# Book of Abstracts

# IN$^2$UB ANNUAL MEETING

Enric Casassas Lecture Hall
Physics and Chemistry Faculties
Universitat de Barcelona

▶ 6th June 2019

Institut de Nanociència
i Nanotecnologia

UNIVERSITAT DE
BARCELONA

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# Foreword

*Dear colleagues,*

*It constitutes an honor to welcome you to the IN²UB Annual Workshop 2019.*

*In the past year we have multiplied our efforts to foster the participation among members to the activities of the Institute and encourage mutual and multidisciplinary collaborations within the organization, conscious that our strength resides in this cooperation. This has crystallized into various collective achievements, such as the creation of a* ***Permanent Commission for Outreach of the IN²UB****, the deployment of a permanent series of* ***IN²UB International Research Seminars*** *or the organization of the forthcoming* ***IN²UB - Medicine Faculty Researchers Meeting****. In this context, the Institute has been able to grant six* ***Cooperative Research Grants*** *(ART), the highest annual amount so far.*

*This past and recent journey has brought us to the current* ***Annual Workshop****, which gathers the largest amount of communications presented so far in any of our workshops. This encouraging engagement by all of you must be interpreted as a sign that the IN²UB is in the right direction and stimulates us to pursue this path.*

*We are conscious of the current potential and strength of the Institute in its various facets; frontier research, teaching excellence and outreach. Recently, the IN²UB has been honored with the award of five "2018 ICREA Academia" prizes among its members, adding to those already awarded in the recent past. It is one of our goals to make sure that this value is recognized and rewarded at the national and international level, and this is one of our primary tasks.*

*The current workshop is an important step in this direction. It gives us the opportunity to learn first-hand information on the collaborative research conducted by the ART grantees, as well as on the projects conducted by all our members. It should constitute a useful opportunity to facilitate further interactions and scientific cooperation. This year we are honored with the presence of two well recognized guest scholars: ERC Grantee Dr. Gonzalo Abellán (Institute of Molecular Science, University of Valencia) and CINBIO Director Prof. Africa González-Fernández (University of Vigo). I thank them for accepting our invitation, all of you for this fantastic turn out and all those that have helped in the organization of this event, especially the members of the Direction team, Dr. Ifigènia Saborit and Dr. Albert Romano.*

*On behalf of the IN²UB, I wish that you enjoy and find this workshop useful.*

*Sincerely,*
**GUILLEM AROMÍ**

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### Plenary

### 2018-ART grantees

### Modeling, Simulation and Nanoscopic Methods (NanoMet)

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## Nanostructured materials (NanosMat)

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# Program

| | |
|---|---|
| **9:00h - 9:30h** | *Registration* |
| **9:30h - 9:45h** | *Welcome*<br>**GUILLEM AROMÍ**<br>*Director of Institute of Nanoscience and Nanotechnology (IN$^2$UB) / Department of Inorganic and Organic Chemistry, Faculty of Chemistry, Universitat de Barcelona (UB)*<br>*Opening*<br>**MERCÈ SEGARRA**<br>*IN2UB, Department of Materials Science and Physical Chemistry, Faculty of Chemistry, Vice-Dean of Research and Transfer of the Faculty of Chemistry of the Universitat de Barcelona (UB)* |
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| **10:45h - 11:10h** | *2018 Art Grantee (ART1)*<br>**Nanostructured Mo$_x$C/ZnO systems for photocatalytic hydrogen production**<br>**PAULINA R. MARTÍNEZ-ALANIS**<br>*IN$^2$UB, Department of Inorganic and Organic Chemistry, Inorganic Chemistry Section, UB* |
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| **12:35h - 13:00h** | *Oral 2 (O2)*<br>**Nonequilibrium self-assembly processes: Formation of meso- and nanostructures with applications to biology and material science**<br>**ANDRÉS ARANGO-RESTREPO**<br>*IN$^2$UB, Department of Condensed Matter Physics, Faculty of Physics, UB* |
| **13:00h - 13:20h** | *Oral 3 (O3)*<br>**Transport and assembly of colloids in liquid crystals**<br>**JOSEP Mª PAGÈS**<br>*IN$^2$UB, Department of Materials Science and Physical Chemistry, Faculty of Chemistry, UB* |
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| **15:00h - 16:00h** | *Plenary 2 (PL2)*<br>**Nanoscience: the future arrived**<br>**ÁFRICA GONZÁLEZ FERNÁNDEZ**<br>*Universidad de Vigo, Director of the Biomedical Research Center (CINBIO), President of the Spanish society for Immunology* |
| **16:00h - 16:25h** | *2018 Art Grantee (ART3)*<br>**Study of oxidation states in the amyloid-magnetite complex related with Alzheimer's disease**<br>**MONICA MIR[1] and LLUÍS LÓPEZ-CONESA[2]**<br>*[1]IN$^2$UB, Nanobioengineering Laboratory, IBEC, Department of Electronics and Biomedical Engineering, Faculty of Physics, UB*<br>*[2]IN$^2$UB, CCiTUB, Department of Electronics and Biomedical Engineering, Faculty of Physics, UB* |
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| **18:15h - 18:35h** | *Oral 6 (O6)*<br>**Iron oxide nanoparticles: From fabrication to bioapplications**<br>**CARLOS MOYA**<br>*IN$^2$UB, Department of Condensed Matter Physics, Faculty of Physics, UB* |
| **18:35h - 18:45h** | *Closing Remarks*<br>**ALBERT ROMANO**, *Secretary of IN$^2$UB, Department of Electronic and Biomedical Engineering, UB* |

# Invited Speakers

**Plenary Lectures**

**ART (Ajut a la Recerca Transversal) Grantee 2018 Call**

## *Invited Speakers* **Plenary Lectures**

### PL1. CHEMISTRY OF 2D-PNICTOGEN NANOMATERIALS

**G. Abellán**[1,2]

[1] Institute of Molecular Science (ICMol), University of Valencia, Paterna, Spain

[2] Joint Institute of Advanced Materials and Processes (ZMP), University Erlangen-Nuremberg, Fürth, Germany

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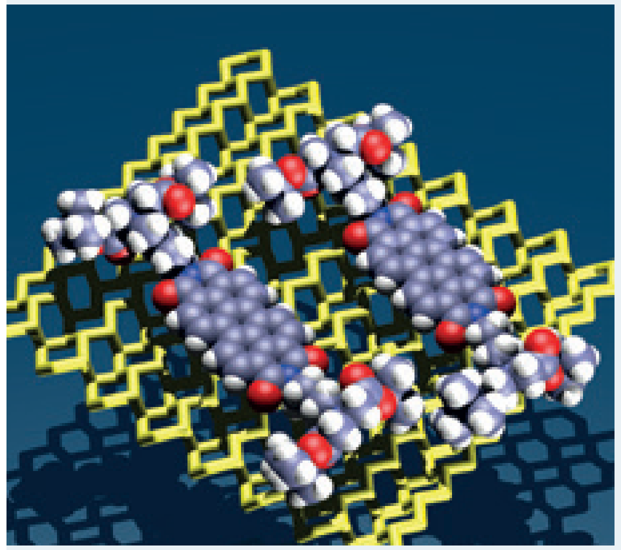
Two-dimensional (2D) materials have attracted great attention in the last years due to their outstanding physical properties and their potential applications in optoelectronics, sensors, energy storage, and catalysis. In contrast to the most studied material graphene [1,2], the layered allotropes of group 15 elements (P, As, Sb, and Bi, also called pnictogens) have been fairly less developed. 2D pnictogens exhibit a marked puckered structure with dative electron lone pairs located on the surface atoms, which results in semiconducting character and good electronic mobility, and also in an increased chemical reactivity. Indeed, 2D-BP (phosphorene) and 2D-Sb (antimonene) exhibit a great ability to easily adsorb and stabilize unsaturated organic molecules through van der Waals interactions [3–6]. Herein we will show novel insights into the oxidation, chemical functionalization (both covalent and non-covalent), intercalation and passivation of 2D pnictogens [7–10]. Moreover, we will prove that 2D-BP and 2D-Sb can act as catalysts in synthetic organic transformations involving unsaturated molecules, in a completely different way as graphene does [11].

*Schematic representation of the non-covalent functionalization of Black Phosphorus with a novel ethylenediaminetetraacetic (EDTA) ligand containing an integral perylene bisimide (PDI) core*



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### PL2. NANOSCIENCE: THE FUTURE ARRIVED

**África González-Fernández**

Director of Centro de Investigaciones Biomédicas (CINBIO). Centro de Investigación singular de Galicia. Universidad de Vigo, Spain. President of the Spanish society for Immunology.

Nanoscience is not longer a future. There are several nanocomponents already being used in many fields, including in a wide range of applications (motor industry, buildings, electronics, chemistry, textile, biomedicine, food, environment, etc.). They can offer alternatives / improve to the current products, due to the interesting properties that they show at the nanoscale.

The potential of nanomaterials is clear, particularly in biomedicine as medical devices, vaccines, biosensors, scaffolds, contrast agents or drug-delivery systems. In this latter aspect, they can offer improved stability, better biodistribution profiles and drug release kinetics, lower immunotoxicity and targeting to specific cell populations. However, their use in biomedicine has been accompanied by a significant concern regarding toxicity and biocompatibility, and their success will depend at some extent on their interactions with cells and other components of the immune system. Although in recent years our understanding of nanoparticle interaction with components of the immune system has improved, many questions still arise requiring more thorough investigation. Nanoparticles can be recognized as "foreign" elements by our organism, inducing responses against them. However, we could take advantages of this process, and nanoparticles can be specifically designed to either target or avoid interactions with the immune system. Moreover, the standardization of studies to understand the potential toxicity induced by nanomaterials is strongly needed.

## Invited Speakers ART (Ajut a la Recerca Transversal) Grantee 2018 Call

### ART1. NANOSTRUCTURED MOXC/ZNO SYSTEMS FOR PHOTOCATALYTIC HYDROGEN PRODUCTION

**P. R. Martínez-Alanis**[1], M. Molina[1], A. Pajares[1,2], F. Güell[3], P. Ramirez de la Piscina[1], N. Homs[1,2]

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[3] Department of Electronic and Biomedical Engineering, Faculty of Physics & Institute of Nanoscience and Nanotechnology (IN$^2$UB). University of Barcelona. C/Martí i Franquès 1, 08028 Barcelona.

The design and optimization of catalytic systems for photocatalytic hydrogen production from biomass-derived alcohols is a great challenge. A small amount of a noble metal added to an oxide semiconductor decreases the rate of recombination of electron hole pairs and produces an increase of the $H_2$ yield.

Transition metal carbides (TMCs) are materials with unique metal-carbon chemical bonds and noble metal-like d-state density around Fermi level [1]. Moreover, TMCs show high thermal stability and mechanical hardness and are considered potential materials to be applied in different processes for fuel production [2]. Usually, TMCs are synthesized by temperature programmed reduction methods (T>1500°C), which employ gas-solid reactions between oxides and hydrocarbon-containing gases ($CH_4$, $C_2H_6$). Among TMCs, molybdenum carbides show an outstanding reactivity with $H_2$ and $CO_2$ and are effective catalysts for the $CO_2$ reduction to CO [1, 3].

The catalytic behavior of molybdenum carbide depends on the preparation method used [4]. Several methods using different molybdenum salts and carbon sources have been reported. However, the complete transformation of the precursors is difficult to achieve lowering the active surface of materials.

The goal of this work is the study of new synthetic methods to obtain nanostructured TMCs by using organic-inorganic precursors involving different carbon sources, and the integration of $Mo_xC$ nanoparticles onto ZnO nanostructures. Ultrasound-assisted precursor generation in the synthesis of $Mo_xC$ is also investigated. The structural and optical characterization of photocatalysts is carried out using different techniques such as X-ray diffraction, scanning electron microscopy and photoluminescence. The photocatalytic performance of $Mo_xC$/ZnO systems in hydrogen production from aqueous solutions of alcohols is discussed.

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### ART2. BIODEGRADABLE PLGA-BASED DEXIBUPROFEN NANOPARTICLES INTERACTIONS WITH AN AGE-DEPENDENT CORNEAL MEMBRANE MODEL

**E. Sánchez-López**[1,2,3,4], A. Ortiz[1,2], G. Esteruelas[1], A. López-Machado[1,2], A. Cano[1,2,3], J. Prat[1,2], M. Muñoz[1,2], M. Espina[1,2], M. Ettcheto[3,4], A. Camins[3,4], A.C. Calpena[1,2], H. Lisette[1,2], M.L. García[1,2,3], M. Pujol[1,2,3]

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Ageing is a biological process that leads to a decline of biological functions and remains as the major risk factor for the most prevalent diseases of developed countries. This process leads to changes in the biological membranes, affecting specially some body structures such as the ocular surface. Specifically, the lipids of the corneal ocular surface exhibit age-related changes which increase the epithelial permeability rendering the corneas more vulnerable to injuries.

Ocular inflammation is one of the most prevalent diseases in ophthalmology, which can affect any part of the eye or the surrounding tissues. Non-steroidal anti-inflammatories (NSAIDs) such as Ibuprofen, are the most widely used as eye-drops drugs to treat ocular inflammation. However, their ocular bioavailability in internal eye tissues is very low (< than 5%). Therefore, drug delivery system such as biodegradable polymeric PLGA nanoparticles constitute a suitable alternative to topical eye administration because improve ocular bioavailability, reducing side drug effects and by their prolonged drug release allow to reduce administrations enhancing patient treatment adherence.

During recent years, new approaches have been developed to study the NPs-membrane interaction by using models of biological membranes, mimicking their bilayer structure, but limited to only a few lipids in composition. In addition, there are just a few reports mimicking the lipid structure of the corneal surface. Hence, the aim of this work will be to develop an in vitro corneal membrane model suitable to study the interactions of drugs or drug delivery systems with their surface.

In order to develop the corneal membrane model, the miscibility of different proportions of lipids was studied using Langmuir Blodget films. Figure 1 shows the miscibility of the lipids used for the corneal membrane model. From here, three different corneal age-dependent membrane models were developed containing a constant ratio of Phosphatidylcholine, phosphatidylethanolamine and phosphatidylserine o (40:50:10). Different amount of cholesterol and sphingomyelin were added in order to obtain three different corneal age-dependent models (kids, adults and old population).

Moreover, several formulations of PLGA based nanoparticles encapsulating Dexibuprofen (active enantiomer of Ibuprofen) were prepared by solvent displacement method using different surfactants (2). The formulations have been characterised and their interactions with the developed corneal membrane model were studied.

So far, a new corneal membrane model has been developed and the interaction between new drug delivery systems and conventional formulations was elucidated.

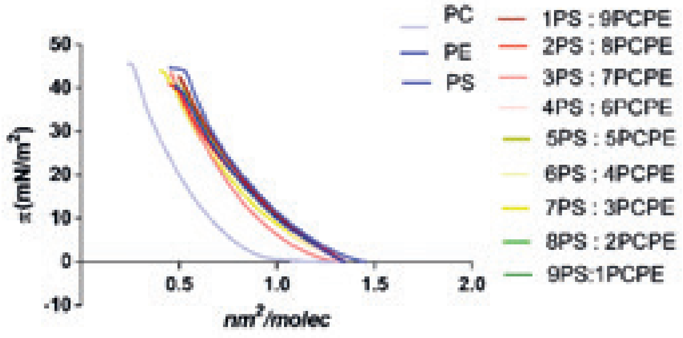

*Figure 1.*
*π - A curves for lipid miscibility study*

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## ART3. STUDY OF OXIDATION STATES IN THE AMYLOID-MAGNETITE COMPLEX RELATED WITH ALZHEIMER'S DISEASE

**Mònica Mir**[1,2,3,4*], **Lluís López-Conesa**[3,4,5], Sònia Estradé[3,4], Francesca Peiró[3,4], Josep Samitier[1,2,3,4]

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The formation of amyloid peptide Aβ42 fibrils is one of the main hallmarks of Alzheimer Disease (AD). However, the presence of an increase of magnetic nanoparticles in AD brains, without an increase of ferritin concentration, the usual iron transporter, has been recently explored. However, the mechanism for biogeneration of magnetite inside the body in AD patients is still unclear. Previously, we have investigated the interaction between these important players in AD and the results support the notion that the magnetite-Amyloid β complex is created before the synthesis of the magnetic nanoparticles, bringing a highly stable interaction of this couple. The capacity of amyloid peptide to bind and concentrate iron hydroxides, benefits the spontaneous synthesis of these nanoparticles with a symbiotic interaction that stabilize both compounds.

A neuronal culture model was used to monitor the activity changes and effective connectivity in amyloid-magnetite affected cultures, showing a clear spontaneous disrupting neuron network community mainly with the amyloid-magnetite dose. To bring some light about the higher toxicity of this couple, a detailed mapping of Fe oxidation state in the magnetic nanoparticles obtained through this amyloid Aβ42-assisted formation is under study with Electron Energy Loss (EELS) Spectroscopy in the Transmission Electron Microscope (TEM).

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## ART4. CONTROLLED GAS INSERTION IN THERMALLY SWITCHABLE MOLECULAR MATERIALS

**D. Aguilà**[1], **O. Casals**[2], R. Diego[1], G. Sanchez[2], L. A. Barrios[1], G. Aromí[1], J. D. Prades[2]

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Molecular-based materials able to absorb and desorb small volatile molecules are an exquisite tool for energy and environmental sciences. The potential of these chemosensors relies on measurable physical changes experienced by the material upon the interaction with the gas molecule, such as color, fluorescence, or other effects.[1] One type of compounds that can exhibit such behavior are Spin-Crossover (SC) systems.[2] These molecular materials are able to switch from high- (HS) to low-spin (LS) state upon an external stimulus such as change of temperature, light irradiation or inclusion of guest molecules. In that sense, we have been involved in the production of a unique family of thermally induced SC molecular materials able to absorb reversibly some volatile molecules at room temperature (acetone, water or alcohols, Figure 1, left) while maintaining, in some cases, its crystallinity.[3] These processes involve important optical, crystallographic and magnetic changes, converting those materials into promising room-temperature switches, sensitive to gases. In order to evaluate such a potential, these materials have been studied in an atmosphere-controlled set up, which has been developed to carefully expose materials to the desired gases (Figure 1, right). This strategy, which involves the synergy between the GMMF (experimental chemistry) and MIND (electronic devices) research groups, allows the possibility of assessing a controlled insertion/remove of different gases in molecular materials at different temperatures in a new range of experiments, which have never been carried out, and approaching these materials to applications. Moreover, the crystal-to-crystal character of the processes could allow a further characterization of the materials accessed using other techniques such as crystallographic or magnetic measurements.

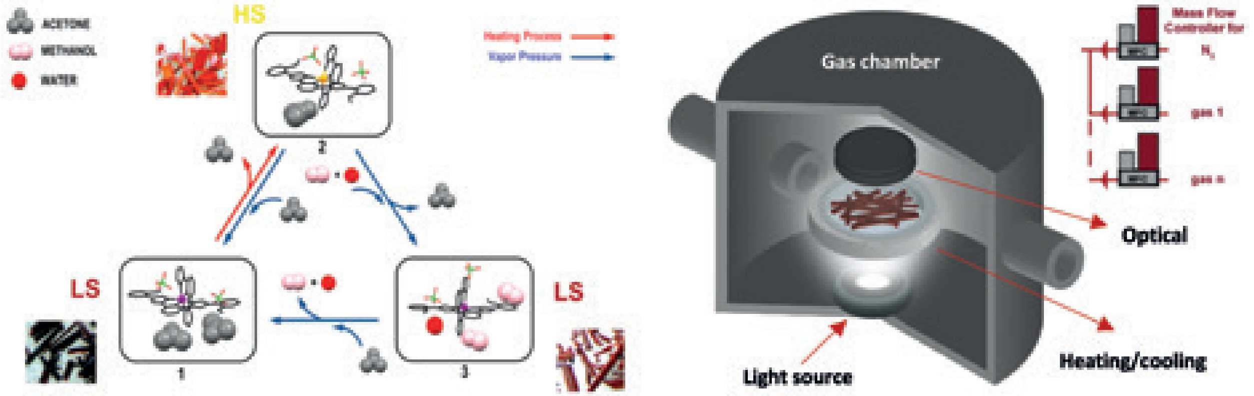

*Figure 1. (Left) Crystal image and structure from a FeII-based SCO compound after absorption/desorption of acetone, methanol and water.3 (Right) Diagram of the set-up for the optical analysis under different atmospheres and at different temperatures.*

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# Oral Presentations

## 01. PEGYLATED NANOPARTICLES OF EPIGALLOCATECHIN-3-GALLATE: A NEW ALTERNATIVE FOR THE TREATMENT OF TEMPORAL LOBE EPILEPSY

**Amanda Cano**[1,2,3], Miren Ettcheto[3,4,5], Marta Espina[1,2,], Elena Sánchez-López[1,2,3], Antoni Camins[3,4], Maria Luisa García[1,2,3]

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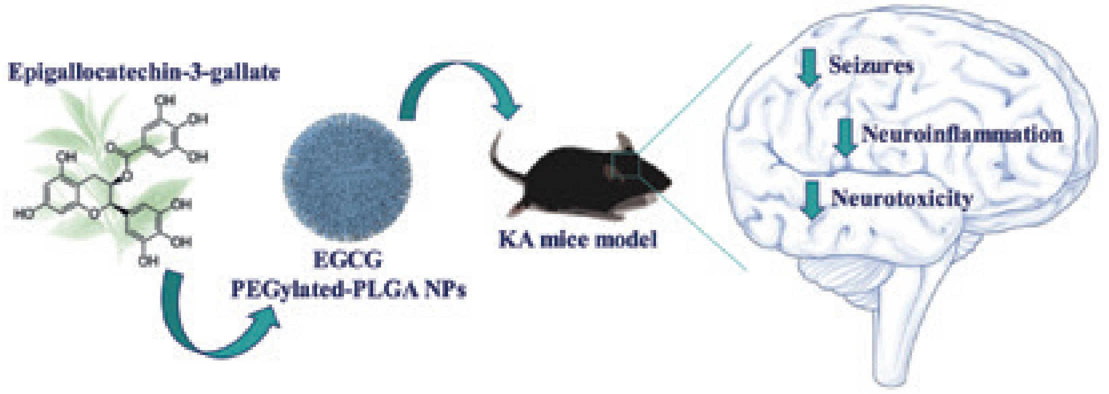
Epilepsy is a brain disorder derived from an imbalance in the neuronal electrical activity, which gives rise to convulsive events [1]. Temporal lobe epilepsy (TLE) is the most common form of pharmacoresistant epilepsy in adults [2], so it is needed to find new compounds for its therapeutic approach. Epigallocatechin-3-gallate (EGCG) has aroused much interest because of its multiple therapeutic effects [3], but its instability compromises the potential effectiveness of this molecule. In recent years, colloidal systems have been increasingly studied due to its potential for highly targeted drug delivery and to protect drugs from external aggression [4]. Thus, PEGylated-PLGA nanoparticles of EGCG (EGCG NPs) were designed. Nanoparticles were prepared by the double emulsion method and *in vitro*, *in vivo* and *ex vivo* studies were carried out to determine their effectiveness in the kainic acid (KA) mice model of TLE. Results obtained showed that EGCG NPs exhibited optimal physicochemical characteristics to reach the brain and promote a sustained release of the drug. Nanocarrier were non-toxic and behavioural test demonstrated that nanoparticles reduced most than free drug the number of seizures and their intensity. Finally, it was observed a reduction of neuronal death and neuroinflammation processes in mice treated with this nanosystem. In conclusion, EGCG NPs exhibit the appropriate characteristics to become a new effective alternative for the treatment of the TLE.



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## 02. NONEQUILIBRIUM SELF-ASSEMBLY PROCESSES: FORMATION OF MESO- AND NANOSTRUCTURES WITH APPLICATIONS TO BIOLOGY AND MATERIAL SCIENCE

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In self-assembling processes, a set of disordered interacting building blocks form ordered structures by means of energy and matter dissipation. The formation of microtubules, gels, virus capsides, cells and living beings among others are prominent examples of self-assembly under nonequilibrium conditions. Nevertheless, a general evolution criterion able to account for why nature selects some structures outside equilibrium and not others is lacking. As a starting point to understand non-equilibirum self-assembly (NESA), gelation is analyzed by using mesoscopic non-equilibrium thermodynamic model that describes the dynamic assembly of the structures. In the model, the evolution of the structures from the initially inactivated building blocks to the final agglomerates is governed by kinetic equations of the Fokker-Planck type. We also propose a model to show the formation of Liesegang rings under non-isothermal conditions to understand NESA process. The model formulates reaction-diffusion equations for all components intervening in the process together with an evolution equation for the temperature. Finally, we show how the architecture of self-assembled structures can be determined from the knowledge of the energy and matter dissipation inherent to its formation. When the amount of dissipation quantified by the total entropy produced in the process is represented in terms of parameters which describe the shape of the assembled structures, its extremes correspond to structures found in experimental situations such as in gelation and Liesegang ring formation. It is found that only a small amount of extra energy is needed to yield smooth changes in the form of the assembled structures. The connection found between the entropy produced and the type of structures formed may constitute a selection criterion which shows why a set of disordered units may give rise to a determined self-assembled structure.

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## 03. TRANSPORT AND ASSEMBLY OF COLLOIDS IN LIQUID CRYSTALS

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Transport of solid inclusions in liquid media has opened new perspectives for both single particle transport and colloidal self-assembly [1]. Of special interest is the use of colloidal microparticles dispersed in a nematic liquid crystal (NLC) medium. In this situation, we present experiments based on the transport of single colloids which are propelled along the nematic director by means of both, free gravity sedimentation and under the application of an external AC electric field, the well-known liquid crystal-enabled electrokinetics (LCEEK) mechanism [2]. From these experiments, we have assessed the diffusive behaviour perpendicular to the nematic director in terms of the elastic distortion of the local nematic director around the inclusions, being superdiffusive for dipolar configurations, while for quadrupolar configurations results barely differ from diffusion. The observed phenomena can be reproduced with different driving methods and propulsion speeds. Moreover, we propose a mechanism based on the geometry of the liquid crystal backflow around the inclusions to justify the persistence of thermal fluctuations and relate it with the obtained superdiffusive behaviour [3]. Going further, and by taking advantage of the LCEEK mechanism, hundreds of particles can be assembled above a photo-induced topological defect. The particles assemble in circular clusters that feature three well-defined regions as time proceed, a solidified central core, where the area fraction of particles ($\phi$) remains mostly constant, is followed by a liquid-like corona ending in a dispersed, gas-like phase. Directly from $\phi$ we can determine the pressure and effective temperature provided by the system [4]. We also develop a theoretical model which captures all the basic physics of the process. Furthermore, simulations agree with experimental data.

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## 04. LASER-INDUCED FORWARD TRANSFER FOR PRINTED ELECTRONICS APPLICATIONS

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In printed electronics conventional printing techniques originally designed for the graphics industry are used for manufacturing electronic components and devices by transferring metal and dielectric inks on a wide variety of substrates. For example, gravure or screen printing (SP) are chosen when considering large production runs for their fast output power and reliability. However, these become expensive when defect repair or customization are required, because rolls or masks need to be produced before printing. Alternatively, direct-write techniques such as inkjet printing (IJP) or laser-induced forward transfer (LIFT) are capable of printing user-defined patterns by depositing ink droplets on demand.

In LIFT, a liquid layer of ink is spread on a transparent substrate called donor and placed in front of the receiver substrate at a certain gap. Then, a laser pulse is focused at the donor film, where it is absorbed and a bubble is created (Fig. 1a). The expansion of this bubble results in the formation of a jet that propels the ink forward until it reaches the receiver and a sessile droplet is thus deposited. Through the repetition of this process in multiple positions of the donor, any pattern can be produced.

Unlike IJP, LIFT is nozzle-free, which implies that inks with large particles in suspension can be deposited free from clogging issues. In turn, a broad range of ink viscosities are printable, from 1 mPa·s to 100 Pa·s. Therefore, almost any ink can be printed using LIFT, quite regardless of its rheology.

In this work we will explore the basic principles of LIFT for depositing inks for printed electronics applications. First, we will discuss a typical LIFT setup and how the transfer mechanism takes place in order to understand its performance. Later, we will focus in our main results obtained in the field of printed electronics. For instance, we have been able to print silver nanowires (Ag-NWs) for producing transparent electrodes on flexible PET substrates (Fig. 1b). Also, high solid content inks typically used in SP have been deposited in regular paper to produce highly conductive tracks (Fig. 1c). This proves the versatility of LIFT for printing almost any type of ink independently of its particle size or viscosity in a digital fashion, which unveils its great potential for printed electronics.

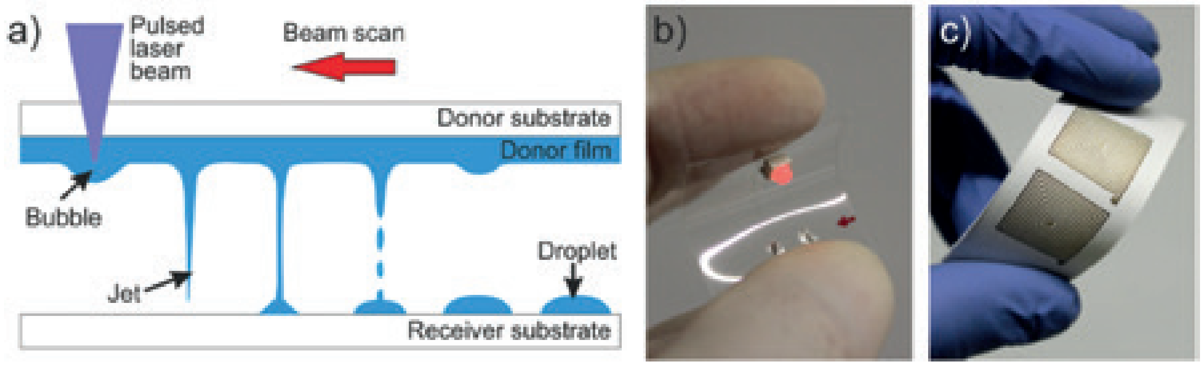

*Figure 1. a) Schematic representation of the transfer mechanism in the LIFT of inks. b) LED connected to a power source through transparent Ag-NWs electrodes deposited on PET. c) Silver SP ink inductors printed on regular paper.*

## 05. SYNTHESIS OF ZnO NANOWIRES: OPTICAL SPECTROSCOPY AND APPLICATIONS

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One-dimensional nanostructures such as nanowires (NWs) have attracted a lot of attention compared to bulk and thin film materials, due to their high surface-to-volume ratio, which increases their response to light. ZnO NWs show remarkable optical properties such as waveguiding effects; and have multitude of applications including ultraviolet (UV) lasers, light emitting diodes, sensors and photocatalysis.

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## 06. IRON OXIDE NANOPARTICLES: FROM FABRICATION TO BIOAPPLICATIONS

**C. Moya**[1], A.M. Abdelgawad[2], N. Nambiar[2], R. Escudero[3], D.C. Malespina[3], M. de la Mata[4], J. Hernández[4], S. Majetich[2], J. Faraudo[3], A. Roig[3], X. Batlle[1], A. Labarta[1]

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Iron oxide nanoparticles ($Fe_{3-x}O_4$ NPs) have been on the focus of many research studies not only for their fascinating magnetic properties, but also for their potential in biomedical approaches. However, there are still some issues in the NP design that limit their optimal response, such as lack of reproducibility, poor control over the NP structure and deficient colloidal stability in biological media. Recently, some of us have developed new strategies to synthesize $Fe_{3-x}O_4$ NPs by the decomposition of organometallic iron compounds with a good control of both the crystal structure and stability in some complex biological media.

Here we report the effect of oleic acid on the fabrication of $Fe_{3-x}O_4$ NPs with tunable shapes and sizes within 7 and 100 nm [1]. Structural and magnetic characterization of the samples indicated highly crystalline NPs with values of saturation magnetization close to the bulk material. Besides, we observed by infrared spectroscopy a strong effect of the oleic acid concentration on both the nucleation temperature and NP growth. Once the concentration of the oleic acid increases, the nucleation temperature raises as well, and consequently the growth process can be tuned. Next, we compared the structural and magnetic properties of single-crystal cubic and spherical $Fe_{3-x}O_4$ NPs obtained by a similar methodology, with comparable volumes and high saturation magnetization, in three sorts of NP assemblies [2]: dilute dispersions with minimal magnetostatic interactions, 2D close-packed monolayers and 3D close-packed arrays. Structural characterization reveals that cubic NPs pack into square 2D lattices or simple cubic lattice 3D platelets. Magnetic properties suggest that the cubes have lower surface anisotropy and therefore lower effective anisotropy than spherical NPs. Moreover, we established a protocol to easily preform a human serum albumin (HSA) corona onto $Fe_{3-x}O_4$ NPs of different sizes in a reproducible maner [3]. The resulting molecular structure was studied by molecular dynamics simulations of the hybrid nanoconjugates. The number of HSA forming the corona and their disposition as a monolayer on the particle surface predicted by molecular simulations was in agreement with dynamic light scattering and electron microscopy analysis. Furthermore, the effect of the HSA corona on the NPs efficiency as magnetic resonance imaging contrast agents in water, human serum, and in saline medium was also evaluated. The protein corona did not affect the efficiency of the $Fe_{3-x}O_4$ NPs as $T_2$ contrast agents but reduced their efficiency for $T_1$ contrast. Finally, we observed a greater stability for HSA-$Fe_{3-x}O_4$ nanoconjugates in both saline and acid media, preventing nanoparticle dissolution in extreme gastric conditions.

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# Posters

**RESEARCH AREAS :**

- Modeling, Simulation and Nanoscopic Methods (NanoMet)
- Nanobioscience, Nanobiomechanics and BioNanotechnology (NanoBio)
- Nanopharmaceutics and Nanomedicine (NanoPharmaMed)
- Nanoelectronics, Nano-optics and Nanophotonics (NanoPhotoElectro)
- Nanomagnetism and Spintronics (NanoMagnetics)
- Nanostructured materials (NanosMat)
- Nanoenergy: Production and Storage (NanoEnergy)

## *Posters* Modeling, Simulation and Nanoscopic Methods (Nanomet)

### P1. STUDY OF DEFECTS AND STRAIN IN GAN NANOWIRES FABRICATED BY TOP-DOWN ETCHING USING PRECESSION ELECTRON DIFFRACTION

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Gallium nitride (GaN) nanowires have attracted much attention, because of their unique material properties, such as wide direct bandgap, high saturation velocity and large breakdown field. There are several methods for the bottom-up synthesis of GaN nanowires. However, GaN nanowires can be also formed by a top-down approach. Although the presence of defects and threading dislocations in GaN nanowires is extensively studied for bottom-up fabrication procedures, that is not the case for GaN nanowires fabricated by top-down methods. Thus, the study of defects and strain through GaN NWs fabricated by top-down etching is relevant.

In this work, five GaN nanowires (NWs) samples have been fabricated by top-down etching from GaN films, which provides an accurate control of their position and dimensions. This top-down approach comprises three conventional nanofabrication steps: (1) electron-beam lithography, (2) reactive-ion etching and (3) wet-chemical etching. Although the fabrication method was the same for all samples, they have been submitted to different fabrication conditions in order to investigate samples comparing two different wet etching approaches, as well as the effect of rapid thermal annealing (RTA) at 750ºC. Finally, one sample has been coated with 30nm of SiNx.

High Resolution Transmission Electron Microscopy (HRTEM) and diffraction contrast in two-beam conditions have been used to study the presence of defects and threading dislocations along GaN NWs. Moreover, strain mappings have been performed along the different GaN NWs in order to evaluate the relationship between the fabrication process and the stress on the nanowire. Strain measurements were carried out by precessed electron diffraction (PED) using the combination of the Digistar beam scanning and precession unit and the TopSpin software from the Nanomegas company.

### P2. ADVANCED EELS AND X-EDS ELECTRON TOMOGRAPHY TECHNIQUES APPLIED TO THE RESOLUTION OF DOPED CEO2 MESOPOROUS STRUCTURES

**Javier Blanco-Portals**[1,2], Federico Baiutti[3], Simone Anelli[3], Marc Torrell[3], Miguel López-Haro[4], Sònia Estradé[1,2], Albert Tarancón[3,5], Jose J. Calvino[4], Francisca Peiró[1,2]

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Cerium Oxide nanocomposites have remained a hot topic in materials science in recent years, partly due to their wide range of possible applications. CeO$_2$ doped with different composites, mainly transition metals and rare earths, has been rutinarly proposed as a solid electrolyte in solid state oxide fuel cells. Variations of the electrical behaviour have been proved to be closely bounded to the distribution of dopants and, thus, a precise analytical characterization of the spatial morphology becomes mandatory for a fine control of the devices performance.

Here, we present the characterization of a mesoporous nanostructure of CeO$_2$ doped with Gd and Pr. Due to the high complexity of the mesoporous morphology, only small localized regions could be analyzed by convential means, showing in these cases a clear segregation of dopants towards the grain boundaries, with the localization of the dopants across the whole structure unresolved. To address this issue, we undertook an analytical electron tomography experiment centred on the X-EDS signals, making the most of the capabilities of the TVM3D algorithm, achieving succesful results under conditions only tested up to this point in phantom models of lower complexity. Dopant segregation was confirmed.

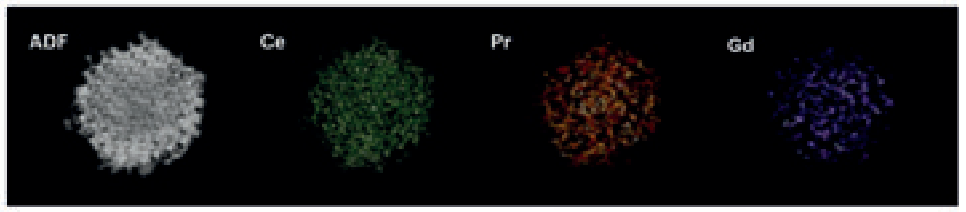

*Figure 1. Volume rendering of the reconstructions for the ADF signal and the X-EDS Ce, Pr and Gd signals.*

## P3. VORTICITY AND QUANTUM TURBULENCE IN THE MERGING OF SUPERFLUID HELIUM NANODROPLETS

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We have studied the merging of two 4He droplets at zero temperature due to their Van der Waals mutual attraction. The merging shows the appearance of density structures evolving in time which closely match the experimental observations by Vicente et al. [J. Low Temp. Phys. **121**, 627 (2000)]. We show that quantized vortex-antivortex ring pairs are nucleated at protrusions on the surface that either shrink and evanesce, or annihilate inside the droplet producing a roton burst. The merging process also nucleate ring structures that in some cases have been identified as quantized vortex-antivortex wrapping the outer droplet surface. Analysis of the energy spectrum discloses the existence of a first regime where turbulence arises from vortex-antivortex ring annihilation characterized by a power law close to that of the Kolmogorov spectrum, followed by another time interval where roton radiation dominates leading to a weak-wave turbulence regime.

## P4. PHASE TRANSITION ANALYSIS BETWEEN LOW DENSITY AND HIGH DENSITY NANOCONFINED WATER

**Luis Enrique Coronas**[1, 2], Valentino Bianco[3], Arne Zantop[4], Giancarlo Franzese[1,2]

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We perform Monte Carlo simulations of a coarse-grained model for confined water that includes many-body interactions associated to water cooperativity. The model is computationally efficient and allows us to equilibrate systems with a great number of water molecules at extreme conditions. Our results show the presence of a liquid-liquid phase transition (LLPT) ending in a liquid-liquid critical point (LLCP) between a low density liquid (LDL) and a high density liquid (HDL) forms of water, and a smooth structural change between HDL and very high density liquid (VHDL), recalling the structural transformation occurring among LD-amorphous, HD-amorphous and VHD-amorphous. Our results are consistent with atomistic simulations and experiments and clarify fundamental properties of nanoconfined water.

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## P5. NANOPARTICLE SIZE EFFECTS IN THE FORMATION OF THE PROTEIN CORONA

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One of the most surprising aspects of the interaction of nanoparticles with cells, that clearly distinguishes them from chemical molecules, is the so-called protein corona which is formed around them when they are found in aqueous solutions containing biomolecules such as blood [1,2]. In essence, chemical molecules interact directly with biological elements, whereas nanoparticles are coated by proteins and lipids. These macromolecules adhere very strongly to the nanoparticle's surface, and as a consequence, the exchange times with the solution are so large that the biological identity of the nanoparticles depends to a great degree on the proteins that coat them rather than on the materials that compose them. The formation of the corona is a complex process that depends on many parameters [3-5]. Here, we perform coarse-grain computer simulations of human serum albumin (HSA), transferrin (Tf) and fibrinogen (Fib) adsorption on a silica nanoparticle (NP) with an implicit water solvent to study how the final composition of the corona changes with the NP size. Our first results show that there is a crossover in the protein with the highest coverage from Fib to Tf at a characteristic radius within the range of 20 – 30 nm.

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## *Posters* Nanobioscience, Nanobiomechanics and BioNanotechnology (NanoBio)

### P6. UNVEILING ACTIVE TURBULENCE IN ACTIVE NEMATICS

**Berta Martínez-Prat**[1,2], Jordi Ignés-Mullol[1,2], Francesc Sagués[1,2]

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One of the most striking phenomenon that active systems show is the so called active turbulence [1,2]. Such a state is characterized by the formation of dynamic patterns of swirls with a characteristic length scale much larger than the size of an active unit itself (Fig. 1a). According to different theoretical studies, instabilities are at the origin of such regime [3]. However, so far, no one has experimentally reported the transition from an unconfined aligned active system towards the final turbulent state. In our lab we have used a very straightforward method to prepare a radially-aligned active nematic [4] based on a kinesin/tubulin system [5] that rapidly evolves forming a concentric pattern, finally dismantled as a result of the nucleation of half integer defects (Fig. 1b). Moreover, we have seen that from the beginning of the instability there is a wavelength selection, which we have rationalized by means of the active gel theory [4]. Besides, we are currently trying to reproduce a theoretical study where it is predicted that active turbulence in active nematics is characterized by a new universal scaling of the flow spectrum and by the absence of energy cascades between length scales.

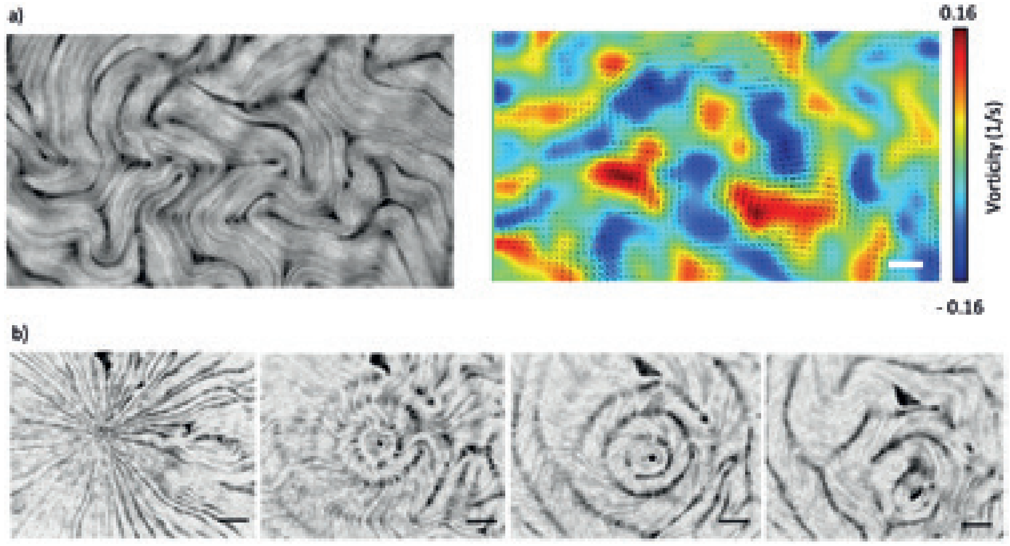

*Figure 1. Active turbulence and its onset. a) Left: An active nematic based on a kinesin/tubulin system. Right: Velocity field and vorticity of the active nematic highlighting the pattern of vortices. b) Pathway of the active nematic from a radially aligned disposition to the final turbulent state. Elapsed times from left to right are: 0, 13, 26 and 47 s. Scale bars: 100 μm.*

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### P7. PHYSIOLOGICAL MICROENVIRONMENTS IN REGENERATIVE MEDICINE: A CHALLENGE FOR NANOTECHNOLOGY

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Currently in tissue repair engineering, the extracellular matrix (ECM) is considered as an active architecture that can instruct cell functions through the introduction of different signals. The understanding of regeneration tissue healing requires a complex study of multiple variables affecting cells, as well as their interaction with the ECM. Stablished study platforms involve 2D culture and in vivo models. First ones can only be trustworthy in limited cases due to their lack of complexity compared to real human biological tissue environments, while second ones often introduce uncertainties, dispersion and many times they are not statistically valid, apart from considering their high cost and ethical issues. We try to shed light on mechanisms affecting cells and ECM by emulating the human biological conditions by the creation of microphysiological environments inside microfluidic chips. To do that, nanotechnology is crucial as tool to recreate the complexity of the cell environment in terms of nanotopography, mechanics and signaling, which is introduced by an accurate design of the biomaterial at the nanoscale [1]. It aids to design these environments that act as release platform of secondary signals such as metal ions, which have demonstrated to be a feasible tool to trigger signals produced by the own cells, acting as own signal regulators. Together with physical and/or mechanical stimuli we can emulate the process of tissue healing, and nanoparticles, electrospinning, microfabrication, electronics and surface engineering can be efficiently combined using nanostructured biomaterials and electrospun ECM-like environments [2].

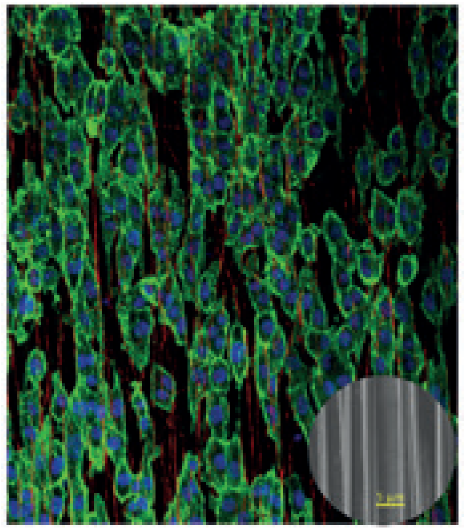

*Figure 1. Nanostructured fibrous topography can modify the shape of cells like cardiomyocytes which can efficiently polarized and matured with a further application of an electrical field.*

Hence, several approaches are presented here involving nanotopographic, nanostructured ion release platforms and electrospun polymeric nanofibers acting as temporary guiding templates (Fig 1). Results showed that these devices are not only a promising and low-cost tools for an efficient tissue mimicking, but also to modulate the whole process of healing and tissue regeneration.

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# P8. ARRANGEMENT OF ACTIVE GELS ON FLUID-SUPPORTED LIPID BILAYERS

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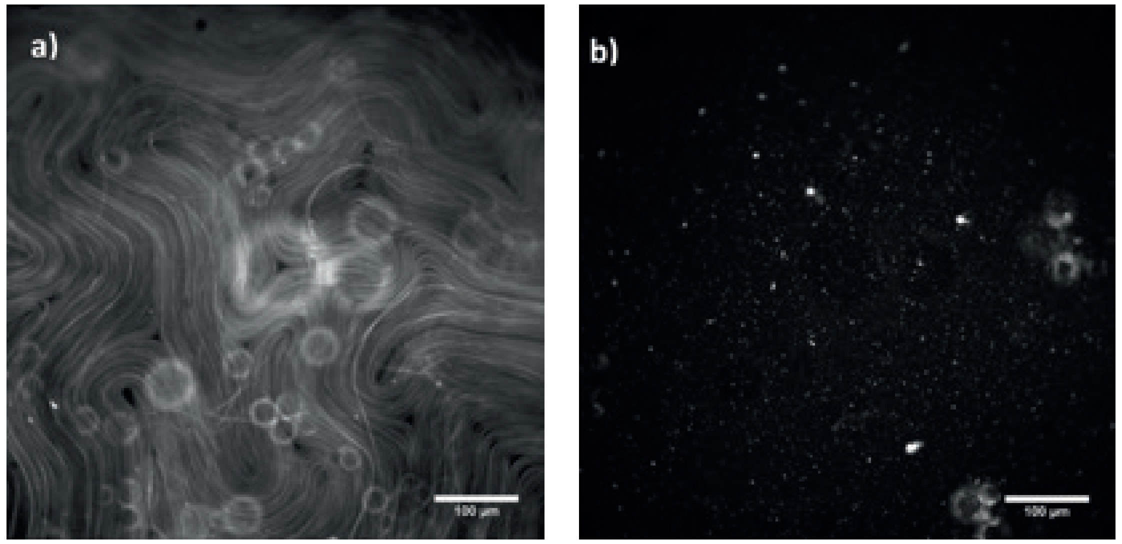

*Figure 1. Fluorescence images of the AN assembly (left) on a segregated fluid-supported lipid bilayer (right). Both images correspond to the same zone. Bright spots are segregated microdomains of the lipid bilayer.*

The interaction between the cytoskeleton and the cell membrane is very important as it regulates cellular interactions and organizes the cell [1]. An Active gel [2], an in-vitro cytoskeleton reconstitution, and supported lipid bilayers (SLB) were used here as model systems to assess this interaction. It is well-known that active gels self-assemble forming an active nematic (AN, where orientational order emerges) in contact with substrates that provide enough mechanical accommodation [3]. Until now, AN formation on SLB has not been achieved presumably because of the low fluidity of the used substrates. Preparation of SLB on a water-oil interphase has been devised to solve this problem and the formation of AN on this system has been achieved in our experiments. Ternary lipid mixtures with DPPC, DOPC and cholesterol result in SLB with phase separation [4]. This non-equilibrium system is a useful platform to study the effect of the AN, another non-equilibrium system, on the lipid bilayer (Fig. 1). We find that the activity of the AN is transferred to the SLB, providing continuous movement to the segregated microdomains. In our experiments, this mixing motion did not lead to a change of domains size.

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# P9. DELIVERY OF POLYPURINE REVERSE HOOGSTEEN HAIRPINS (PPRHS) AGAINST SURVIVIN IN PROSTATE CANCER CELLS USING GOLD NANOPARTICLES

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PolyPurine Reverse Hoogsteen (PPRH) hairpins are single-stranded DNA molecules formed by two antiparallel polypurine mirror repeat sequences linked by a five-thymidine loop, thus forming intramolecular reverse-Hoogsteen bonds between both domains. Upon binding to their polypyrimidine target in the dsDNA, PPRHs provoke strand displacement of the polypurine tract of the duplex producing inhibition of transcription or altering splicing, thus causing a specific gene silencing effect [1,2]. In the past, we demonstrated the effect both *in vitro* and *in vivo* of a PPRH designed against the promoter region of the *survivin* gene in PC3 prostate cancer cells. The PPRH led to a high decrease in cell viability, mRNA levels and protein levels. We also observed a reduction in tumor volume and tumor weight in a subcutaneous xenograft tumor model of PC3 prostate cancer cells [3]. The delivery of PPRHs both *in vitro* and *in vivo* was performed using cationic liposomes such as DOTAP and PEI. Currently we are exploring new PPRH delivery methods that could be non-toxic, efficient and cell/tissue specific. Gold-nanoparticles (AuNPs) are highly customizable, and can be designed and optimized for cellular uptake, bypassing the degradative machinery of the cells and improving gene expression in the nucleus. Therefore, AuNPs coated with polyethylene-glycol (PEG) were bound to a PPRH designed against *survivin*. This complex was stabilized using plasmid DNA following the process described at United States Patent Application 20180318424 [4]. Next, PC3 cells were incubated with the nanosomes for 4 hours and cell viability was determined after 5 days, showing the efficacy of this nanodelivery method.

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**Acknowledgements**

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# P10. HOLOGRAPHIC IMAGE PROJECTION WITH ACOUSTO-OPTIC DEFLECTORS

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We demonstrate a two-dimensional projection system for laser intensity patterns and videos based on acousto-optic deflectors. Acousto-optic deflectors (AODs) are light modulating devices that have a wide range of applications because of their immense speed and accuracy. Their main functionality is the angular deflection of a laser beam. They typically achieve 100.000 different deflection angles per second. This functionality is used e.g. in material processing [1] to steer a laser beam to thousands of positions on a substrate per second, or in confocal microscopy [2] to scan fluorescent samples point-wise with a laser beam. Although AODs excel with their high switching speeds, the amount of points which they can address in a certain amount of time is finite. That limits the throughput in material processing applications and the scanning speed of confocal microscopes. Other applications, such as video projections, are not possible at all, because images typically consist of millions of pixels which are impossible to project at a video rate by simply deflecting the laser beam.

To overcome this limitation, we investigate the combination of acousto-optic modulation with digital holography what enables AODs to form two-dimensional laser patterns and to address multiple positions simultaneously with a single laser beam. The holographic information is encoded in the electronic signals that drive the AODs. We demonstrate the potential of our holographic signals by applying a setup of two crossed AODs as image projector. The obtained image quality is excellent, and the projection speed is orders of magnitudes higher compared to the application of AODs as deflectors.

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# P11. DESIGN AND CHARACTERIZATION OF A NASAL NANOEMULSION LOADED WITH DONEPEZIL AND PIOGLITAZONE FOR THE TREATMENT OF ALZHEIMER'S DISEASE

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Pioglitazone (PGZ) is an agonist of Peroxisome proliferator-activated receptor-gamma (PPAR-γ) used to treat type 2 diabetes mellitus while Donepezil (DPZ) is a non-competitive and reversible acetylcholinesterase inhibitor widely used in the treatment of Alzheimer's disease. Several studies have reported that PGZ could be used in the treatment of inflammatory processes. The aim of this study was to develop and characterize a nanoemulsion loaded with PGZ and DPZ (PGZ/DPZ-NE) administered through the nasal route for the treatment of Alzheimer's disease. Solubility studies and three pseudoternary phase diagrams were carried out to establish the composition of the formulation. Physicochemical characterization including pH, droplet size, polydispersity index, viscosity and rheological behavior were evaluated. The physical stability of the PGZ/DPZ-NE was evaluated by its transmission profile of samples stored at 25 and 40 °C for 60 days. The tolerability was evaluated by cytotoxicity studies and histological analysis after PGZ/DPZ-NE administration using *in vivo* models. The obtained nanoemulsion was transparent and homogeneous with an optimal pH value (6.1) for nasal formulations. PGZ/DPZ-NE showed droplets with a nanometric size of 230 nm and spherical shape. The rheological profile showed Newtonian behavior with a linear relationship between shear stress and strain rate whereas the viscosity remained constant when the shear rate increased. This analysis was supported by mathematical modeling. The physical stability studies of the formulation did not detect signs of destabilization over a span of 60 days of study at 25 and 40 °C. Tolerability studies by cytotoxicity assays using human nasal cells showed viability greater than 80% in the dilutions assayed. Similarly, the histopathological analysis of porcine nasal mucosa showed no infiltration of inflammatory mediators after spray application of PGZ/DPZ-NE.

## P12. THYMIDYLATE SYNTHASE GENE SILENCING BY POLYPURINE REVERSE HOOGSTEEN HAIRPINS IN PROSTATE CANCER CELLS AS CANCER THERAPY

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The Thymidylate synthase enzyme (TS) is widely studied as an anti-cancer target because of its role in the synthesis the novo of dTTP. Treatment with TS inhibitors (e.g. 5-FU) can lead to tumour resistance through overexpression of TS, either by chromosome aberrations or by alteration of molecular mechanisms that regulate gene expression of this gene. It has been proposed that G-quadruplex nucleic acid sequence motifs may regulate translation as well as transcription. Therefore, in the present work, we have explored the incidence of G-quadruplex motifs in the 5′ untranslated regions (5′-UTR) of the mRNA of the thymidylate synthase gene as potential targets in cancer treatment. By using the QGRS mapper, a software for searching putative quadruplex forming G-rich sequences, we found a predicted G-quadruplex (G4). This prediction was confirmed by circular dichroism and UV melting measurements for the RNA sequence. In consequence, and to develop new therapeutic agents that could overcome resistance to TS inhibitors, we designed a Polypurine Reverse Hoogsteen hairpin (HpTYMS-G4-T-PPRH) against the complementary strand of this G4 sequence.

First, we demonstrated the ability of binding of the PPRH to its target sequence by gel-shift assays. HpTYMS-G4-T was able to bind to the template strand of the TS ds DNA target sequence in in vitro assays. Next, as TS is involved in dTTP synthesis, we compared the effect of this PPRH in PC3 cells incubated either in the presence or the absence of thymidine. The HpTYMS-G4-T PPRH was cytotoxic in both media, decreasing cell viability to less than 5% for at a concentration of 100 nM. These results raised the concept that TS could be involved in other proliferation pathways. The response of PC3 cells after treatment with HpTYMS-G4-T was dose dependent. This PPRH could be altering the transcription of TS gene at this site or the regulation of a G4 structure at this point. In conclusion, our results show the ability of the designed PPRH to bind to its target sequence of TS and to decrease PC3 cells viability. Therefore, PPRHs can be considered as a new type of molecules to modulate TS expression and overcome the resistance produced by traditional treatments.

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## P13. FROM BIOMASS TO SUSTAINABLE NEW MATERIALS: NOVEL ASPECTS ON CELLULOSE UTILIZATION

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Nowadays, enormous efforts are being done in the scientific community in order to develop sustainable alternatives to petrol derivatives like plastics for all kinds of applications, including packaging, building blocks, or biomedical devices, among others.

In this context, cellulose is an extraordinary renewable material for both its versatility and its abundance; it accounts for more than one third of the existing organic carbon sources on earth.

Considering this, as a group of Microbial Enzymes for Industrial and Environmental Applications, we are working on the biotransformation of natural polymers like vegetal cellulose, including the development of enzymes that catalyse its modification, hydrolysis, and/or synthesis. In addition, we are exploring the potential of bacterial cellulose, as an innovative source for new biomaterials, including its utilization as a platform for anchoring proteins, antimicrobial agents and other functionalization.

We have deep experience on the study of molecular biology of carbohydratases and esterases, and the identification and design of enzymes for biotechnological applications in pulp bleaching and paper recycling, production of biofuels, synthesis of new compounds from wastes, improvement of textile fibers, food industry, and development of new materials based on lignocellulose. With different approaches, we have expanded the toolbox of new enzymes, or their improvement by protein-engineering strategies, available for the community.

We aim at combining basic research with applied studies and innovation, and within this combination, we explore the development of new materials obtained through sustainable processes, and their modification in mild conditions by replacing chemical pollutants with enzymatic components. The developed materials display exceptional physicochemical properties, such as an ultrafine reticulated structure, high crystallinity, high tensile strength, high hydrophilicity and biocompatibility. These unique properties are allowing us to develop new biocomposites and to evaluate their applicability in several fields.

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## P14. DEVELOPMENT OF A SUPERFAST CONFOCAL MICROSCOPY TECHNIQUE THROUGH ENHANCED ACOUSTO-OPTIC MODULATION

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The major part of human knowledge regarding processes at the cellular and subcellular level has come from its direct visualization. For that reason, nowadays there is available a large catalogue of microscopy techniques compatible with living samples. In this framework, it is mandatory to specially mention fluorescence microscopy, because the possibility of direct observation of specific cellular components through specific labelling.

Moreover, confocal microscopy is one of the most used methods to extend resolution in optical microscopy because the reduction of the out-of-focus background. Confocal microscopy also allows fast imaging at hundreds of frames per second by multi-point scanning using spinning disk devices. However, using a mechanical component such as a rotating disk has its drawbacks, such as a remarkable inflexibility (scanning of arbitrary regions of interest or use of low magnification objectives is difficult) and low optical efficiency (typically 3-5% of excitation light reaches the sample).

For that reason, using its previous experience in holography and microscopy, our group has developed a new confocal microscopy technique by using acousto-optic deflectors (AODs) driven by complex radio-frequency (RF) signals computed according to methods of digital holography. With the AODs, all mechanical elements are removed from the set-up. By using an arbitrary wave-from generator (AWG) coupled to RF amplifiers, we are able to introduce the complex signals into the AOD devices (what we call acousto-holograms) and generate programmable multi-point patterns for sample-scanning. Combining the velocity of the AODs with virtual pinholing, a technique that performs the confocal filtering at the camera sensor, we are able to reach imaging rates up to 300 fps without many of the limitations of current high-speed confocals.

In this communication, we present the technique developed by our group, explaining the basic operation principles and the initial design carried out. Results obtained with the first prototype are also shown.

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## *Posters* Nanopharmaceutics and Nanomedicine (NanoPharmaMed)

## P15. PRANOPROFEN LOADED NANOSTRUCTURED LIPID CARRIERS: PREPARATION AND CHARACTERIZATION

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Pranoprofen (PF) (2-(5H-[1]benzopyrano-[2, 3-b]-pyridin-7-yl)propionic acid) is a NSAID which can be used as a safe treatment in skin local inflammation. Nanostructured Lipid Carriers (NLC) are colloidal nano-carriers systems composed of high melting point solid lipid/lipids as a core coated by surfactants and they are a great drug delivery system. The aim of the work is to prepare NLC containing PF for dermal use in order to obtain a sustained release formulation for the treatment of skin inflammatory diseases.

### MATERIALS AND METHODS

The lipidic components of the PF-NLC were: Lanette® as solid lipid, and castor oil and LAS (PEG-8 Caprylic/Capric Glycerides) as liquid lipids. The surfactant used was Tween® 80. The NLC were obtained by ultrasound method: treated for 15 min in a sonication probe (13 mm diameter) at 40% power amplitude [VCX 500 (Sonics & Materials Inc., Newtown, CT, USA)]. Characterization of lipid nanoparticles, namely the mean particle size (Z-ave), polydispersity index (PI) and zeta potential (ZP) were assessed by photon correlation spectroscopy (PCS, Zetasizer Nano ZS, Malvern, UK). The entrapment efficiency (EE) of PF in NLC was determined by indirect determination of the concentration of non-entrapped drug in the dispersion medium by a validated reversed phase high-performance liquid chromatography (RP-HPLC). The non-entrapped PF was separated using a filtration/centrifugation technique. Each sample was diluted with PBS pH=7.4 (1:20) prior to filtration/centrifugation

The rheological measurements were performed at 25ºC by using Thermo Scientific, Haake Rheo Stress 1 with cone rotor C60/2-Ti (60 mm diameter, 2º angle). Short physical stability was assessed at 25ºC by multiple light scattering analysis of backscattering (BS) profiles of a pulsed near-infrared light source (λ = 880 nm) using the Turbiscan®Lab (Formulaction Co., L`Union, France).

### RESULTS

The results showed size of 300 nm, PI of 0.3, ZP of -12.5 mV and EE >90%. The rheological evaluation of the formulations showed pseudoplastic behavior. The BS profiles of selected PF-NLC stored at 25°C confirmed good stability with BS variations minor than ± 10%, 60 days after production.

### CONCLUSION

The novel PF-NLC formulation proposed is a stable system during at least two month and its rheological behavior allow an excellent alternative for dermal application in skin inflammatory diseases.

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## P16. RGD AND PENETRATIN PEPTIDES: DUAL-RECOGNITION SITES IN LIPOSOME FOR TARGETED NANO-ONCOLOGICAL DRUG DELIVERY

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Cells in developing tissues and organs have evolved mechanisms to promote cooperative interactions with their neighbors. Uncooperative cells can be wiped out from the tissue by a dynamic process called cell competition. Cell competition allows proliferating cells to adapt to changes in their environment and promotes developmental robustness and optimal fitness [1]. However, this mechanism can be exploited by cheater cells to proliferate as occurs in cancer, resulting also in the overexpression of biochemical compounds such as integrins. Integrins [2] are main cellular adhesion receptors that through multifaceted roles as signaling molecules, mechano-transducers and key components of the cell migration machinery are implicated in nearly every step of cancer progression from primary cancer development to metastasis.

Drug carriers nanotherapy has acquired a sizable portion in the development of cancer treatment. The nanoscale size in combination with aptitude of poorly hydrosoluble drug encapsulation, enables nanoparticles as promising material to successfully accumulate at specifically damaged site by EPR effect [3]. Furthermore, nanoparticle surface chemistry characteristics and drug release profile [4] are fundamental parts when designing drug carriers. Current noticeable efforts are put into the development of combination therapies including co-encapsulation of drug with other molecules including specific recognition sites.

Taking into consideration all these aspects, our group has developed a system by combining specific dual-recognition sites with liposomes (lip) as nanocarriers to enhance drug delivery. Arginylglycylaspartic acids (RGD) and penetratin peptide (pAnt) have been incorporated into liposome for being cell recognition and attachment sites for several extracellular matrix proteins. In addition, RGD/pAnt-lip were fabricated and evaluated with methotrexate (MTX) as a model drug for the treatment of cervical cancer cells (HeLa). Liposomes were prepared by the thin film hydration method and characterized for their various physicochemical and physiological properties. Potential cytotoxicity of the different systems was evaluated after remaining 24 hours with them or with cell culture media (control) in three independent experiments by MTT assay. Results, expressed as percentage of viable cells related to control ones, show that the complex RGD/pAnt-lip are more effective that RGD-lip, pAnt-lip and control (7.0±0.1, 14.6±0.3, 13.4±0.1, and 44.1±0.4, respectively). These results support the proposed dual-targeting strategy of MTX-containing liposomes as a promising approach for cancer treatment.

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## P17. DESIGN, DEVELOPMENT AND CHARACTERIZATION OF A NANOEMULSION USING A PHOSPHODIESTERASE-4 INHIBITOR FOR THE TREATMENT OF INFLAMMATION

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Phosphodiesterase-4 (PDE4), which is found in immune cells, epithelial cells, among others, is presented as an intracellular enzyme without receptor that modulates inflammation and epithelial integrity. The inhibition of PDE4 triggers various effects through the elevation of the level of cyclic adenosine monophosphate (cAMP) and the subsequent regulation of a wide range of proteins and genes. It is known that PDE4 is a promising therapeutic target for the treatment of various diseases, in which we find dermatological ones. The purpose of this study was to design, develop and characterize a nanoemulsion (NE) loaded with a PDE4 inhibitor to evaluate its effectiveness in the treatment of inflammatory diseases of the skin. Solubility studies and optimization of the formula were carried out using ternary phase diagrams to establish the composition of the NE. Physicochemical characterization included particle size, polydispersity index (PDI), viscosity, rheological behavior and transmission electron microscopy (TEM). *In vitro* release and permeation studies were performed on human skin using Franz diffusion cells. The cytotoxicity of the formula was studied to determine the tolerance of the same. The study of the biomechanical properties due to water loss (TEWL) and hydration of the stratum corneum (SCH) was carried out in 12 volunteers. Finally, accelerated stability studies were carried out at different temperatures (4 °C, 30 °C, 40 °C) by the light transmission detection technique. The results of the solubility studies showed that Transcutol-p and Labrasol present the best characteristics for the optimization of NE, resulting in a transparent and homogeneous NE. The NE presented a particle size around 70 nm, PDI less than 0.4. Rheologically it showed a Newtonian behavior. The release mechanism of the NE followed hyperbolic kinetics and the ex vivo permeation profile showed that the PD4 inhibitor did not cross the layers of the skin, which would suggest an effectiveness at the site of administration. The *in vitro* cytotoxicity study showed that the formula exceeded a cell viability higher than 80%. No significant changes in the particle size and PDI were observed during the three months of stability. The results suggest that the developed NE can be used in local treatment for inflammatory skin diseases.

## P18. LEISHMANICIDAL ACTIVITY OF A NANOSTRUCTURED EMULSION LOADED A POLLENIC MACROLIDE ANTIBIOTIC

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Leishmaniasis is a neglected tropical disease, endemic in tropical countries. The World Health Organization (WHO) recommends the use of antimony salts as the treatment of choice, although this treatment is not available in countries where the poverty index is very high [1]. This is why pollenic macrolide antibiotics such as Amphotericin B (AmB) are suggested as second-line treatment. The AmB is characterized by having approximately 7 conjugated double bonds, they have amphoteric characteristics besides being highly lipophilic molecules. Nanoemulsions are thermodynamically stable, transparent, dispersions of oil and water stabilized by surfactants molecules having the droplet size less than 100 nm recommended for skin application [2]. In this case we have developed a nanoemulsion loaded Amphotericin B (AmB) studying its leishmanicidal activity.

### MATERIALS AND METHODS

Formulation: Nanoemulsion of AmB 0.3 % (AmB-NE) was prepared with a previous optimization formula [3].

Promastigote Assay: The IC50 was calculated using the quantification method with Resarzurin to carry out the infection with L.tropica promastigites described by Kulshrestha *et al.* [4]

Amastigote Assay: The IC50 was calculated using the quantification method described by Fernandez O. *et al* working certain modifications, using RAW cells to carry out the infection with L.tropica promastigites. [5]

### RESULTS

The IC50 values AmB-NE versus L.tropica were below 1,0 µg / mL (0,26 ± 0,09 µg/mL-promastigote and 0,73 ± 0,02 µg/mL-amastigote, respectively). The nanoemulsion without AmB (Blank) showed action against L.tropica promastigote and amastigote (0,16 ± 0,03 %-promastigote and 0,39 ± 0,02 %-amastigote, respectively), this could be due to the ability of the mixture of components enhancing the effect of the drug improving the activity with respect to AmB-free (0,73 ± 0,02 µg/mL-promastigote and 1,79 ± 0,02 µg/mL-amastigote, respectively).

### CONCLUSION

Taking into account the values of AmB retained in the skin [3], the density of the hydrated skin and the low values of IC50 in front of both stages of the parasite, we could conclude that our nanoemulsion might exert an adequate effect in cases of cutaneous Leishmaniasis.

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## P19. EX-VIVO PERMEATION OF CARPROFEN NANOPARTICLES AND CARPROFEN SOLUTION: A COMPARATIVE STUDY BETWEEN THE TWO FORMULATIONS IN PIG CONJUNCTIVA

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Carprofen (CP) [(+)-6-Chloro-*alpha*-methylcarbazole-2-acetic-acid] is a non-steroidal anti-inflammatory drug (NSAID) that reduces the production of inflammatory effusion primarily through inhibition of cyclooxygenase-2 (COX-2). CP is widely used in veterinary medicine and there are several studies about the role of this drug in several species [1]. However, CP permeation studies in swine conjunctiva have not been found among the consulted literature. The local administration of NSAIDs has been explored as a potential strategy to avoid the first pass effect and the gastrointestinal disorders that may occur when NSAIDs are administered orally [2]. When treating inflammation by directly applying the NSAID on the affected area, it should be ensured that the drug reaches the site of action at determined concentrations and within effective therapeutic range. Therefore, the use of polymeric nanospheres could be considered as a strategy to enhance the bioavailability of topically administered drugs.

### PURPOSE

The main objective of this work was to study the *ex vivo* permeation of CP nanoparticles and CP solution in swine conjunctiva and compare them.

### METHODS

Nanoparticles with a matrix structure containing CP and a solution at the same concentration of CP as the nanoparticles were prepared. *Ex vivo* permeation studies in conjunctival membrane were carried out using Franz Diffusion Cells with an area of 0.64 cm$^2$ and Phosphate Buffer Solution (PBS) pH 7.4 at 32 °C as receptor phase. Samples (300 µL) were withdrawn from the receptor compartment at predetermined times over 6 hours and replaced by an equivalent volume of fresh PBS at the same temperature. The amount of CP in the samples taken in the *ex vivo* permeation study was determined by a validated technique of high performance liquid chromatography (HPLC) with UV detection. Permeation parameters such as: permeability coefficient ($K_p$), lag time ($T_l$) and flux (J) were estimated by biopharmaceutical evaluation and the results were expressed as the mean of 6 replicates.

### RESULTS

Permeation parameters are exposed in the next table expressed by median and range:

| | **J** (mcg/h/cm$^2$) | **$K_p$*103** (cm/h) | **$T_l$** (h) |
|---|---|---|---|
| Carprofen Nanoparticles | 4.19<br>(0.50-7.80) | 2.20<br>(2.62-4.14) | 0.31<br>(0.19-0.43) |
| Carprofen Solution | 9.40<br>(9.00-9.50) | 4.93<br>(4.50-4.99) | 1.45<br>(1.40-1.46) |

### CONCLUSIONS

With regards to the obtained results it can be concluded that CP incorporated in both nanoparticles and solution is able to permeate through mucosa membrane of swine conjunctiva, which suggests that this route can be used as an alternative method to achieve its anti-inflammatory effect. In addition, the J, Kp and Tl results demonstrate that nanoparticles of CP are more favorable for local anti-inflammatory effects in conjunctiva mucosa than CP solution.

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## P20. PRANOPROFEN LOADED NANOSTRUCTURED LIPID CARRIERS IN PLURONIC® P407 GELS

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Skin inflammation is one of the most common skin problems. Pranoprofen (PF) is a non-steroidal anti-inflammatory drug which can be used as a safe treatment in skin local inflammation. Nanostructured Lipid Carriers (NLC) are a great drug delivery system, which can improve the biopharmaceutical profile of the drug. The selected PF-NLC loaded in Pluronic® P407 gels are a novel method for the treatment of inflammatory skin diseases.

### MATERIALS AND METHODS

The lipidic components of the PF-NLCs were: Precirol ATO5 as solid lipid, and Castor oil and LAS as liquid lipids. The surfactant used was Tween® 80. The NLCs were obtained by high pressure homogenization method. These selected PF-NLC were incorporated in thermoreversible Pluronic® P407 gels. The morphological examination of the selected gels was performed by Scanning Electron Microscopy (SEM) using a Phenom ProX microscope (Paralab, Spain). Short physical stability was assessed at 25ºC by multiple light scattering analysis of backscattering (BS) profiles of a pulsed near-infrared light source ($\lambda$ = 880 nm) using the Turbiscan®Lab (Formulaction Co., L`Union, France). Data were acquired at 5, 8, 15 and 30 days.

### RESULTS

These P407 gels show thermoreversible properties. The medium size of the PF-NLC was about 300 nm as showed the SEM images. The BS profiles of selected PF-NLC stored for different periods at 25ºC confirmed good stability with BS variations minor than ± 10%, 30 days after production, which means that no particle size variation phenomenon occurred over the analyzed periods.

### CONCLUSIONS

The selected PF-NLC loaded in Pluronic® P407 gels exhibited an optimal size for dermal application as the results of the SEM analysis showed. Additionally, stability assays revealed good physical stability during at least one month. After an accurate galenic and clinic development, this formula could be a novel method for the delivery of PF in inflammatory skin diseases.

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## P21. INFLUENCE OF SURFACE PROPERTIES ON CELL BEHAVIOR IN BIOMEDICAL APPLICATIONS

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Cell adhesion between cells and surfaces is a crucial controlling parameter on biological processes ranging from activation, differentiation, migration and proliferation. Changes in cell adhesion have been detected in a wide range of diseases such as arthritis, cancer, osteoporosis and atherosclerosis, where cell-matrix as well as cell-cell interactions have been reported to be cell type- and oncogene-specifics. Interfacial interactions between cells and surfaces correlate quite well with many important phenomena in biological systems and have been considered to the development of several artificial biomaterials and applications. When the *in vitro* biocompatibility of a biomaterial is determined, it depends mainly on its own surface properties, such as stiffness, surface charge, chemical functionalities, roughness and wettability [1]. Besides this, the culture medium and conditions as well as the type of cell are important parameters that also modulate the behavior of cells. As a first example this work includes the study of the influence of coatings at different degree of hydrophobicity on cell response [2]. Polyester fabrics have been coated by mixed organic-inorganic coating resulting in moderated to highly water repellence. *In vitro* experiments have been performed in order to establish the influence of surface modification on adhesion of representative model mammalian cell lines.

The second example of this work is related to the use of interference microscopy as a non-invasive technique for studying living cells and other biological materials. Although this technique is a commonly used tool in semiconductor and microelectronics manufacturing, where it affords nanometer dimensional precision in height measurement, over wide fields of view, interference microscopy make possible to examine living cell's biophysical properties to infer a cell's state and its changes in response to various stimuli [3]. Cells themselves act as biological sensors that integrate local biochemical and biophysical signals into a physiologically relevant, functional readout. A key advantage of using this technique is that it does not require labeling with fluorescent proteins or optically active dyes. Recently, 3D confocal interferometric scanning profilometry have been used to carry out imaging and surface analysis with nanometric resolution to characterize single cells morphology in real time in case of response of cells to external chemical stimuli, in comparison with conventional endpoint methods. The analysis of the profilometry profiles suggests that changes in cell volume [4] can be used to trigger early stages of either necrosis or apoptosis processes during the loss of cell viability.

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# P22. NEW STRATEGIES FOR PRION DISEASES: DRUGS FOR STABILIZATION OF GLOBULAR DOMAIN OF THE CELLULAR PRION PROTEIN INTERACTING IN THE COPPER(II) BINDING REGION

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The availability of high-resolution structures of PrPC (obtained by NMR and X-ray crystallography) allows the potential identification of novel PrPC ligands by employing computer-based methodologies. The globular domain of PrPC has been scouted to define solvent-accessible pockets that could be targeted with small molecules. To achieve this goal, two recently described, complementary methods have been employed: (i) fpocket, an empirical high-throughput method, and (ii) MDmix, which is physics-based and more reliable, but with a lower throughput. Combined, these methods will be applied to a large set of target candidates to obtain good confidence on positive predictions. This method also reveals the interactions preferences of the protein and identifies non-displaceable water molecules. Preliminary studies, performed using human PrP (1QLZ.pdb) and vole PrP (2K56.pdb), suggest the presence of a druggable region around His187 residue. Importantly this region corresponds a copper(II) binding region that is essential for the aggregation of native PrP in its infectious form. The prion protein (PrP) binds copper that, under some conditions, can facilitate its folding into a more protease resistant form. Hence, copper levels may influence the infectivity of the scrapie form of prion protein (PrPSc). Our research team is intensely involved in the design of small peptides as potential biocompatible agents to remove copper(II) ions from senile plaques (Alzheimer's disease; AD). We have recently demonstrated that several tripeptides have great potential for the design/development of potential anti-Alzheimer drugs and/or diagnostic agents showing that tripeptides of the type HXaaH (namely histidine-any aminoacid-histidine) have a strong affinity for copper(II) ions (through the formation of a highly stable ATCUN motif). These copper chelators oligopeptides have been tested in the PrP model obtaining promising results in the preliminary *in-vitro* tests.

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# P23. STABILITY STUDIES OF LYOPHILIZED LACTOFERRIN LOADED PLGA NANOPARTICLES

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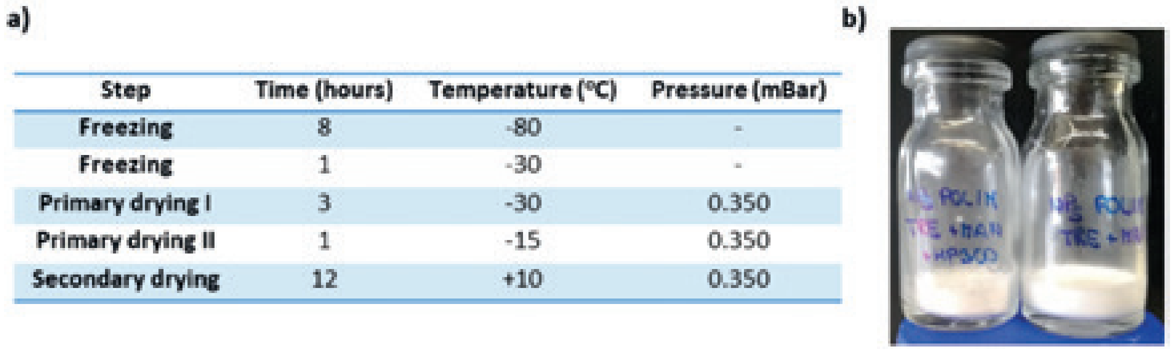
Physicochemical instability is the main drawback limiting the use of nanoparticles (NPs) in the drug delivery field. This is mostly noticed when these NPs suspensions are stored for extended periods. To overcome this problem, water must be removed, and freeze-drying is the principal technique to achieve the long-term stability [1]. The main objective of this work is to carry out the stability study, optimizing the freeze-drying process and selecting the best cryoprotectants for lactoferrin (LF) loaded poly(lactic-co-glycolic acid) NPs, to treat ocular inflammatory diseases due to anti-inflammatory and antioxidant properties of LF.

LF-NPs were prepared using the double emulsion method and optimized by design of experiment (DoE) approach. Average NP size and polydispersity index (PI) were analyzed. The entrapment efficiency of LF in the NPs was determined indirectly by measuring the non-entrapped drug in the dispersion medium by a reverse-phase high-performance liquid chromatography (RP-HPLC) method [2].

In order to obtain the optimal cryoprotection, different cryoprotectants (fructose, trehalose, mannitol, sucrose and HPβCD) was analyzed to assess their possible combinations in order to preserve the formulation against freeze drying. Furthermore, these molecules were used to get a suitable osmolarity for ocular drug delivery (305-316 mOsm/kg).

The lyophilization process was carried out using a Labconco freeze-dryer (Labconco Corporation, USA). Different lyophilization cycles, with and without annealing, were carried out in order to get the optimized NPs dried.



| Step | Time (hours) | Temperature (°C) | Pressure (mBar) |
|---|---|---|---|
| Freezing | 8 | -80 | - |
| Freezing | 1 | -30 | - |
| Primary drying I | 3 | -30 | 0.350 |
| Primary drying II | 1 | -15 | 0.350 |
| Secondary drying | 12 | +10 | 0.350 |

*Figure 1. a) Optimized lyophilized cycle. b) White shell after freeze-drying*

Freeze-dried LF-NP powders were sterilized by γ-irradiation applying a dose of 25 kGy (Aragogamma, Spain), and these lyophilized were stored at three different temperatures (4, 25 and 38 °C). Afterwards, NPs have been resuspended once a month for 3 months. Morphometric parameters and drug encapsulating efficiency were measured after resuspending. Samples presented no significant changes in the physicochemical properties. Being 4 °C the most proper temperature of storage.

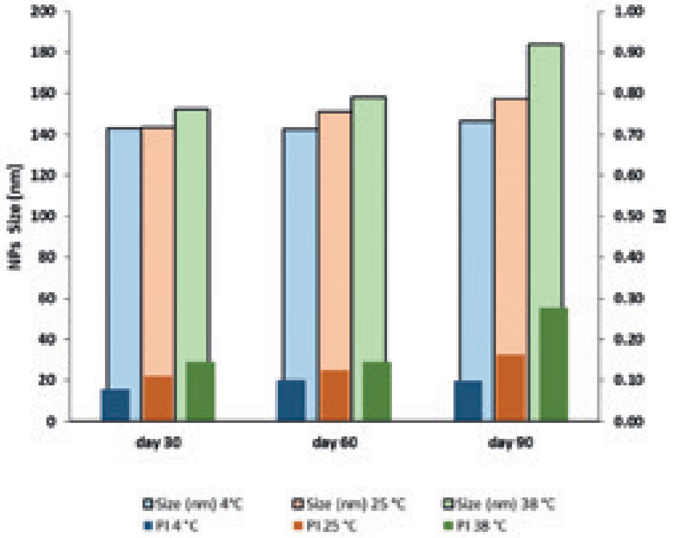


*Figure 2. Morphometrical parameters of resuspended LF-NPs*

An optimal ocular formulation has been successfully developed allowing a long-term storage by freeze-drying and maintaining their physicochemical properties as well as appropriate osmolarity and sterility.

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# P24. TRANSFERRIN-CONJUGATED DOXORUBICIN-LOADED PLGA NANOPARTICLES: PREPARATION, CHARACTERIZATION AND IN VITRO CYTOTOXICITY EVALUATION

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Polymeric nanoparticles (NPs) represent an important strategy to circumvent the cardio-toxicity and multidrug resistance caused by one of the most used anticancer drug, doxorubicin (DOX). The active targeting approach can be exploited to trigger the drug release in the cancer sites by including proteins, antibodies, hyaluronic acid or folate in their structure, as well as throughout pH physical stimuli [1,2]. Transferrin (Tf) protein binds directly to specific receptors of Tf (TfR), which are over-expressed in tumor cells [3]. The surfactant 77KS (Nα,Nε-dioctanoyl lysine with an inorganic sodium counterion) was described elsewhere as an biocompatible and efficient pH-sensitive promoter of the DOX release [4]. Therefore, the objective of this study was to develop Tf-conjugated DOX-loaded poly (lactic-co-glycolic acid) (PLGA) NPs (Tf-DOX-PLGA-NPs), with complete characterization and in vitro cytotoxicity evaluation. The NPs were prepared by nanoprecipitation method [5], resulting in a structure with spheroidal shape as seen by cryogenic transmission electron microcopy (Cryo-TEM). The suspensions showed mean particle size about 99 – 108 nm and polidisperity index lower than 0.23, both measured by dynamic light scattering, indicating a monodisperse system. The zeta potential was slight negative, which is due to the PLGA charge. By HPLC analysis, 0.29 ± 0.02 $mg.mL^{-1}$ of drug content was verified, while the Tf conjugation rate, achieved by BioRad® assay, was 0.55 ± 0.13 $mg.mL^{-1}$. The cytotoxicity evaluation was performed after 24h, 48h and 72h of incubation, comparatively between Tf-DOX-PLGA-NPs, NPs without the protein (DOX-PLGA-NPs), unloaded-NPs and free DOX, against one tumor and other normal cell line (HeLa and HaCaT, respectively), by MTT viability endpoint. The response of free DOX and DOX-loaded NPs in inhibiting cell growth were time-dependent and the unloaded-NPs exhibited low cytotoxicity effects against both cell lines over the 72h. There was a substantial reduction in cell viability when HaCaT were treated with DOX-loaded NPs; however, this effect certainly is due to the intrinsic DOX activity. Even so, it is worth mentioning that the Tf-DOX-PLGA-NPs were able to protect this cell line comparing to free DOX (60% and 18% of cell viability, respectively, in the lowest concentration at 72h). Fortunately, Tf-conjugated NPs were more active on HeLa cell line than DOX-PLGA-NPs and free DOX, resulting in 32%, 64% and 65% of viable cells at 72h, respectively. Thus, the set of results allows us to conclude that the Tf-DOX-PLGA-NPs are a promising drug delivery system to reach specifically the cancer cells, reducing, thus, the side effects promoted by the traditional chemotherapy. The future perspective is to study these NPs suspensions against a multidrug resistant cell line.

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## P25. NANO APPROACH TO LESSEN AMYLOID-ß TOXICITY AND COPPER-PROMOTED DAMAGE IN ALZHEIMER'S DISEASE

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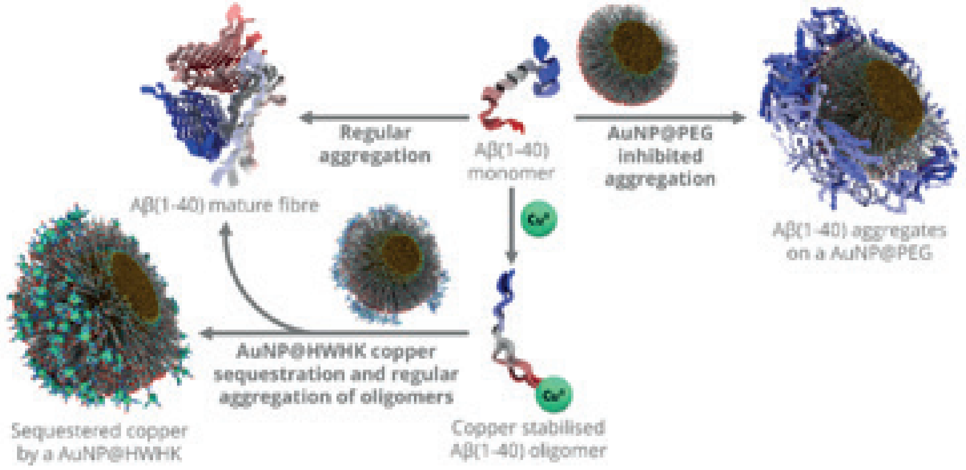
Alzheimer's disease is considered the world's 5th leading cause of death, with more than 35 million patients suffering from this type of dementia. One of the hallmarks of the disease pathogenesis is the toxicity of amyloid-ß related species. Protein aggregation and formation of senile plaques have been related to neuroinflammation and toxic oligomers to synaptic disruption inducing cell death [1]. We are proposing the use of functionalised gold nanoparticles as a mean for lessening amyloid-ß related toxicity in Alzheimer's disease. The nanoparticle biostability, low cytotoxicity, high loading capacity, high surface-to-volume ratio and permeability through the blood-brain barrier will further enhance the effectiveness of this method. We have observed that polyethylene glycol-coated gold nanoparticles can dramatically affect the aggregation of Aß(1-40), possibly preventing the formation of senile plaques. Colloid concentration, nanoparticle core size, surface charge and effective surface area are crucial regulatory factors for rationalizing such effect. On the other hand, by using gold nanoparticles functionalised with amino-terminal copper and nickel binding (ATCUN) peptides, we have been able to sequester copper(II) ions from toxic copper-stabilised oligomers [2], favouring the aggregation of the protein, generating less harmful fibres. Combining both effects, *viz.* copper redox silencing and aggregation inhibition, might lead to synergistic effects to tackle the toxicity due to amyloid-ß.



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**Acknowledgements**

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## P26. IN VITRO AND EX VIVO EVALUATION BY LEAD MODIFICATION STRATEGY FROM NATURAL FLAVANONE USING NANO SYSTEM FORMULATIONS

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The inflammatory diseases are becoming common in society throughout the world [1]; many therapeutical drugs have disadvantage to display side effects. Alternative to that are derivative natural products [2]. The (2S)-5,7-dihydroxy-6-(3-methyl-2-buten-1-yl)2-prenyl-2,3dihydro-4H-1-Benzopyran-4-one (1) was isolated from Eysenhardtia platycarpa and reported anti-inflammatory, antioxidant and cytotoxic properties.3,4 Different structural modification were semi-synthesized from (1) as a suitable strategy to obtain new compounds such as (8S)-5-hydroxy-2,2-dimethyl-8-phenyl-7,8-dihydro-2H, 6H-Benzo[1,2-b:5,4-b´]dipyran-6-one (**1a**) with improved biological efficacy.4 Nano system formulations (**NSF**) are thermodynamically stable dispersions used as drug delivery systems. The aim of this study was to evaluate a new formulation through *in vitro* drug release, *ex vivo* transdermal drug penetration and retention amount of (**1a**).

### MATERIALS AND METHODS

The components of the nano system formulation of **1a** (**NSF1a**) 5%w/w were: labrasol, labrafac, plurol oleique and propylene glycol. The drop size was measured by Zeta-Sizer, Malvern Instruments. *In vitro* release assay were performed in Franz Diffusion Cells with dialysis membrane. As receptor phase was used ETOH:$H_2O$ (70:30) kept at 32 °C and stirred continuously. The diffusion area was 2,54 cm$^2$. Samples (300 μL) for 89 h. *Ex vivo* permeation study used human skin as a membrane. The donor side was filled with 0,3 g of **NSF1a**. Samples (300 μL) at 19, 23, 27, 29 h. All studies were conducted in sixplicate. Extraction: The amount retention in the skin of **1a** was carried out with a mixture of ETOH:$H_2O$ (70:30) under sonication. Samples of the *in vitro* and *ex vivo* studies were quantified by means a validated HPLC method $H_2O$:ACN (30:70) as mobile phase; 280 nm. *In vitro* and *ex vivo* data were analyzed by GraphPad Prism software with Weibull model and were estimated permeation parameters: J, TI, P1, P2 and $A_{ext}$.

### RESULTS

The average drop size of the **NSF1a** was 383 nm with PI=0,4. The kinetic release model that best describes the amount of (**1a**) load at any time is representing by the function named as Weibull, $Q_t = Q_\infty\left[1 - e^{-\left(\frac{t}{t_d}\right)^{\beta}}\right]$, where: Q = 48,4 ± 16,1 and $t_d$ = 41,5 ± 33,2. Permeated amount of **1a** after 29 h were 1,5 μg. The (J) was 6,5 x $10^{-2}$ μg/h and TI was 7,9 h. While the P1 and P2 were 9,6 x $10^{-4}$ cm and 2,1 x $10^{-2}$ 1/h, respectively. The $A_{ext}$ was 9,6 μg/cm$^2$.

### CONCLUSIONS

The **NSF1a** displayed a drop size 383 nm with PI=0,4. P1 and P2 justified **NSF1a** action in drug diffusion transport in human skin. The **NSF1a** is a promising alternative to administrate anti-inflammatory modified drug.

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**ACKNOWLEDGE**

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## *Posters* Nanoelectronics, Nano-optics and Nanophotonics (NanoPhotoElectro)

### P27. SERS IN ARRAYS OF GEOMETRICALLY FRUSTRATED PLASMONIC NANOLEMENTS

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Plasmonic nanoelement arrays have been widely used for a variety of applications including enhanced spectroscopies, perfect absorbers or energy harvesting. The collective modes of these arrays can be different from the plasmon response of individual noble metal elements. On the one hand, when nanostructures are very close, near field interactions appear. On the other hand, the lattice long-range order can support collective modes. The interplay of these two excitations may yield much more intense resonances than those of single particles. In this work, surface enhanced Raman spectroscopy (SERS) measurements were carried out on substrates with arrays of geometrically frustrated plasmonic Au nanolements. The samples were fabricated by electron beam lithography and electron beam evaporation using metal-insulator-metal configuration, without lift-off procedure, which allows the formation of Au asterisks of 450 nm at the bottom of asterisk-shaped cavities and the corresponding inverse gold structure on the top. Fourier Transform Infrared (FTIR) spectroscopy revealed high absorption peaks around the visible or/and near-infrared regions. These structures are thus of interest for both enhanced spectroscopies and applications related to light absorption. As a proof of concept, the samples showed their usefulness as substrates for SERS after functionalizing them with 4-mercaptopyridine.

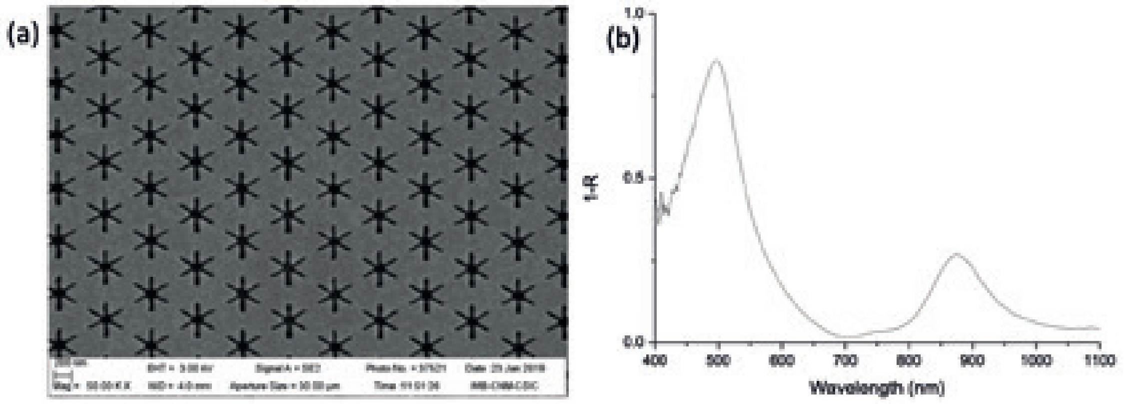

*Figure 1(a) SEM image of an array of Au asterisk-shaped cavities. (b) FTIR measurements of the array in (a)*

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### P28. ITO/ZNO/P-SI RESISTIVE SWITCHING DEVICES PROPERTY IMPROVEMENT VIA TB-DOPING

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Resistive switching (RS) consists in the tuning of the resistance of a material by an applied bias voltage. Different oxide compounds such as $TiO_2$, $HfO_2$, $SnO_2$, or ZnO have been used as active materials in RS switching devices, being the last one particularly interesting because of its non-toxicity, earth abundancy and transparency in the visible range of light. One possible way to improve the properties of ZnO RS devices is doping them with rare earths. These materials attract oxygen ions, limiting their diffusion and improving the resistance ratio and stability of the devices. Here, ZnO and ZnO:Tb RS devices deposited by sputtering are characterized. In this work it is shown that, in RS cycles induced with voltage sweeps, the operating current of doped devices can be lowered, which improves their endurance and resistance ratio, reaching the latter a value of 109. There is also an improvement in behavior of the devices using voltage pulses, increasing their stability and resistance ratio. The doped devices also exhibit light emission that depends on their resistive state, which would permit the reading of said state via optical means.

## P29. RESISTIVE SWITCHING READOUT THROUGH SILICON NANOCRYSTALS ELECTROLUMINESCENCE

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In the last decade, research efforts have been devoted to the field of memristors and resistive switching (RS), the latter being a phenomenon consisting of a controlled resistance change between two or more states, a very promising property to be exploited in the next generation of non-volatile memories and neuromorphic circuits. As well, the research with silicon nanocrystals (Si NCs) has explained the difference in electronic properties with the bulk material due to the quantum confinement effect. Electroluminescence (EL) emission of Si NCs has been tailored thanks to their growth within a multilayer (ML) structure, which allows for size control of the NCs, thus making them suitable for light emission applications. Silicon oxides have already proven to be suitable materials for RS, but little has been studied regarding its combination with EL-emitting Si NCs to achieve optical readout of the resistance state, which in turn paves the way to the successful integration of RS applications into optoelectronics.

In this work, we present a device with a structure of ZnO/Si NC MLs/Si, in which the NCs stack simultaneously exhibits EL and RS properties. The formation of conductive filaments associated to the RS process was found to strongly influence the EL emission of the Si NCs. ZnO is used as a transparent top electrode that allows performing both electrical and optical characterization. Additionally, defects in ZnO also yield a characteristic emission when properly excited. As a result, the RS state during a reading process can be directly identified through the EL emission, thus paving the way to novel integrated optical memristors.

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## P30. FABRICATION AND SIMULATION OF PHOTONIC CRYSTALS BASED ON SILICON NANOPILLARS

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Integrated photonic devices are, currently, one of the most important trends in the optoelectronics field of investigation. They are devices that aim to drive photons through them as electronic integrated systems do with electrons. One of the most versatile structures used in these integrated devices are photonic crystals. Photonic crystals are defined as periodic distributions of two dielectric materials with different refraction indexes. Depending on the characteristics of this periodical arrangement, photons can behave in them analogously as electrons do in solid-ionic crystals. Thus, the apparition of photonic bands and band gaps is promoted giving an absorption, reflection and transmission spectra strongly bounded to the geometrical distribution of materials over the photonic crystal [1]. Due to their potential applications, a vast number of papers have been oriented towards their theoretical simulation and modulation in different and imaginative ways during the last decades. However, experimental development of these advanced structures, based on photonic crystals, have been scarcely reported due to the difficulty of their fabrication at the nanoscale. Despite of that, thanks to the advanced knowledge on silicon nanofabrication and manipulation, the fabrication of photonic devices based on silicon is, nowadays, possible [2].

The aim of our investigation is to develop nanostructures based on hexagonal distribution of silicon nanopillars. The main goal of these structures is to behave as mechanical sensors due to the strong susceptibility of the absorption, reflection and transmission spectra to geometrical changes over these crystals. Accordingly, we would expect that any mechanical deformation of the pillars would induce a change in these spectra profiles.

The work carried out until now have been based on, both, the simulation of the structures and their fabrication in clean room facilities.

Simulations have been performed using MEEP (https://meep.readthedocs.io/en/latest/), what is an open-source software package that uses Finite-Difference-Time-Domain (FDTD) method for electromagnetic computational simulation. Different structures have been simulated varying both the radii of the nanopillars and the lattice parameter, or pitch. Moreover, the introduction of defects has been taken under account in our simulations. Their presence in the crystal can introduce new artifacts in the measured spectra that can be easily detected and that are strongly sensitive, as well, to geometrical changes [3]. The defects considered in our simulations have been the introduction of cavities in the crystal, removing or changing the radii of one or more pillars, and the introduction of waveguides, removing partially or completely a line of pillars.

At the same time, the nanofabrication of the structures has been optimized. The fabrication process has been implemented in a clean room environment, using electron beam lithography (EBL), followed by a lift-of process and the final nanopillars obtention via chemical reactive ion etching. The last experiments have resulted in structures consisting on a 660x660 μm$^2$ nanopillars zone with different waveguides, enclosed by a 20 μm-wide wall, and with 4 square-shaped grating structures, attached to the centre of each wall side, of 150x150 μm$^2$. The morphological characterisation of the nanostructure has been carried out via scanning electron microscopy (SEM). SEM shows the correct pattern fabrication, the almost perfect cylindrical shape of the 2 micrometres-tall pillars and the differences of the pillar's radii of the photonic crystal and those in the waveguide. These structures are shown in Figure 1.

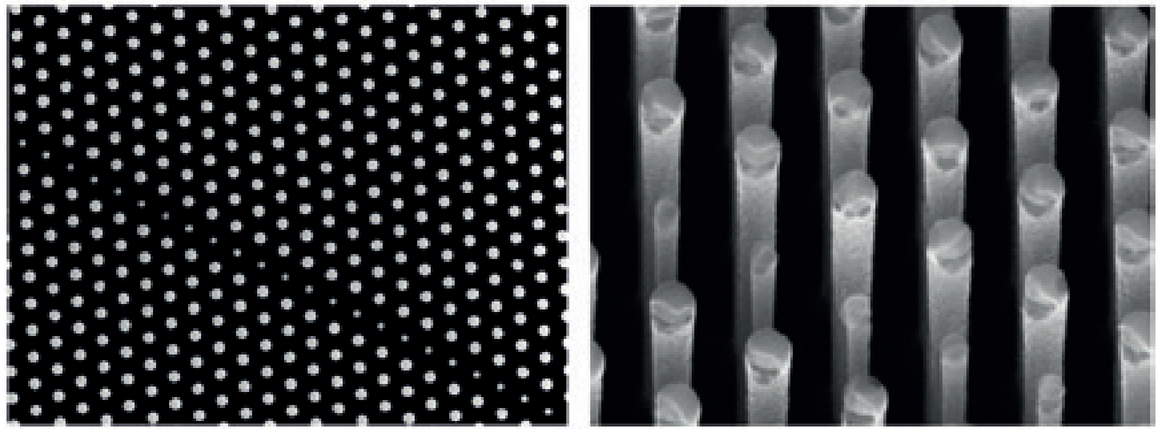

*Figure 1. Overview of the fabricated crystal with a waveguide (left); Nanopillar's of different radii (right)*

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## P31. LIGHT EFFECT ON THE RESISTIVE SWITCHING PROPERTIES OF ZNO-BASED DEVICES

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The fast scaling in electronics has arisen a great interest in memory technologies, being the resistive random access memory (ReRAM) one of the most promising memory candidates. In this kind of devices, the formation and destruction of conductive filaments across a dielectric permits to switch between a high resistance state (HRS) and a low resistance state (LRS). In metal oxides, this structural modification is typically governed by oxygen vacancies, being the combination of the applied voltage and the injected current necessary to trigger this process. The use of light in reading the resistance state of the memory has been recently addressed, in particular in devices where the variation of the transmittance of the active layer occurs under external voltage stress. However, in this case, the light does not directly influence in the switching process, being only used to read the optical state. Instead, involving light in the writing process, i.e., the active modification of the inner dielectric structure, is currently an issue under investigation.

In this work, the control of the conductive nanofilament formation during the electroforming in ITO/ZnO/*p*-Si pristine devices is studied by analyzing the electrical properties before, during and after illumination. The application of light not only allows decreasing the required voltage to form conductive nanofilaments, but also achieving stable intermediate resistance states. The injection of additional carriers from the p-Si substrate due to photogeneration plays a crucial role to induce this progressive structural modification. As well, a similar behavior has been observed using pulsed voltages, by gradually increasing the write voltage combined with the application of light.

# P32. LASER-INDUCED FORWARD TRANSFER OF NANOSTRUCTURED MATERIALS FOR PRINTED ELECTRONICS

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In the last years printed electronics has become a promising and cost-effective alternative to silicon-based electronics in applications such as flexible, wearable or organic electronics. In printed electronics, circuits are typically manufactured using rolls or masks when printing on a large scale. Nonetheless, these techniques become too expensive when considering short runs, customization or defect repair. In this case, direct-write (DW) techniques become an interesting alternative because they are able to print patterns directly from a digital file. The most extended one, inkjet printing (IJP), relies on the deposit of droplets of ink on-demand from an output nozzle. However, the presence of this orifice limits the range of printable ink rheologies: only viscosities of 1-50 mPa·s and particle sizes smaller than 1/100th of the orifice can be routinely printed. Another DW technique, laser-induced forward transfer (LIFT), has none of these constrains.

In LIFT, a liquid layer of ink is deposited on a transparent substrate which is flipped and placed at convenient gap in front of the receiver substrate. Then, through the action of a focused laser beam on the donor film, part of the ink is propelled forward till it reaches the receiver and a droplet is deposited. By the successive repetition of this process in several positions of the donor film, multiple droplets can be deposited and thus complex patterns can be produced. Since the transfer occurs through a jet instead of a flying droplet, as in IJP, LIFT has a broader range of printable viscosities. In addition to that, liquids with nanostructured materials in suspension (nanotubes, nanowires or particles) can be transferred since there is no nozzle through which the ink must be ejected.

In this work we explore some of the advantages of LIFT over other DW techniques by printing nanostructured materials for electronic devices. In order to do that we demonstrate the feasibility of LIFT by depositing inks containing silver nanowires (Ag-NWs) on glass (Fig 1a), which is otherwise very difficult to achieve through IJP. Later, the optimal printing parameters for obtaining conductive and stable lines are found by systematically varying the laser fluence and the scan speed. These printed structures are then characterized in order to study their functionality and prove their performance. Finally, a device consisting of Ag-NWs is fully printed with LIFT as a proof of concept of the technique (Fig 1b).

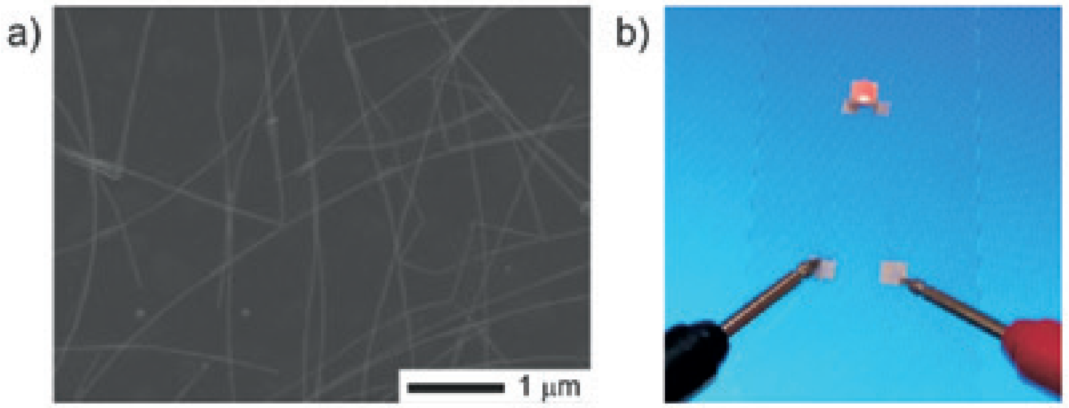

*Figure 1. a) SEM image of Ag-NWs deposited by LIFT. b) Circuit with the deposited transparent Ag-NWs electrodes*

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# P33. ROOM TEMPERATURE HUMIDITY SENSORS BASED ON INDIVIDUAL GA$_2$O$_3$ NANOWIRES GROWN VIA CARBOTHERMAL REDUCTION

**G. Domènech-Gil**[1,2], I. Peiró[1], E. López-Aymerich[1], M. Moreno[1,2], P. Pellegrino[1,2], S. Barth[4], I. Gràcia[3], C. Cané[3], A. Romano-Rodríguez[1,2]

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Gallium oxide is a wide band gap semiconductor material that is used in electronics for high-power technologies and has been widely studied during the last three decades, in form of thin films, for its high-temperature (> 600 °C) sensing properties towards oxygen and reducing gases [1]. With the reduction of dimensions of sensing devices, the interest in the nanowire (NW) form of this material has grown, thanks to the resulting high surface-to-volume ratio.

In this work is presented the growth of monoclinic gallium oxide ($\beta$-$Ga_2O_3$) NWs, using a metal-assisted vapor-liquid-solid (VLS) process [2] via carbothermal reduction at temperatures between 800 and 950°C using a solid precursor. The structural and optical characterization confirms that the NWs are monocrystalline $\beta$-$Ga_2O_3$ nanostructures, exhibiting average lengths of tens of µm and diameters below 100 nm. Individual NWs have been electrically contacted using focused electron beam induced deposition (FEBID) techniques for their use as gas sensors in the form of chemoresistors.

For the gas sensing response of these devices, twelve single NW-based resistors were tested against relative humidity, $H_2$, CO, $NO_2$ and $O_2$ at temperatures between 25 (RT) and 200°C. Fast, stable and reproducible responses were measured towards water vapor at RT, with a power consumption in the nW range. For the other gases, no response was observed, which agrees with reported results for this material [1], also indicating high selectivity of these sensors towards humidity. The reaction promoting this response cannot be due to the $Ga_2O_3$ surface, but can be related to residual carbon resulting from the carbothermal reduction process. This is in agreement with results from charcoal, which shows a significant water adsorption and charge transfer when exposed to humidity [3].

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## *Posters* Nanomagnetism and Spintronics (NanoMagnetics)

### P34. CHALLENGES IN THE SYNTHESIS OF HYBRID NANOSTRUCTURES WITH MAGNETIC AND PLASMONIC PROPERTIES

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Superparamagnetic Iron oxide nanoparticles (SPIONs) have attracted great attention in nanomedicine due to their high magnetization at room temperature, low magnetic anisotropy and biocompatibility. However, their magnetic properties depend on several parameters such as size, shape and crystallinity so that a careful control of the synthesis is needed to optimize the magnetic response. On the other hand, gold nanoparticles, exhibiting strong localized surface plasmon resonance (LSPR) in the visible and/or near-infrared (NIR) wavelengths, are also suitable nanostructures for biomedical applications due to the easy-synthesis in aqueous media, biocompatibility, low toxicity, and optical properties which made them good candidates for biomedical applications. The combination of these two materials pave the way to synergies between magnetic and plasmonic properties. Therefore, this work is focused on the synthesis of hybrid structures to achieve multifunctional materials. Magnetite NPs are synthetized through thermal decomposition method, which allows obtaining monodispersed nanoparticles with high-crystal quality in a range from 5 nm to 20 nm. Then the NPs are transferred to water by exchange ligand to improve the biocompatibility and allow gold attachment.

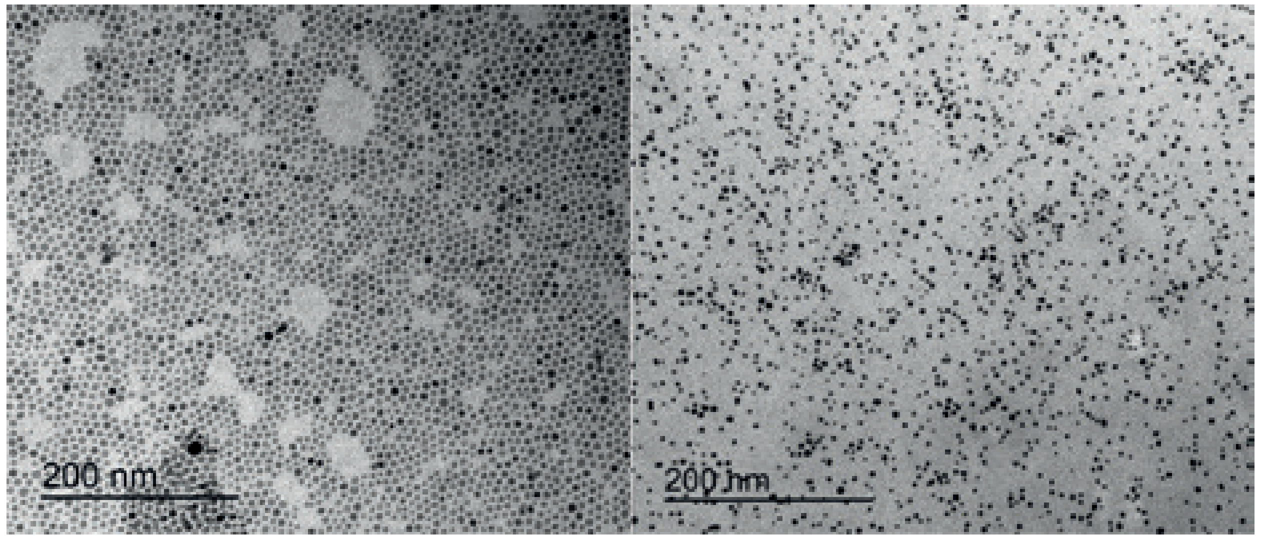

*Fig.1. Left. Magnetite nanoparticles of 8.2 ± 1.2 nm. Right. Gold nanoparticles of 4.6 ± 0.9 nm*

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*This work was supported by Spanish MINECO (MAT2015-68772- P, BES-2016-077527) and the European Union FEDER funds.*

### P35. SYNTHESIS AND FUNCTIONALIZATION OF IRON OXIDE NANOPARTICLES FOR TARGETED CANCER THERAPY

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Over the last decades, nanoparticles as drug carriers have attracted a lot of attention as potential systems for targeted drug delivery. Their tunable size and properties have opened a wide variety of possibilities to design future drug vehicles.

On the other hand, Polypurine Reverse Hoogsteen Hairpins (PPRHs) molecules are DNA hairpins bound via Hoogsteen bonds. The PPRHs can bind by WatsonCrick bonds to the desired DNA sequence. In this particular case, the PPRHs are synthetized to act against the survivin production, which is an antiapoptotic protein, so its inhibition provokes cellular apoptosis, as it has already been proved and reported in literature.

In this work, a new system for targeted cancer therapy is presented from the combination of superparamagnetic iron oxide nanoparticles (SPIONs) and the PPRHs. Monodisperse SPIONs are synthetized and functionalized with dopamine, hyaluronic acid and PPRHs. Dopamine acts as an anchor to the nanoparticle, whereas hyaluronic acid is a known ligand to the CD44 receptor, apart from preventing the SPIONs to agglomerate. The paramagnetic behavior of these nanoparticles, along with their tunable size, makes them a very promising system for future cancer treatments.

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## P36. A SPIN-CROSSOVER MOLECULAR MATERIAL DESCRIBING FOUR DISTINCT THERMAL PATHWAYS

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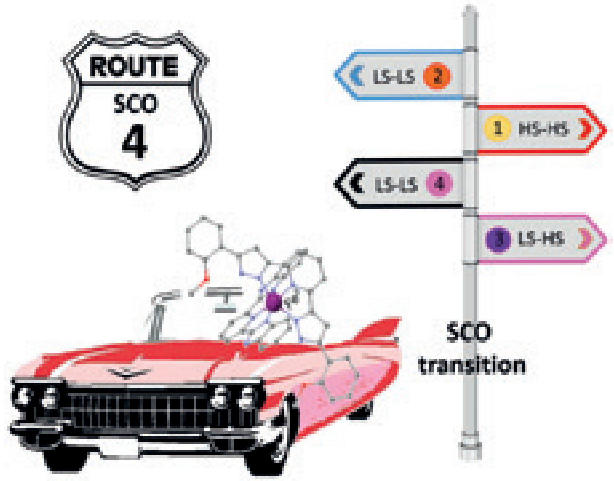
The spin crossover (SCO) is a fascinating phenomenon that concerns any $d^4$-$d^7$ transition metal complex due to their ability to reach to different spin states, depending on the energy of the $t_{2g}$ vs. $e_g$ orbital splitting in relation of the necessary for pairing two electrons within on d orbital [1]. The origin of this transition lies in the molecular scale even so structural phase transitions (SPTs) influence greatly the behaviour within crystalline structures due to different effects of cooperativity. Coordinating tris-imine like ligands with Fe (II) produces dense network of intermolecular interactions that offers analysing the crystal breathing and the understanding of the solid-state transformations[2]. The heteroleptic complex, [FeL(bpp)](ClO$_4$)$_2$ (L and bpp are tris-imine ligands, (1), is an ideal robust systems that allow making a connection between SCO and SPTs through single X-ray diffraction (SCXRD). Magnetometry and SCXRD measurements unveil a succession of SCO and crystallographic phase transformations never seen before[3]. Starting form a fresh crystal of 1 (a mixed spin state HS-LS) containing one molecule of acetone per Fe center (1·ac), a fully HS (1α phase) state is reached upon warming. This crystallographic phase converts into another one (1β) upon cooling and accessing to LS state. Warming of 1β induces a new SCO coupled to another crystallographic phase transition, 1β→1γ (HS-LS). This last phase cycles between the HS-LS and the LS states through superimposable pathways. We present here four different thermal SCO routes gives rise to four different magnetic responses within a range of temperatures near to ambient conditions.



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## P37. DINUCLEAR [LN$_2$(2-FBZ)$_6$(TERPY)$_2$] COMPOUNDS. SMM BEHAVIOUR AND LUMINESCENT PROPERTIES

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Lanthanide ions possess interesting luminescence properties, emitting light when appropriately sensitized by a ligand. The 2-fluorobenzoate ligand (2-FBz) interacts strongly with the Ln(III) via the carboxylate group and possesses a conjugated aromatic ring that confers luminescence properties to the compounds it forms [1]. Moreover, lanthanide atoms are also well known to exhibit large magnetic moments and strong magnetic anisotropy and therefore they are considered good candidates for the elaboration of Single Molecule Magnets (SMMs) [2]. The use of 2-FBz and 2,2′:6′,2″-terpyridine (terpy) has led to a new family of isostructural homodinuclear compounds with general formula [Ln$_2$(μ$_2$-2-FBz)$_2$(2-FBz)$_4$(terpy)$_2$] (Ln(III) = La, Nd, Sm, Eu, Gd, Tb, Dy, Er and Yb). The dysprosium derivative (Figure 1) presents SMM behaviour at zero applied field and luminescent properties. In this work, we present the magnetic and luminescent properties of this family of compounds.

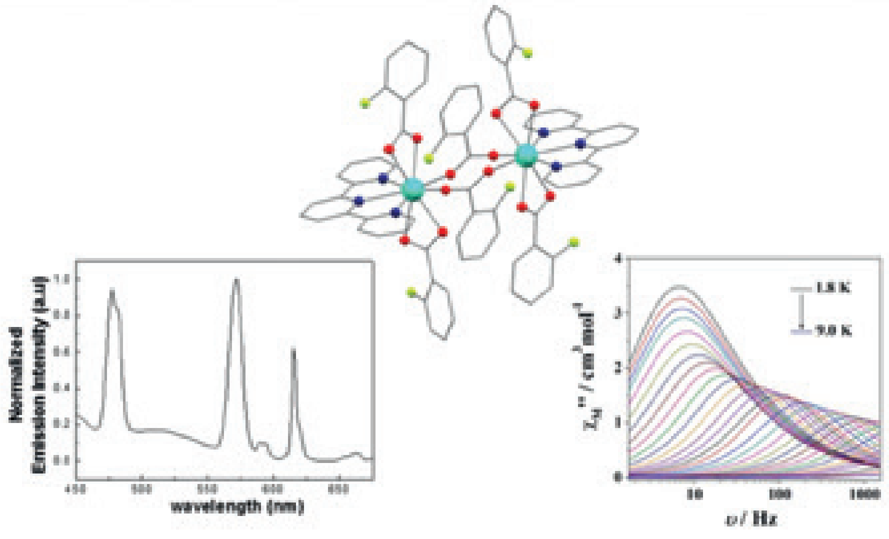

*Figure 1. Structural representation (top centre), luminescence spectra (bottom left) and ac magnetic measurements (bottom right) of the dinuclear compound [Dy$_2$(μ$_2$-2-FBz)$_2$(2-FBz)$_4$(terpy)$_2$].*

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## P38. GEOMETRIC FRUSTRATION IN ORDERED ARRAYS OF PLASMONIC NANOELEMENTS

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Frustration has largely been studied in magnetism where the term refers to situations in which one or more spins in the magnetic unit cell do not find a proper orientation to fully satisfy all the interactions with the neighboring spins, either by the existence of competing interactions or by the actual geometry of the structure itself. Inspired by this, we recently introduced the concept of geometric frustration in the field of plasmonics [1]. In this work, we study the plasmonic response of four types of arrays of Au nanoelements, three with triangular symmetry and one with square symmetry, all of them showing features that are a consequence of geometric frustration for the dipolar excitation of the gaps between neighboring nanoelements through near-field interactions [2]. The key point is to hamper the excitation of these low-energy modes boosting in turn collective lattice modes corresponding to high-Q resonances and longer lifetimes [1,2]. All the arrays show high absorption sharp peaks in the visible and/or the NIR (Figure 1), as well as extended time responses with an echoed excitation of the collective modes that remain excited at long times due to the frustrated dipolar polarization of the gaps [2]. This behaviour, together with the fact that the electric field extends over much larger areas as compared to strongly coupled dimer antennas, makes these plasmonic arrays suitable for enhanced Raman or fluorescence spectroscopies.

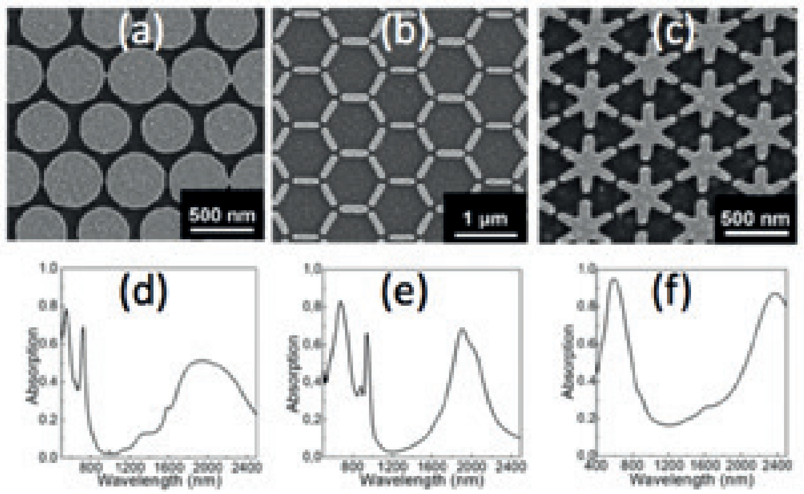

*Figure 1. (a-c) SEM micrographs and absorption spectra for different types of arrays of Au nanoelements.*

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## P39. CHIRAL OPTICAL RESPONSE IN TRIANGULAR LATTICES OF PLASMONIC NANOELEMENTS

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Chirality is one of the basic features of living systems. Many biologically important species (such as nucleic acids, proteins or certain drugs) are chiral. In most cases, the enantiomers of chiral molecules show clear differences in biochemical activity, metabolic mechanism, transport pathway, and toxicity. Thus, the detection of enantiomers of chiral molecules is of great practical importance in the biochemical and pharmaceutical fields.

We aim to develop novel, chiral plasmonic structures with a strong chiral optical response. Our approach is to exploit the apparent emergence of dark plasmon modes in geometrically frustrated arrays of plasmonic nanoelements [1,2] to develop a new mechanism for direct dark mode excitation based entirely in the lattice symmetry of the arrays. By exciting the structures with right-/left-handed circularly polarized light, an asymmetric optical response of the modes is expected, which could be exploited to make active chiral structures. In Fig. 1, we show Finite Difference Time Domain (FDTD) simulations showing the potential of our approach. The absorption spectra and the spatial distributions of both the electric field enhancements and the electric charge have been simulated for single nanoelements as well in finite lattices of nanoelements with triangular symmetry such as that depicted in the inset to Fig. 1. A remarkable chiral optical response is found for the absorption peaks in the visible, both in their average magnitude (Fig. 1(a)) as well as in the corresponding local charge and electric field enhancement distributions (Fig.1(b)). Our work paves the way to detect chiral molecules functionalized with this kind of plasmonic nanostructures by probing the chirality of the latter.

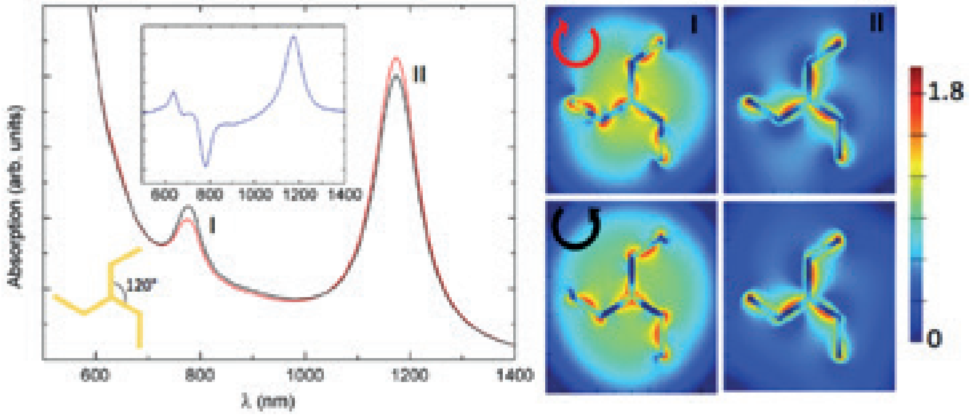

*Fig. 1. (a) Simulated absorption spectra for clockwise and anti-clockwise circularly polarized light of the structure depicted in the inset, formed by 6 bars of 225 nm in length and 30 nm in width and thickness, using a Metal-Insulator-Metal configuration with a $SiO_2$ spacer of 100 nm. A difference close to 20% in absorption through the structure between left- and right-circularly polarized light is found.*
*(b) $Log(|E|^2/|Eo|^2)$ of the peaks labeled as I and II in (a) for clockwise and anti-clockwise circular polarization.*

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## *Posters* Nanostructured materials (NanosMat)

## P40. SYNTHESIS AND CHARACTERIZATION OF NANOSTRUCTURED Pt-Ag-BASED CHALCOGENIDE SEMICONDUCTORS

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Platinum-based chalcogenides have been gaining a lot of attention due to the special electrical and catalytic properties stemming from both the platinum presence and the semiconductor nature of the material [1]. Colloidal nanocrystal synthetic strategy was found to be a perfect candidate to form homogenous and compositionally complex nanostructured systems [2]. Thus, a set of synthesis were designed by changing reaction parameters such as temperature, amount of reactants and also varieties of capping agents in order to form such nanostructured systems. The characterization results suggested that the silver chalcogenide nanocrystals have successfully transformed into compositionally more complex systems by using oleyamine as capping agent at certain temperature by means of cation exchange reaction. Structural and chemical characterization of these novel system suggests the formation of a ternary material with a Ag$_3$PtSe$_2$ stoichiometry.

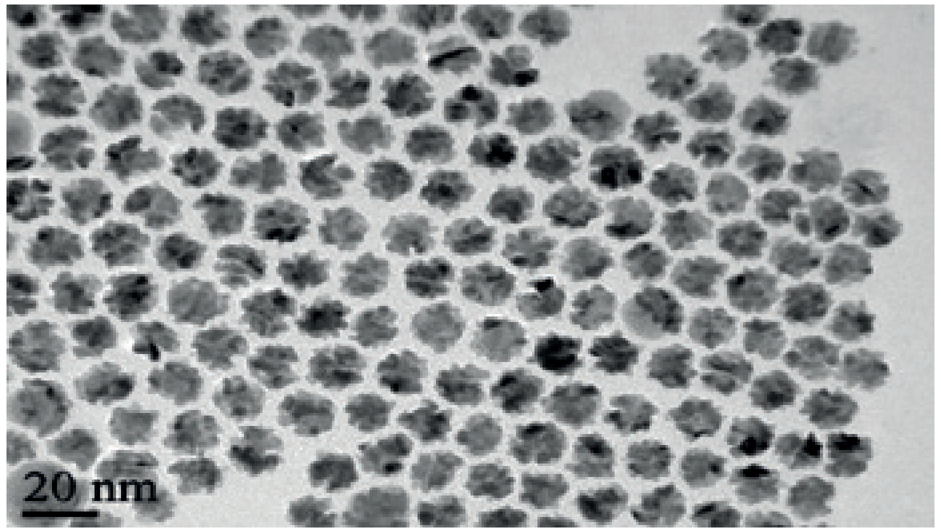

*Figure 1. TEM micrographs of nanocomposite systems at 120 °C*

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## P41. SYNTHESIS AND STUDY OF METAL CHALCOGENIDE NANOPARTICLES: TOWARDS TAILORING HYBRID STRUCTURES

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Achieving control over the design and structure of a material has always been key to the optimization and functionalization of such material [1]. In order to develop novel nanostructured materials, an excellent choice for a synthetic approach is colloidal chemistry, since it allows for a thorough control of both the size and architecture of the materials that can fit in several applications [2]. In this work, we have tailored the composition, morphology and structure of Ag$_2$Se and Cu$_{2-x}$Se nanoparticles (NPs). The understanding of the nature and behavior of these systems led to the synthesis of hybrid nanostructures of the type Ag$_x$Au$_y$X and Cu$_{2-x}$Au$_y$X (where X can be Se or S).

These ternary systems are proving to be very interesting materials. The synthesized Ag$_2$Se NPs have shown to be luminescent in the NIR-I, with tuning possibilities towards lower wavelengths depending on the size of the NPs. Since Ag$_2$S NPs perform fluorescence in the NIR-II, a combination of both chalcogenides is expected to be optically active and tunable. Regarding Cu$_{2-x}$Se NPs, they show a noticeable plasmon resonance band (LSPR) despite being a semiconductor material, which could be modulated by doping it with gold. The Cu$_{2-x}$Au$_y$Se ternary system would be a novel material on its own. Early results suggest that the doping can be tailored, leading to different structures and hybrid materials.

Advanced atomic-resolution electron microscopy techniques are required for the proper characterization and study of these nanomaterials, due to their complex chemical distribution. Local measurements have proven to be essential for the understanding of these systems, relating them to their optical properties so as to gain solid knowledge of their nature.

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## P42. UTILIZING LANGMUIR-BLODGETT METHOD FOR PREPARING OF SERS SUBSTRATE TO DETECT ORGANIC AND WATER POLLUTANT

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Nanoparticle self-assembly is a sturdy and adaptable strategy for the development of functional nanostructured materials, self-assembly methods offering low-cost and scalable methods that can be fine-tuned for many different specific applications. In this work, we prepared a pathway for the fabrication of tailorable two-dimensional lattices of gold nanoparticles to be used as a substrate in Surface Enhanced Raman Scattering (SERS) technic in order to detect of biomolecules and water pollutants. As a first step, nanoparticles are spread in the form of monolayer at the water/air interface at different surface pressures and compressed and tuned to a target lateral density in a Langmuir–Blodgett trough, then transferred monolayer to a properly functionalized solid surface. Once firmly adhered to the substrate, the lattice of nanoparticles can be directly used or be further processed using electroless gold deposition to let the nanoparticles grow, thus tuning the plasmonic response and SERS enhancement. Various organic molecules and water pollutant such as 4-MBA, Carbaryl and Thyram were adsorbed on the substrates in order to detect with SERS technique. The resonance was observed in the peak of SERS graphs of 4-MBA and water pollutants under the optimum condition (10 nm Gold nanoparticle size and 13-14 mNm-1 as surface pressure).

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## P43. CARBON BASED MATERIALS GROWTH PROCESS EFFECT ON 304 STAINLESS STEEL SUBSTRATES

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Carbon based materials have earned a well-deserved reputation. Thanks to their physical, chemical, electronic, thermal, mechanical and optoelectrical properties, research and industrial groups all over the world are constantly improving their production. They are a versatile material that can be obtained by different ways. In addition, flexible displays, sensors, and energy storage devices can be manufactured using this kind of material. The development of energy storage devices is one of the applications in which carbon based materials, as carbon nanotubes (CNTs) or graphene nanowalls (GNWs), stand out. Another interesting aspect of these materials is that they can be obtained on conductive materials, such as nickel, copper or steel. The last one is precisely one of the substrates that we and other research groups have selected to support the carbon-based materials. In a hydrogen-rich atmosphere, at temperatures in the range 600 to 730 °C, with the use of precursor gases (acetylene or methane) and using plasma technology, uniform forests of these structures have been obtained on the surface of 304 stainless steel. However, the growth process can produce counterproductive effects on the steel substrates. Above all, decrease its flexibility, increase the crystal size or decrease its corrosion resistance. In that way, we believe it is appropriate to present some of our results observed in 304 stainless steel during our experiments. SEM images, XPS analysis and XRD allowed us to document changes in the surface and also in the bulk material.

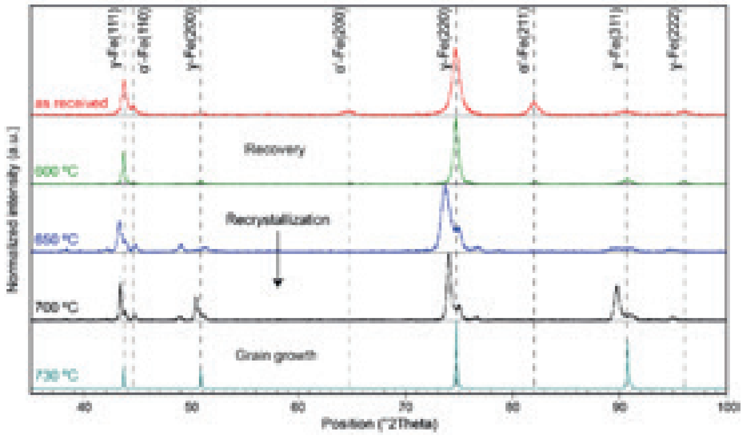

*Figure 1. XRD patterns of untreated and reduced samples of 304 stainless steel at 600, 650, 700 and 730 °C*

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## P44. SUPER-CAPACITIVE PERFORMANCE OF MANGANESE DIOXIDE/GRAPHENE NANO-WALLS ELECTRODES DEPOSITED ON STAINLESS STEEL CURRENT COLLECTORS

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Graphene nano-walls (GNWs) are promising materials that can be used as an electrode in electrochemical devices. We have grown GNWs by inductively-coupled plasma-enhanced chemical vapor deposition on stainless steel (AISI304) substrate. In order to enhance the super-capacitive properties of the electrodes, we have deposited a thin layer of $MnO_2$ by electrodeposition method. We studied the effect of annealing temperature on the electrochemical properties of the samples between 70°C and 600°C (Fig.1). Best performance for supercapacitor applications was obtained after annealing at 70°C with a specific capacitance of 104 $F\cdot g^{-1}$ at 150 $mV\cdot s^{-1}$ and a cycling stability of more than 14k cycles with excellent coulombic efficiency and 73% capacitance retention. Electrochemical impedance spectroscopy, cyclic voltammetry, and galvanostatic charge/discharge measurements reveal fast proton diffusion ($1.3\times10^{-13}$ $cm^2\cdot s^{-1}$) and surface redox reaction after annealing at 70°C.

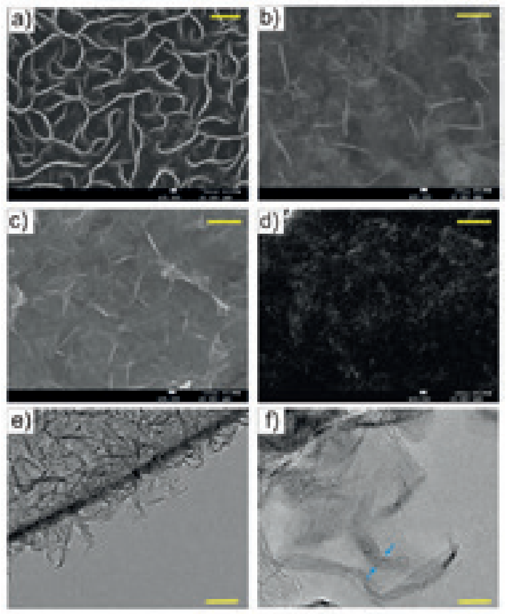

*Figure 1. a) SEM images of MLGNWs grown on SS; b) $MnO_2$/MLGNWs without thermal treatment; c) $MnO_2$/MLGNWs with annealing at 200°C; d) 600°C and e) f) TEM images of as grown MLGNWs. Arrows indicate the thickness of the nanowalls. Scale bars correspond to 500 nm in (a-d). 100 nm in (e) and 10 nm in (f)*

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## P45. STRUCTURAL OPTIMIZATION OF THE DIINDOLOCARBAZOLE CORE AS SEMICONDUCTOR FOR ORGANIC THIN-FILM TRANSISTORS

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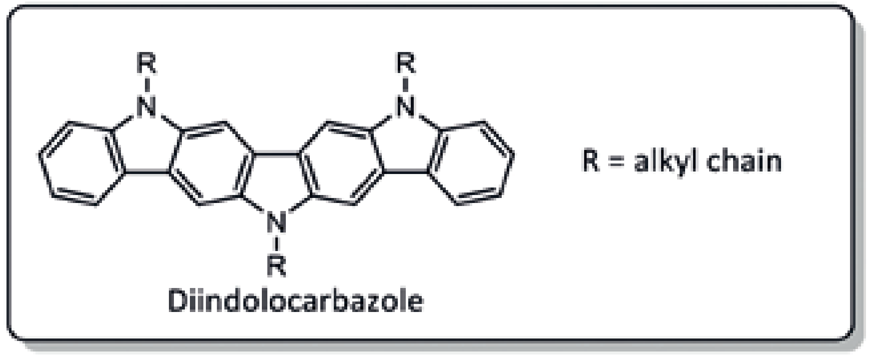
Carbazole-based semiconductors have been gradually setting as important materials within the optoelectronic technology [1]. Derived structures, such as indolocarbazole and triindole, show high thermal stability, π-stacking capability and optoelectronic properties [2]. Thus, carbazole is a very promising building block for constructing novel organic semiconductors with effective charge carrier transport. The aromatic expansion of molecules that mimic pentacene, which remains as one of the top organic semiconductors in terms of charge mobility, combined with the aforementioned properties attached to the carbazole core, was considered in this study both synthetically [3] and in terms of application in vacuum-deposited Organic Thin-Film Transistors (OTFTs).

Herein we present the study of the novel diindolocarbazole core displaying a series of structural variations related to the attached alkyl chains. In fact, the position and length of the alkyl chains affect the intermolecular organization, and thus, the charge-transporting properties of the thin films. Alongside the characterisation of their optoelectronic properties, the integration in OTFTs with different organic dielectrics has confirmed the potential of this new family of materials.



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## P46. GROWTH TEMPERATURE STUDY OF MULTI-LAYER GRAPHENE NANO-WALLS.

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Temperature is one of the significant growth factors for graphene nanowalls. The temperature in PECVD process can be provided by an external source or by the plasma itself or by combining both. It is reported that a temperature above 500°C is in demand for obtaining carbon nanostructures [1,2]. Much lower temperature growth is possible using microwave plasma CVD or helicon plasma enhanced CVD, which permit to grow multi-layer graphene nano-walls (MLGNWs) in 400-700°C temperature range. The optimum growth temperature was established with the aid of transmission electron microscopy, scanning electron microscopy, and Raman spectroscopy. From this temperature study, we have concluded that, the successful MLGNWs grown process starting at 650°C. In addition, we observed that activation energy is at least 2 times lower for graphene grown by PECVD than by CVD. The lower value of activation energy (0.42 eV) allows deposition at low-temperature. The morphology of the MLGNWs grown on different substrates shows a higher nanowalls density and height with increasing growth temperature. The Raman scattering showed the different behaviour of MLGNWs grown on stainless steel (SS304) and c-Si substrates. In the case of MLGNWs/SS304 the number of defects, for the temperature range of 650°C-800°C, was higher than for MLGNWs/c-Si. Moreover, MLGNWs grown on c-Si substrate had a small number of graphene layers in the temperature range of 650-750°C and above 750°C, the number of layers increases due to the graphitic structure formation. For MLGNWs/SS304, the graphite structure (more than 15 graphene layers) was observed over the entire temperature range and for that reason the difference is not noticed at 800°C. MLGNWs synthesis on different substrates at different temperatures depends on the number of the radicals in the gas phase, ions and other active species formed during the plasma deposition. For temperature range 650°C-750°C the hydrocarbon and atomic hydrogen radicals did not show sudden changes. These decreased intensities resulted in differences in the dissociation mechanism of hydrocarbon precursor, such as for temperatures 550°C and 800°C.

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## P47. CARBON NANOSTRUCTURES ON STAINLESS STEEL SUBSTRATE AS ELECTRODES FOR MICROBIAL FUEL CELLS

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Microbial fuel cells (MFCs) are bioelectrochemical systems that can produce bioelectricity from organic matter. Wastewater from urban, domestic or industrial origin can be used as a fuel to produce electricity. In addition, the amount of pollutants and contaminants decreases during the production of bioelectricity [1,2]. Thus, such bioelectrochemical systems produce renewable energy and, simultaneously, can be used as a novel technology for wastewater treatment. However, the efficiencies obtained are still too low and the output voltage of the MFCs need to be increased. In addition, the overall cost of the cell has to be reduced in order to promote this technology into the market. Here, we have studied the growth of graphene nanowalls and carbon nanotubes on stainless-steel substrate 304 (SS), which can be used as electrodes in air-cathode MFCs. Growth parameters have been optimized to obtain vertically aligned and dense carbon nanostructures on both SS foil and mesh. MFCs with different electrodes have been prepared to study the effect of different parameters and to determine whether the presence of carbon nanostructures results in an increase of the electrochemical efficiency. The effect of an oxygen plasma treatment on the properties of the electrodes has been studied as well as the presence of $MnO_2$ catalyst on the cathode, which has been electrochemically deposited to catalyze the oxygen reduction reaction (ORR).

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## Posters Nanoenergy: Production and Storage (NanoEnergy)

### P48. NOBLE METAL-LIKE BEHAVIOR OF MOLYBDENUM CARBIDE-BASED CATALYSTS FOR $CO_2$ REDUCTION AND PHOTOCATALYTIC $H_2$ PRODUCTION

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Nowadays, there is a big interest in the use of $CO_2$ as C1 carbon source; this could contribute to the diminution of $CO_2$ concentration in the atmosphere helping to mitigate the greenhouse effect. One of the methods for $CO_2$ valorization is the reverse water gas shift (RWGS) reaction [1,2], which converts $CO_2$ and $H_2$ into CO and $H_2O$, this reaction is considered a prior step for the production of added value chemicals from $CO_2$/CO/$H_2$ mixtures. The RWGS is an endothermic reaction, which is catalyzed by noble metals.

On the other hand, the energetic scenery is a big issue to be considered for a sustainable development. The use of hydrogen as energy vector has been proposed because its high energy density and clean and efficient use in appropriate fuel cell systems. Solar photocatalytic water splitting is one of the most promising methods for hydrogen production [3]. However, the hydrogen yields are still very low. The photocatalytic transformation of aqueous solutions of biomass-derived alcohols can increase the hydrogen yield and simultaneously generate oxidized products with a higher added value than the initial alcohol. A semiconductor and a co-catalyst, typically a noble metal, usually form the photocatalytic systems. The co-catalyst plays an important role facilitating the separation of photo-induced charges, increasing the lifetime of electron-hole pairs generated in the semiconductor; thus, increasing the $H_2$ yield.

Several transition metal carbides such as molybdenum carbide have been proposed as alternative catalysts to noble metals because they can be prepared from different inexpensive metallic precursors and show Pt-like catalytic behavior. Molybdenum carbides could be proposed as catalysts for reactions involving $H_2$ and $CO_2$ because they interact appropriately with them.

In our group, we are studying new catalytic systems based on transition metal carbides, particularly on molybdenum carbide. Different phases of molybdenum carbide were synthesized ($Mo_2C$ and MoC) by novel sol-gel methods, avoiding the use of conventional reducing and carburizing agents, such as $H_2$ and/or $CH_4$, and thermal treatments at high temperatures. Moreover, new methods of preparation of supported catalysts containing MoxC nanoparticles are proposed. Supports, such as, $Al_2O_3$, $SiO_2$ and $TiO_2$ are used for the preparation of catalysts which resulted highly active and selective for the RWGS reaction. We are also exploring the use of some of these systems in the photocatalytic transformation of aqueous ethanol solutions for $H_2$ production.

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### P49. STUDY OF VC-BASED CATALYSTS FOR $CO_2$ CONVERSION TO CO

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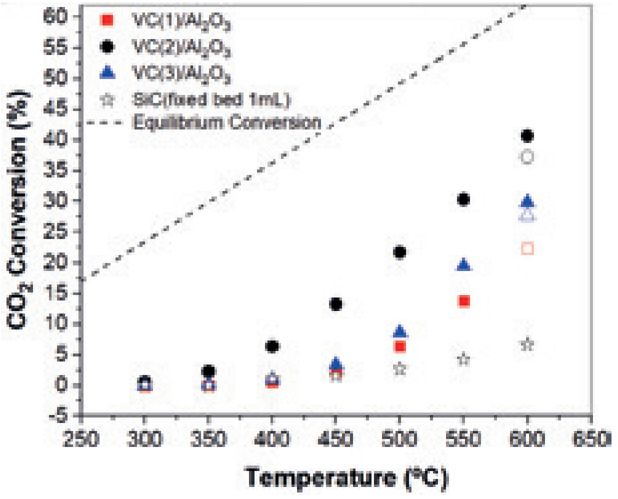
Efforts are in progress in order to reduce the atmospheric concentration of emitted $CO_2$. In this context, the chemical recycling of $CO_2$ and its reuse in the production of fuels or other chemicals is highly attractive. Among different utilization processes, $CO_2$ reduction for CO production, through the reverse water gas shift reaction (RWGS) is an option, which can be contemplated as a previous step for the production of high-added value chemicals and fuels, through well-known technologies as methanol or Fischer-Tropsch synthesis.

Transition metal carbides have recently received much interest because of their activity and selectivity in the RWGS reaction [1,2]. Vanadium carbide-based catalysts (VC) have been scarcely studied in this reaction. Here, we report on new VC systems prepared using a novel sol-gel method and their catalytic behavior in the RWGS reaction. The preparation has been studied as a function of different factors, such as the metal precursor used, the carbon/metal ratio and the conditions of thermal treatment. Subsequently, $Al_2O_3$-supported VC catalysts were also prepared (VC(1)/$Al_2O_3$, VC(2)/$Al_2O_3$ and VC(3)/$Al_2O_3$). The catalysts were characterized by different techniques before and after reaction (Table 1), and their characteristics related to the preparation method used. The catalytic behavior in the RWGS reaction was tested at atmospheric pressure, using $CO_2$/$H_2$=1/3, and between 300°C and 600°C. All catalysts were active under the conditions used (Figure 1) and their catalytic performance are related to their characteristics.

*Table 1. Several characteristics of VC/Al2O3 catalysts.*

| Catalyst | Crystallite size (XRD) (nm) | B.E.T. area fresh ($m^2 g^{-1}$) | B.E.T. area used ($m^2 g^{-1}$) |
|---|---|---|---|
| VC(1)/$Al_2O_3$ | 38 | 150 | 144 |
| VC(2)/$Al_2O_3$ | 6 | 234 | 210 |
| VC(3)/$Al_2O_3$ | 39 | 257 | 248 |

*Figure 1. $CO_2$ conversion of $Al_2O_3$-supported VC catalysts in the RWGS as a function of reaction temperature. Empty symbols represent conversion after 4 h at 600°C.*



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# P50. CUFE$_2$O$_4$ MAGNETIC NANOPARTICLES: SYNTHESIS OPTIMIZATION, STRUCTURES, AND MAIN MAGNETIC AND MECHANICAL PROPERTIES

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Magnetic nanoparticles are a family of materials with an increasing interest in advanced technological applications. More specifically, magnetic ferrites are commonly used in applications such as biomedicine [1], [2], electronics [3], [4], or energy storage [5], [6]. Furthermore, this kind of materials are every time more demanded for microwaves applications [7]–[9] as radar or telecommunications, for instance. They are unique materials for these applications due to their high electrical resistivity, which minimizes the eddy current losses at high frequencies.

These materials are actually prepared by a wide range of chemical methods. Over all the possible options, wet chemical methods offer the possibility to prepare high purity products with a great control over the process variables. Some examples are thermal decomposition [10], hydrothermal [6], [11], solvothermal [12], co-precipitation [13], [14], or sol-gel methods [15]–[17].

In this work, copper ferrite ($CuFe_2O_4$) nanoparticles are synthesized by two wet chemical methods: co-precipitation and citrate sol-gel. Additionally, sol-gel process has been optimized by a *Design of Experiments* (DoE) approach in order to maximize the purity and minimize the particle size of the product. Interesting results have been found when comparing both chemical routes: the control over particle size and purity is different for each approach. Moreover, an important fact stands out: the formation of different crystal structures (cubic or tetragonal) in each method. It opens an important opportunity for designing new materials by controlling the chemical synthesis process.

Finally, their magnetic and mechanical properties are investigated. Pellets are fabricated from the powder samples and are tested by nanoindentation in order to study the dependence of the elastic modulus (E) and hardness (H) with the sintering treatments applied.

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