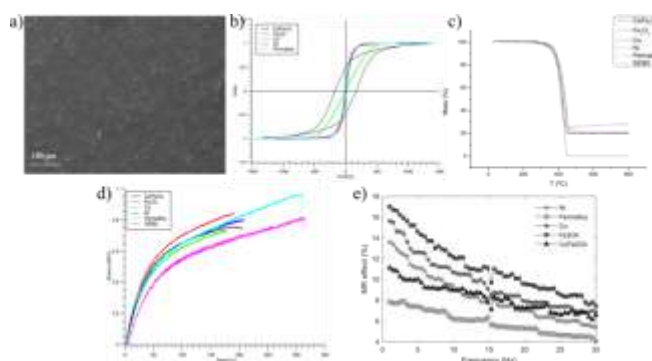


Figure 1: a) SEM image of the CoFe_2O_4 @ SEBS composite. b) Magnetic properties measured by VSM. c) TGA curves of the composites. d) Mechanical properties of the samples. e) Magnetorheological effect of the prepared composites.

Carbon based materials in epoxy resin composites for self-heating applications

Pedro Garcés

C. Mocan¹, O. Galao¹, I. Martín Gullón², B. Del Moral¹, F.J. Baeza¹, E. Zornoza¹, B. Calderón², I. Rodríguez², N. Arnaiz², M.D. Romero Sánchez².

¹ Dept. of Civil Engineering. University of Alicante. Carretera San Vicente, s/n. Alicante

² Applynano Solutions, S.L. Scientific Park of Alicante. Carretera San Vicente, s/n. Alicante

Contact@E-mail: pedro.garces@ua.es

Abstract

This research studies the feasibility of an epoxy resin composite incorporating carbon based materials as a self-heating material for preventing ice-formation and de-icing applications (automotive, aeronautic and wind energy sectors). Carbon based materials may provide electrical conductivity when incorporated to polymeric matrices (i.e. epoxy resins, typically insulating materials) and are responsible of the Joule effect (the heat release of a material due to the movement of electrons when applying an electrical voltage), therefore providing materials with intelligent and self-responsiveness properties, such as self-heating.

In this work, self-heating capacity of epoxy resins containing carbon-based materials has been evaluated for preventing ice-formation and de-icing applications. Tests for characterization were carried out in laboratory conditions with fixed voltages of

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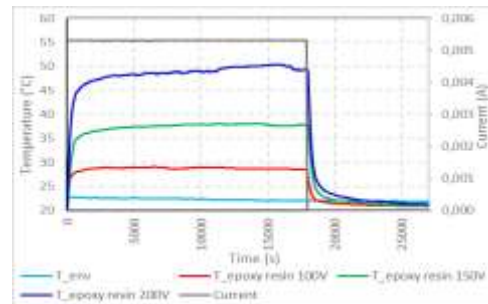


Figure 1. Laboratory conditions tests performed at different fixed voltages.

100, 150 and 200V DC. After that, prevention of ice-formation and de-icing tests were performed at -15 °C with a fixed voltage of 200 V DC. Results showed that carbon-based materials can increase the epoxy composites temperature up to 6.8 °C, 17.7 °C and 30 °C, respectively for the aforementioned voltages, in laboratory conditions, and up to 7.5 °C with an environmental temperature of -15 °C, and 200 V DC fixed voltage.

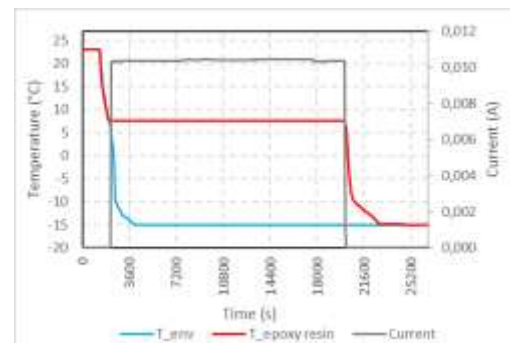


Figure 2. Ice-prevention test performed at 200V DC fixed voltage.

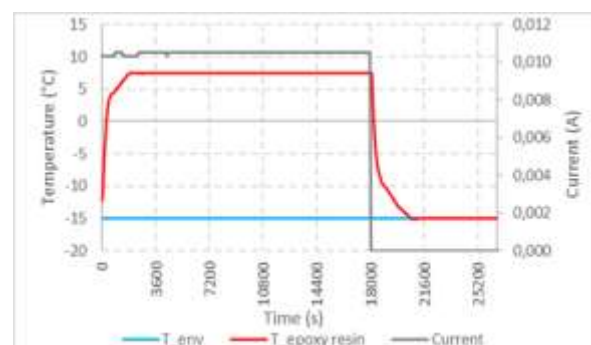


Figure 3. De-icing test performed at 200V DC fixed voltage.

Green synthesis of gold nanoparticles supported in nanocrystalline cellulose (AuNPs@CNCs) with catalytic activity

Eva Rodil¹

Laura Hernandez², Mandana Tavakolian²,
Nathalie Tufenkji²

¹CRETUS Institute, Department of Chemical Engineering, Universidade de Santiago de Compostela, Santiago de Compostela, Spain

²Department of Chemical Engineering, McGill University, Montreal, Quebec, Canada

Contact@E-mail eva.rodil@usc.es

Hairy nanocellulose functionalized with carboxylic groups, known as electrostatically stabilized nanocrystalline cellulose (CNC)¹, was used to facilitate the synthesis of gold nanoparticles (AuNP). The CNC was used as an AuNP support and, as a result, the AuNPs@CNC nanocomposites were formed through a cost-effective and easy method by UV radiation in a chamber. The nanocomposites were characterized by ultraviolet-visible spectroscopy (UV-vis), transmission electron microscopy (TEM), and x-ray photoelectron spectroscopy (XPS). The results indicate that size distribution and shape of the Au nanoparticles changes with radiation time, Au concentration and the carboxylic content of the CNC.

The catalytic activity of the nanocomposites was tested for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol with an excess amount of NaBH₄. Gold nanoparticles supported on CNC showed better catalytic activity and stability than other Au-nanocomposites previously reported^{2,3}. This green method contributes to undergoing efforts for sustainable development of nanomaterials.

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Figures

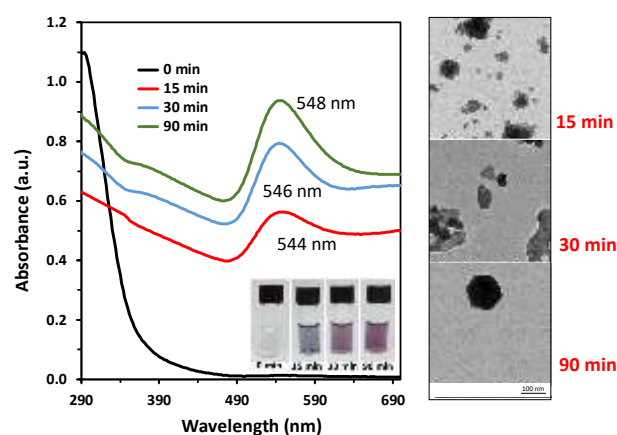


Figure 1: TEM Images and UV-vis absorption spectra of formed AuNPs@CNC nanocomposite after different UV radiation times with CNC (-COOH 6.1 mmol/g and hydrodynamic diameter 280 nm) and Au concentration of 0.25 mM HAuCl₄

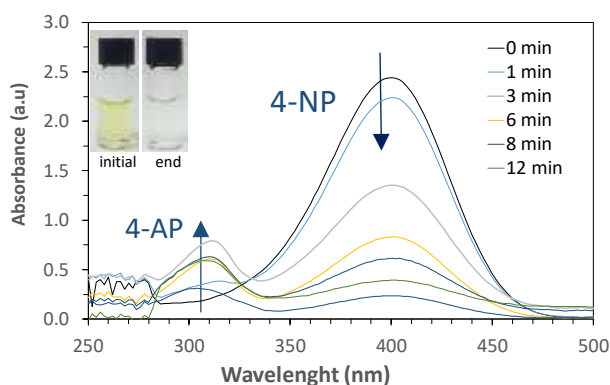


Figure 2: Time dependent UV-spectra for the reduction of 4-NP catalysed with the nanocomposite formed by 15 min uv radiation in a chamber, AuNPs(0.25mM)@CNC(-COOH 6.1 mmol/g and hydrodynamic diameter 280 nm), with an excess amount of NaBH₄ in aqueous media.

What it is 1



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... with opportunities for industrial, business and institutional development

2 Its objectives



Flagship Areas 3

Neurobiosciences



Quantum Technologies (QT)



NeutriOnics



High Performance Computing & Artificial Intelligence (HPC-AI)



4 Expected impact

Research personnel



+400

Publications



+4.000

EPO Patents



+30

Spin offs



+20

Turnover



+350 M€

Employment



+3.200

5 Governance

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Basque Foundation for Science

Recruitment and attraction of research personnel

Management of IKUR funds

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HEZKUNTZA SAILA



Fundación Biofisica Bizkaia
Biofisika Bizkaia Fundazioa

Neurobiosciences



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Materials Physics Center

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Scientific Direction of IKUR's Flagship Areas