2018
IN^{2}UB Annual Meeting

BOOK OF ABSTRACTS

5th June 2018

PARANYMPH HALL
FACULTY MEDICINE
UNIVERSITAT DE BARCELONA

Institut de Nanociència
i Nanotecnologia

UNIVERSITAT DE BARCELONA

Editorial Board and Scientific Management: Ifigènia Saborit Villarroya
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Foreword

Dear colleagues,

It is a great pleasure to welcome you to the IN^{2}UB Annual Workshop 2018. As a new director of the Institute, it constitutes a great challenge for me to maintain or improve the legacy laid by the previous two Directors, Prof. Amilcar Labarta and Prof. Jordi Borrell.

Since the year of its creation in 2006, the IN^{2}UB has continuously enhanced its visibility and increased its impact through innovation, technology transfer and education. This is the fruit of its members' efforts to work on crosslinked multidisciplinary and ambitious research. It is also the result of showcasing the IN^{2}UB as a prestigious and attractive platform for the transfer of knowledge. This success also arises from the devotion of the IN^{2}UB researchers to enrich, from their privileged perspective, the Nanoscience teaching programs entertained by the University of Barcelona.

The IN^{2}UB is prepared now to engage on a qualitative leap in its performance during the forthcoming years. For example, the collaborative work between its researchers has intensified with a view to reach the label of Excellence "María de Maeztu" in the near future. Its members have also participated actively to put in place an internationally coordinated Erasmus Mundus Joint Master Degree (EMJMD). With hard work, we aim at partaking of a selected group of most prestigious Institutes from the University of Barcelona.

The IN^{2}UB annual workshop represents an important tool towards the realization of these goals. Indeed, it provides a unique opportunity to foster the exchange of scientific information among its members, as well as personal experiences. It is very pleasing to realize that the attendance of the current edition lies among the highest ever registered, since it reflects on the dynamism and good health of the organization.

For these reasons, I thank all of you for your participation, and specially or international guests Prof. Michael Sherrat (University of Manchester) and Prof. Pere Roca i Cabarrocas (CNRS-Université Paris Saclay). My gratitude goes also to the people that have helped in the organization of the Workshop, most especially Dr. Ifigènia Saborit, Secretary of the Institute.

On behalf of the IN^{2}UB, I wish that you enjoy and take maximum profit from this event.

Sincerely,
GUILLEM AROMÍ

Program

9:00h - 9:30h REGISTRATION

9:30h - 9:45h
WELCOME: **GUILLEM AROMÍ**
Director of Institute of Nanoscience and Nanotechnology (IN^{2}UB)
Dep. Inorganic and Organic Chemistry, Faculty of Chemistry, Universitat de Barcelona

OPENING: **DOMÈNEC ESPRIU**
Vice-Rector for Research Universitat de Barcelona

SESSION 1

GUSTAVO EGEA Department of Biomedicine, Faculty of Medicine, Universitat de Barcelona

09:45h - 10:45h
PLENARY:
MICRO-COMPUTED X-RAY TOMOGRAPHY: 3D IMAGING IN CARDIOVASCULAR DISEASE, INTERVERTEBRAL DISC DEGENERATION AND BREAST CANCER
MICHAEL J. SHERRATT
Senior Lecturer in Molecular Biochemistry /Academic Lead for Year 2 PEP / Division of Cell Matrix Biology and Regenerative Medicine / School of Biological Sciences / Faculty of Biology Medicine and Health / University of Manchester

10:45h - 11:15h
2017-ART GRANTEE:
MICROSCOPIC ORIGIN OF ELECTROSTATIC SURFACE POTENTIAL OF PHOSPHOLIPID LANGMUIR-BLODGETT MONOLAYERS
CARLES CALERO
Department of Condensed Matter Physics, Faculty of Physics, Universitat de Barcelona

11:15h - 12:00h COFFEE BREAK and POSTER SESSION

SESSION 2

PATRICK GAMEZ Department of Inorganic and Organic Chemistry, Faculty of Chemistry, Universitat de Barcelona

12:00h - 12:30h
2017-ART GRANTEE:
DEVELOPMENT OF OXIDIZED CELLULOSIC MICROFILMS AS PLATFORMS FOR MICRODEVICES APPLICATIONS
DANIEL SANCHEZ and XAVIER ANDRÉS
Department of Genetics, Microbiology and Statistics, Faculty of Biology, Universitat de Barcelona

12:30h - 13:00h
DEVELOPMENT OF AN ELECTROCHEMICAL IMMUNOSENSOR FOR ALZHEIMER'S DISEASE DIAGNOSIS
J. MARRUGO
Department of Electronics and Biomedical Engineering, Faculty of Physics, Universitat de Barcelona

13:00h - 13:30h
MODULATION OF β-AMYLOID AGGREGATION WITH FUNCTIONALIZED GOLD NANOPARTICLES
ANA B. CABALLERO
Department of Inorganic and Organic Chemistry, Faculty of Chemistry, Universitat de Barcelona

13:30h - 15:00h LUNCH

SESSION 3

ENRIC BERTRAN Department of Applied Physics, Faculty of Physics, Universitat de Barcelona

15:00h - 16:00h
PLENARY:
LOW TEMPERATURE PLASMA DEPOSITION PROCESSES: FROM AMORPHOUS SILICON TO CLUSTERS, NANOCRYSTALS, NANOWIRES, AND EPITAXIAL GROWTH
PERE ROCA I CABARROCAS
Research Director at CNRS / Director of PICM Laboratory and FedPV / Laboratory of Physics of Interfaces and Thin Layers (LPICM) / L'École polytechnique / Université Paris-Saclay

16:00h - 16:30h
EFFECTS OF SHAPE AND SPATIAL ARRANGEMENT OF NANOPARTICLE ASSEMBLIES ON THEIR HYPERTHERMIA PERFORMANCE
ÒSCAR IGLESIAS
Department of Condensed Matter Physics, Faculty of Physics, Universitat de Barcelona

16:30h - 17:15h COFFEE BREAK and POSTER SESSION

SESSION 4

ALBERT ROMANO Department of Electronics and Biomedical Engineering, Faculty of Physics, Universitat de Barcelona

17:15h - 17:45h
2017-ART GRANTEE:
NANOPARTICLE-ASSISTED LAB-ON-A-CHIP (LOC) FOR MONITORING CANCER CELL TREATMENTS
ROMEN RODRIGUEZ-TRUJILLO
Department of Electronics and Biomedical Engineering, Faculty of Physics, Universitat de Barcelona

17:45h - 18:15h
LIVING FLOWS IN CONFINEMENT
JÉRÔME HARDOÜIN
Department of Materials Science and Physical Chemistry, Faculty of Chemistry, Universitat de Barcelona

18:15h - 18:30h
CLOSING REMARKS: **JORDI BORRELL**
Department of Pharmacy and Pharmaceutical Technology and Physical-Chemical,
Faculty of Pharmacy and Food Sciences, Universitat de Barcelona

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NANOMAGNETISM, NANOELECTRONICS AND NANOPHOTONICS [NELECTROMAGΦ] RESEARCH AREA

NANOSTRUCTURED MATERIALS [NMATERIALS] RESEARCH AREA

NANOENERGY: PRODUCTION, STORAGE AND ENVIRONMENT [NENERGY] RESEARCH AREA

INVITED SPEAKERS

PLENARY LECTURES

ART (AJUT A LA RECERCA TRANSVERSAL) GRANTEE 2017 CALL

INVITED SPEAKERS

PLENARY LECTURES

MICHAEL J. SHERRATT

Senior Lecturer in Molecular Biochemistry I Academic Lead for Year 2 PEP I Division of Cell Matrix Biology and Regenerative Medicine I School of Biological Sciences I Faculty of Biology Medicine and Health I University of Manchester

MICRO-COMPUTED X-RAY TOMOGRAPHY: 3D IMAGING IN CARDIOVASCULAR DISEASE, INTERVERTEBRAL DISC DEGENERATION AND BREAST CANCER

In contrast to conventional methods for visualising the 3D structure of tissues and organs, phase contrast micro-computed X-ray tomography (microCT) can rapidly image the internal morphology of large volumes of unstained, native tissues at sub-micron resolutions. When combined with advanced image analysis techniques (digital volume correlation) and high X-ray flux (synchrotron) sources microCT imaging can also be used to quantify 3D strain in dynamically deformed tissues. This presentation will discuss the application of microCT to cardiovascular diseases (Marfan syndrome and atherosclerosis), intervertebral disc structure, mechanics and degeneration and the biophysical causes of raised mammographic density (an important risk factor for breast cancer).

Biography

Following PhD and postdoctoral positions with Prof. Cay Kielty at the University of Manchester, Mike was awarded an AgeUK Fellowship and then Senior Fellowship. He is currently a Senior Lecturer in Molecular Biochemistry at the University of Manchester and director of the BioAFM (biological atomic force microscopy) Facility at the same institution. He has served as treasurer for the British Society for Research on Ageing and is an editorial board member for the journals Maturitas and Scientifi Reports.

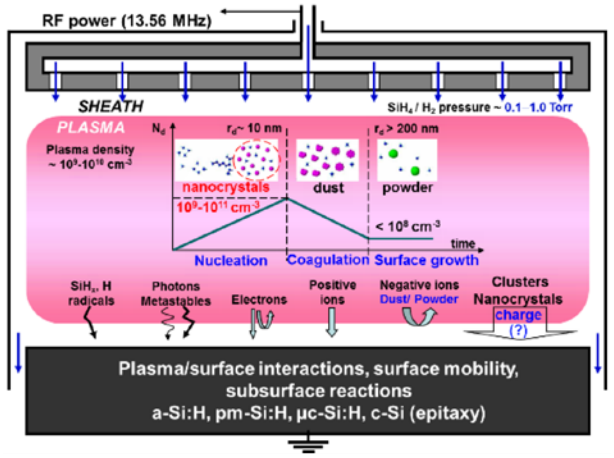
His research is focused on characterising the causative mechanisms and the structural and mechanical consequences of ageing in extracellular matrix rich tissues including skin, arteries, breast and cartilage. In order to achieve these goals Mike's lab has:
i) developed novel atomic force microscopy and microCT methodologies to visualise tissue architecture,
ii) demonstrated that elastic fibre associated proteins are key targets of ultraviolet radiation,
iii) shown that bioinformatic approaches can be used to identify novel ageing biomarkers and iv) demonstrated that raised mammographic density (a risk factor for breast cancer (is associated with localised collagen re-organisation and stiffening.
He is the author of more than 100+ academic works which collectively have been cited more than 2600 times.

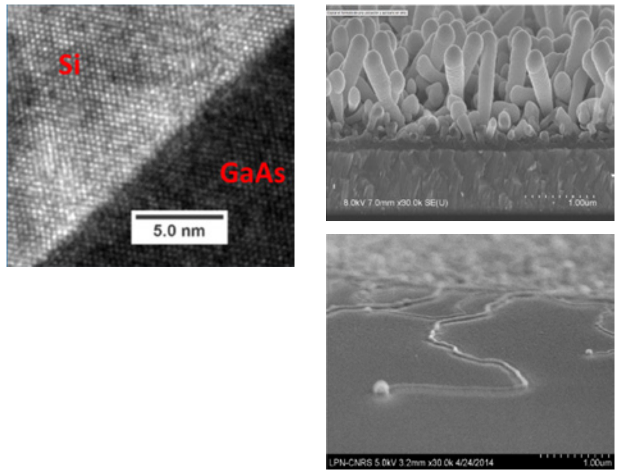
PERE ROCA I CABARROCAS

Research Director at CNRS Director of PICM I Laboratory and FedPV I Laboratory of Physics of Interfaces and Thin Layers (LPICM) I École Polytechnique I Université Paris-Saclay

LOW TEMPERATURE PLASMA DEPOSITION PROCESSES: FROM AMORPHOUS SILICON TO CLUSTERS, NANOCRYSTALS, NANOWIRES AND EPITAXIAL GROWTH

Silicon thin film technology has been driven by hydrogenated amorphous silicon thin films which are routinely produced using silane and silicon tetrafluoride plasmas. While SiH_3 is often considered as the main radical for the obtaining of such films, we have shown that changing the process to conditions where silicon clusters and nanocrystals are produced in the plasma can lead to high deposition rates and improved materials, such as hydrogenated polymorphous silicon and polycrystalline silicon [1,2]. Moreover, by changing the substrate from glass to crystalline silicon, it is possible to produce epitaxial thin crystalline silicon films which can be transferred to foreign substrates for flexible solar cells and electronic devices [3,4]. Even more interesting, this low temperature epitaxy can be extended to doped films as well as to germanium and SiGe alloys and their heteroepitaxial growth on GaAs [5], which opens their way to high efficiency tandem solar cells. Last but not least, combining PECVD with low melting temperature metal particles such as indium and tin opens the way to the plasma-assisted VLS growth of vertical silicon nanowires, which allow to achieve efficient light trapping and carrier collection in radial junction solar cells [6] or even to growth the c-Si nanowires in-plane for stretchable electronic applications [7].





Schematic diagram of a RF glow discharge reactor. A wide range of thin films can be obtained, from amorphous a-Si:H to ordered epitaxial films and silicon nanowires

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Biography

Prof. Pere Roca i Cabarrocas, is an Electrical Engineer from the "Universitat Politécnica de Barcelona". In 1984 he moved to Paris, where he received his PhD from University Paris VII in 1988. After a post-doc position in Princeton University he joined the Laboratory of Physics of Interfaces and Thin Films at Ecole Polytechnique where he holds a position as a CNRS director of research and as a professor. Since 2012 he is the director of LPICM and the French Federation on PV since 2014. He has thirty years of experience in the field of plasma deposition of silicon based thin films for large area electronic applications. His topics cover the study of RF discharges for the deposition of amorphous, polymorphous and microcrystalline silicon thin films. He has used in-situ diagnostic techniques such as UV-visible ellipsometry, Kelvin probe and time resolved microwave conductivity to understand the growth of these materials and apply them to the production of devices such as solar cells, thin film transistors, particle detectors, sensors,… More recently he has been applying silicon nanocrystals synthesized in the plasma as building blocks for the epitaxial growth of silicon thin films and Si/Ge quantum wells. On the other hand, he has extended the plasma processes to the growth of vertical silicon nanowires for third generation solar cells and of horizontal ones for planar electronic applications. He was the recipient of the Médaille Blondel in 2004, of the Innovation Award at Ecole Polytechnique in 2009 and the Silver medal from CNRS in 2011. Since 2016 he is invited professor at Nara Institute of Technology. He has over 450 papers in peer reviewed journals, holds 34 patents and has supervised 47 PhD students.

INVITED SPEAKERS

ART (AJUT A LA RECERCA TRANSVERSAL) GRANTEE 2017 CALL

MICROSCOPIC ORIGIN OF ELECTROSTATIC SURFACE POTENTIAL OF PHOSPHOLIPID LANGMUIR-BLODGETT MONOLAYERS

C. Calero[1,2], F. Chiricotto[3] , O. Domènech[2,4], J. Hernández-Borrell[2,4], G. Franzese[1,2]

[1] Departament de Física de la Matèria Condensada, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona
[2] Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, Spain
[3] Dipartimento di Matematica e Fisica, Università di Roma Tre, Via della Vasca Navale 84, 00146 Roma Italy
[4] Departament de Fisicoquímica, Universitat de Barcelona, Avinguda Joan XXIII 27-31, 08028 Barcelona

Phospholipid Langmuir-Blodgett monolayers are used as model systems to understand the interaction of phospholipids with other phospholipids and biomolecules present in biological membranes (such as proteins and cholesterol), of great relevance since their interaction determine the fluidity and the correct performance of the membrane's functions. In particular, the electrostatic potential drop across Langmuir-Blodgett monolayers and its dependence on lateral pressure are used to gain insight on the configuration of lipids and their interaction with membrane proteins, cholesterol and water. Despite being a macroscopic quantity measured over the whole monolayer, it is correlated with the orientation of lipids with respect to the plane of the monolayer and with the configuration of hydration water, although the relation is complex and only interpretations using oversimplified models have been used. As a consequence, the anomalous behavior of the electrostatic potential (or the perpendicular dipolar moment) in a range of lateral pressures of biological significance is still unexplained.

Here, we propose a combined effort with experiments and computer simulations to ascertain the correlation between the macroscopic electrostatic potential generated by the monolayer and the local configuration of lipids and hydration water. We perform extensive all-atom molecular dynamics simulations of phospholipid Langmuir-Blodgett monolayers in a range of lateral pressures which capture the electrostatic properties measured in experiment. The atomic detail of the simulations allows us to investigate the dominant contributions to the electrostatic potential and identify the origin of the measured anomaly. In addition, the results from the simulations are used to test the range of validity of the current theoretical models.

DEVELOPMENT OF OXIDIZED CELLULOSIC MICROFILMS AS PLATFORMS FOR MICRODEVICES APPLICATIONS

D. Sánchez[1], X. Andrés[1], J. Martínez[1,2], P. Díaz[1,2], F.I.J. Pastor[1,2], E. Xuriguera[2,3], Ò. Domènech[2,4], S.V. Valenzuela[1,2]

[1] Department of Genetics, Microbiology and Statistics, Faculty of Biology, Universitat de Barcelona, Av. Diagonal 643, 08028 Barcelona, Spain
[2] Institute of Nanoscience and Nanotechnology (IN^{2}UB), Universitat de Barcelona, Spain
[3] Department of Materials Science and Physical Chemistry. Faculty of Chemistry, Universitat de Barcelona, Martí i Franquès, 1-11, 08028 Barcelona, Spain.
[4] Department of Pharmacy and Pharmaceutical Technology and Physical Chemistry, Faculty of Biology, Universitat de Barcelona, Joan XXIII, 27-31, 08028 Barcelona, Spain.

Cellulose is the major component of lignocellulose and the most abundant source of renewable carbon on earth. It has become one of the most powerful and sustainable alternatives to petroleum as a platform for generation of biofuels, chemicals, and solvents and recently, great efforts have been done for the development of bio-based new materials. Nevertheless, it has not yet been possible to fully exploit industrial applications of cellulosic materials, due to their recalcitrant nature. The study on lignocellulosic degrading enzymes mainly involves hydrolytic enzymes, but this paradigm has been completely revolutionized by the recent discovery of Lytic Polysaccharide MonoOxygenases or LPMOs: these non-hydrolytic enzymes are able to disrupt the polymer by an oxidative mechanism, as follows: 1) LPMOs cleave glyosidic bonds that are inaccessible to polysaccharide hydrolytic enzymes through a mechanism dependent on copper ion, boosting the overall efficiency of enzymatic biomass degradation, 2) The activity of LPMOs has been demonstrated by the release of oxidized soluble cello-oligosaccharides from cellulosic substrates, but the mode of action of these enzymes on the solid surface of the polymer remains still unclear.

Oxidative chain cleavages in crystalline areas of cellulose are expected to cause local disruptions of the ordered structure of cellulose; therefore, LPMOs might facilitate the action of hydrolytic enzymes. To provide relevant insights based on direct evidence, a serial of cellulosic substrates with decreasing degrees of crystallinity will be produced, treated with LPMOs and analysed by AFM. Once the effect of the LPMOs is determined, the development of oxidized cellulosic microfilms as platforms for the design of sustainable microdevices for industrial applications is projected.

NANOPARTICLE-ASSISTED LAB-ON-A-CHIP (LOC) FOR MONITORING CANCER CELL TREATMENTS

John González-Murillo[1,2], Marta Monge-Azemar[2,5,6], María José García-Celma[2,5], Winnie E. Svendsen[4], Josep Samitier[1,2,3], Mauricio Moreno[1,2], Albert Romano-Rodríguez[1,2] and Romen Rodríguez-Trujillo[1,2,3]

[1]Department of Electronics and Biomedical Engineering, Universitat de Barcelona, Barcelona, 08028, Spain
[2]Institute of Nanoscience and Nanotechnology (IN2UB), Universitat de Barcelona, 08028 Barcelona, Spain
[3]Nanobioengineering Group, Institute for Bioengineering of Catalonia (IBEC-BIST), 08028 Barcelona, Spain
[4]Department of Micro- & Nanotechnology, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark
[5]Department of Pharmacy and Pharmaceutical Technology and Physical Chemistry, Universitat de Barcelona, Barcelona, 08028, Spain
[6]Institute of Advanced Chemistry of Catalonia (IQAC-CSIC), CIBER in Bioengineering, Biomaterials and Nanomedicine, Jordi Girona 18-26, 08034, Barcelona, Spain

The design of biocompatible nanocarriers to treat or tag specific tumor or diseased cells is a challenge. Nanoparticles have demonstrated to be excellent carriers for drug delivery and can facilitate increased intracellular uptake of them to specific cellular targets [1]. The ability of monitoring the viability of cancer cells treated with a specific drug can determinably influence the applied therapy and have a strong effect on the associated morbidity rates. In particular, it has been reported that cancer cells experiment morphological membrane changes when exposed to some therapeutic drugs that induce apoptosis, altering overall electrical properties that differ from non-treated cells [2]. Single-cell electrical impedance spectroscopy (sc-EIS) is a label-free technique, which brings the possibility to detect cancer cells viability based on their intrinsic electrical properties. It permits identifying the changes in the electrical properties of cells without the need of any kind of pre-treatment steps used typically in commercial flow cytometers or colorimetric assays.

In this work, a sc-EIS microcytometer [2] has been used in order to address the viability test. The chip is made in a glass wafer by means of standard UV photolithography and metal evaporation. It is composed by 100nm thick gold coplanar electrodes, a 30 μm thick layer of SU8 to make a microfluidic channel and a flat PDMS gasket used to seal the channel. The Poly(lactic-co-glycolic acid) (PLGA) nanoparticles have been produced from nano-emulsions by the PIC method using the PBS 0.16 M (W)/polysorbate 80 (S)/[4 wt% PLGA in ethyl acetate] (O) system. A HeLa cells suspension, previously treated with PLGA nanoparticles drug-loaded with Paclitaxel, was injected into the microcytometer. Impedance signals acquired were processed to make the cell viability assessment by comparing the amplitude of the high (HF) and low frequency (LF) components.

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ORAL PRESENTATIONS

ORAL PRESENTATIONS

MODULATION OF Β-AMYLOID AGGREGATION WITH FUNCTIONALIZED GOLD NANOPARTICLES

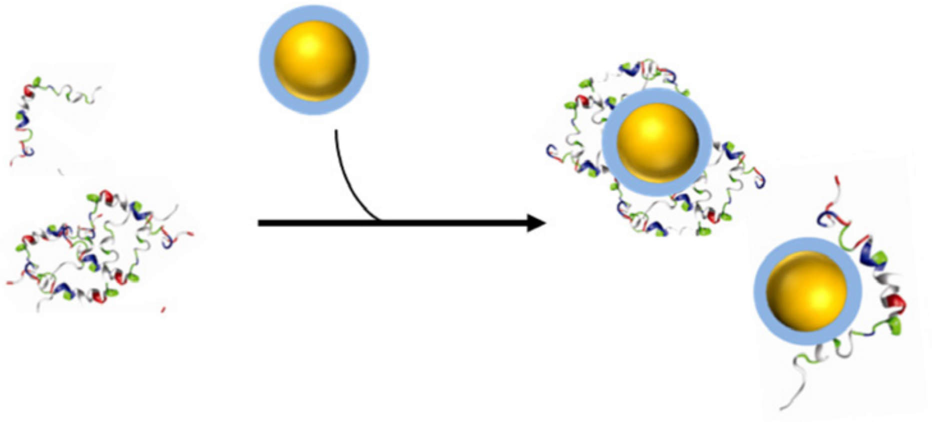
Ana B. Caballero[1], Guillem Vázquez[1], Francesca Canyelles[1], Raimon Sabaté[2], Patrick Gámez[1,3]

[1] *Dept. Inorganic and Organic Chemistry, Facultat de Química, Universitat de Barcelona, Martí I Franquès, 1-11, 08028 Barcelona (Spain)*
[2] *Dept. Physical Chemistry, Faculty of Pharmacy, Avda. Joan XXIII 27-31, Universitat de Barcelona, 08028 Barcelona*
[3] *Institució Catalana de Recerca i Estudis Avançats (ICREA), Passeig Lluís Companys 23, 08010 Barcelona (Spain).*
E-mail ana.caballero@qi.ub.es

Amyloid aggregates are associated with a wide range of neurodegenerative disorders such as Alzheimer's disease. To date, research has been intensely devoted to the inhibition of amyloid aggregation by small molecules. Only very recently, nanomaterials have been reported as effective agents to suppress amyloid aggregation, and some have shown remarkable potential as diagnostic tools. However, the nature of the protein-nanomaterial interaction and thus their mechanism of action are not well understood yet [1, 2, 3].

In our group, we are developing polymer-coated gold nanoparticles with the aim of "rationalizing" their mode of action against amyloid beta aggregation. To this end, the role of key factors, such as the size or the surface functionalization, on the kinetics and thermodynamics of this aggregation process has been investigated.

In the present communication, the state of the art of this rapidly emerging topic will be briefly described together with our latest results. Further discussion on the perspectives regarding the use of rationally designed nanodrugs to treat amyloid-related diseases will be encouraged with conference participants.



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Acknowledgements

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LIVING FLOWS IN CONFINEMENT

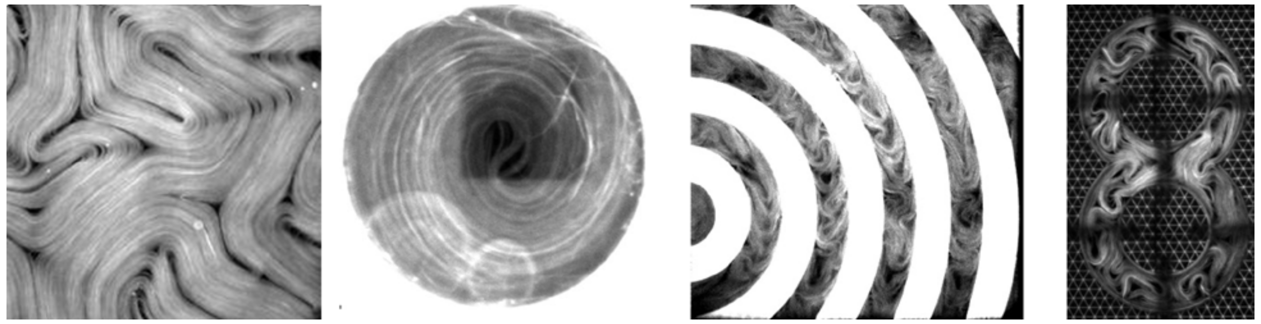
Jérôme Hardoüin[1,2], Teresa López[3], Jordi Ignés-Mullol[1,2] and Francesc Sagués[1,2]

[1] *Departament de Ciencia Materials i Quimica Fisica, Universitat de Barcelona, C. Marti i Franques 1, 08028 Barcelona, Spain*
[2] *Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, 08028, Barcelona, Spain*
[3] *Laboratoire Gulliver, UMR CNRS 7083, ESPCI Paris, Barcelona, PSL Research University*

Despite the outstanding variety of shape transformations that living cells can undergo, their elementary source of motion is a fairly universal mechanism involving two main components: rigid filaments, such as microtubules, and molecular motors, that move along the microtubules with cargo-carrying capabilities. Undefined microscopically, the macroscopic features of deformation (transport, directionality, vorticity) become emerging properties of the microtubule collective motion.

These properties are sensitive to external parameters, such as confinement or chemical signaling. In this work, we study the the dynamics of an in vitro active gel composed of microtubules and motors. When clustered by depletion and segregated to a water/oil interface, such a dense suspension of microtubules can develop a nematic liquid crystal phase, where topological defects spontaneously form and move in a chaotic way [1]. Previous work in the lab has demonstrated the possibility to control the active flows through addressable soft interfaces such as liquid crystals under a magnetic field. The aim of the present study is to investigate the role of surface confinement and curvature.

Recent simulations have shown that, when confined to narrow channels, the initially chaotic motion of the defects transits to more ordered flow regimes, where vortex lattices and laminar flows can be observed [2]. In this talk, we will show experimental evidence of the spontaneous transitions from chaotic to ordered regimes induced by confinement. We use 3D printing to produce flat confining cells that we place at a water/oil interface, where the active nematic is formed. By tuning the activity of the gel as well as the geometry and topology of the confining cell, we validate the simulation predictions and show that confinement in toroidal geometries can lead to spontaneous net active transport.



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Acknowledgements

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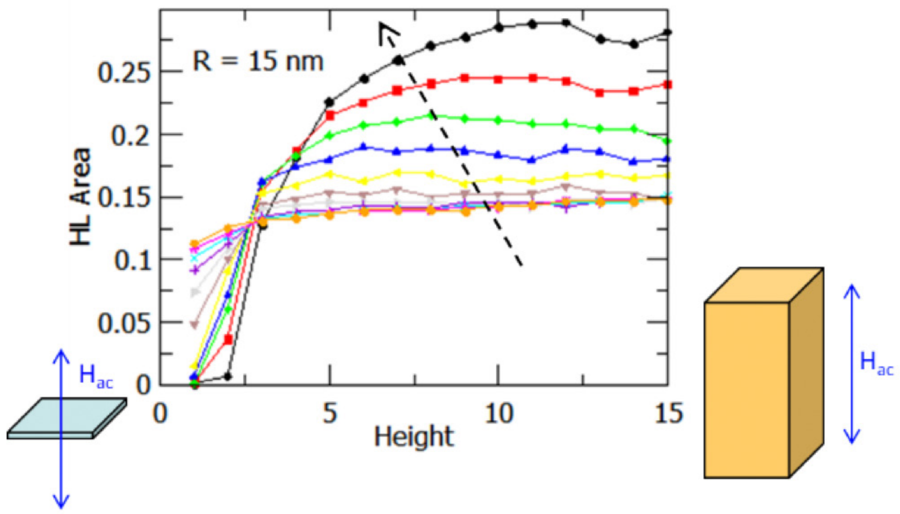
EFFECTS OF SHAPE AND SPATIAL ARRANGEMENT OF NANOPARTICLE ASSEMBLIES ON THEIR HYPERTHERMIA PERFORMANCE

Òscar Iglesias[1], Xavier Martín-Rey[1]
[1] *Dpt. de Física de la Matèria Condensada and IN^{2}UB, UB, Av. Diagonal 647, 08028 Barcelona, Spain*

Magnetic hyperthermia is one of the most promising biomedical applications of magnetic nanoparticles (NP) and is intended to be alternative to cancer therapies based on drug delivery and radiotherapy. It is based on the fact that magnetic NP dissipate heat when an oscillating magnetic field is applied to them in a quantity (specific absorption rate, SAR) that is closely related to the area of the hysteresis loop. The main problem in the field has become to find the suitable range of parameters that maximize SAR for a given material [1], SAR depends of course on the amplitude of the applied magnetic field and its frequency, but also on intrinsic parameters of the NP such as saturation magnetization, anisotropy, shape and size [2]. Although the role of external parameters is somehow well contrasted, there is still ongoing controversy on the role that particle interactions play on SAR because both enhancement and suppression when increasing the NP concentration have been reported. Here, we will present the results of theoretical modelling and Monte Carlo simulations of assemblies of NP interacting through dipolar interactions (DI) in the macrospin approximation [4], studying the effects that interparticle separation, particle size and spatial arrangement of the NP have on SAR. In particular, we will show results for spin chains, randomly placed NP with varying concentrations, and assemblies in SC lattices with different shape. It is found that formation of chain-like arrangements or in assemblies with prolate , lead to considerable increases in SAR due to DI. (Work supported by Spanish MINECO (MAT2015-68772-P), Catalan DURSI (2014SGR220) and EU FEDER funds (Una manera de hacer Europa) also CSUC for supercomputer facilities).



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DEVELOPMENT OF AN ELECTROCHEMICAL IMMUNOSENSOR FOR ALZHEIMER'S DISEASE DIAGNOSIS

J. Marrugo[1,2], J. Samitier[1,2,3], M. Mir[1,2]
[1] *Nanobioengineering Laboratory, Institute for Bioengineering of Catalonia (IBEC), Baldiri Reixac 10-12, Barcelona, Spain*
[2] *Department of Electronics, Barcelona University, Marti i Franques 1, Barcelona, Spain*
[3] *Centro de investigación Biomédica en Red de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), María de Luna 11, 50018, Zaragoza, Spain*

AD is a neurodegenerative disorder mainly characterized by a functional deterioration of the brain due to an accumulation of several biomarkers. Currently there are selected biomarkers for diagnosis in Cerebrospinal Fluid (CSF); however, the extraction of this type of sample is risky and painful for the patient. Therefore, there is an urgent need for a detection method using sensitive and selective biomarkers from blood, such as KYNA, a biomarker related with inflammatory processes. This paper describes the development of an electrochemical immunosensor for KYNA detection, based on successive modification steps of a multi-electrode gold array. The resultant sensors were characterized using cyclic voltammetry (CV), chronoamperometry (CA), and electrochemical impedance spectroscopy (EIS). Two different sensor platforms were studied for this purpose, showing a better performance the one based on an organized monolayer of bioreceptors. The proposed biosensor could respond to KYNA with a linear calibration range from 10 pM to 100nM using CA and EIS, obtaining a LOD of 22.6 pM and 23.9 pM, respectively. This new biosensor exhibited a fast response, high sensitivity and selectivity, and can be served as a significant step towards the real application of the immunosensor in clinical diagnosis and prognosis monitoring.

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POSTERS

RESEARCH AREAS:

- MODELING AND SIMULATION OF SYSTEMS AND PROPERTIES OF MATTER IN THE NANOSCALE (NANOMODELS)
- NANOBIOTECHNOLOGY (NBIOTECH)
- NANOPHARMACOTHERAPY (NPHARMA)
- NANOMAGNETISM, NANOELECTRONICS AND NANOPHOTONICS (NELECTROMAGΦ)
- NANOSTRUCTURED MATERIALS (NMATERIALS)
- NANOENERGY: PRODUCTION, STORAGE AND ENVIRONMENT (NENERGY)

POSTERS

MODELING AND SIMULATION OF SYSTEMS AND PROPERTIES OF MATTER IN THE NANOSCALE (NANOMODELS) RESEARCH AREA

1 TOWARD A COHERENT PICTURE OF THE LOW-DENSITY, HIGH DENSITY AND VERY HIGH-DENSITY FORMS OF BULK WATER

L.E. Coronas[1], V. Bianco[2], A.W. Zantop[3], and G. Franzese[1,4]

[1] *Departament de Física de la Matèria Condensada, Universitat de Barcelona, 08028 Barcelona, Spain*
[2] *Faculty of Physics, University of Vienna, 1090, Vienna, Austria.*
[3] *Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany*
[4] *Institut de Nanociència i Nanotecnologia (IN²UB), 08028 Barcelona, Spain*

We study, by Monte Carlo simulations, a coarse-grained model for bulk water that includes many-body interactions associated to water cooperativity. The model is computationally efficient and allows us to equilibrate water at extreme low temperatures in a wide range of pressures. Our results show the presence of a low density liquid (LDL) and a high density liquid (HDL) forms of water, separated by a liquid-liquid phase transition (LLPT) ending in a liquid-liquid critical point (LLCP) 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 clarify fundamental properties of bulk water that are consistent with the available experimental data.

2 NANOPARTICLE SIZE EFFECTS IN THE FORMATION OF THE PROTEIN CORONA

S. Samatas[1,2], M. Fernández[1], O. Vilanova[1,2], and G. Franzese[1,2]

[1] *Departament de Física de la Matèria Condensada, Universitat de Barcelona, 08028 Barcelona, Spain*
[2] *Institut de Nanociència i Nanotecnologia (IN²UB), 08028 Barcelona, Spain*

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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NANOBIOTECHNOLOGY (NBIOTECH) RESEARCH AREA

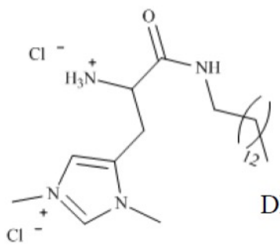
3 CATIONIC COLLOIDAL SYSTEM BASED ON AMINO ACID-BASED SURFACTANTS: PHYSICOCHEMICAL AND BIOLOGICAL CHARACTERIZATION

Vanesa Álvarez[1,2], Lourdes Pérez[1], Ramon Pons[1], Aurora Pinazo[1] and M.Carmen Morán[2,3]

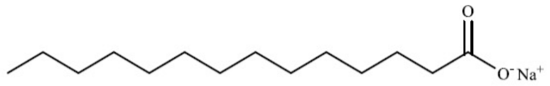
[1] *IQAC-CSIC Institut de Quimica Avançada de Catalunya, 08034 Barcelona, Spain*
[2] *Departament de Bioquímica i Fisiologia-Secció Fisiologia, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, 08028 Barcelona, Spain*
[3] *Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, 08028 Barcelona, Spain*

Nowadays, the design of efficient liposomal system for drug delivery is of considerable biomedical interest. Vesicles prepared from surfactant mixtures may offer several advantages due to their spontaneous formation and their long term stability [1]. However, despite the significant scientific interest and promising potential, the safety of vesicles systems remains a growing concern because of their unpredictable biological effects.

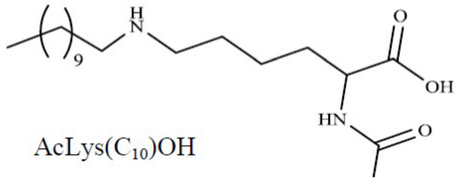
Recently our group has prepared monocatenary cationic histidine-based surfactants of different alkyl chain length. The polar head of these surfactants consists of the histidine amino-acid with methylene groups at N(π) and N(τ)-positions on the imidazole group of histidine. Given their simple chemical structure these new surfactants can be prepared using a straightforward and economical procedure. The C14 homologue (DMHNHC14) showed remarkable growth inhibition activity against several Gram-positive and Gram-negative bacteria as well as fungi [2].



DMHNHC$_{14}$



C$_{13}$COOH



AcLys(C$_{10}$)OH

Cationic colloidal systems composed by mixtures of the C14 homologue (DMHNHC$_{14}$) with sodium miristate (C$_{13}$COOH) or N-acetyl,N-Lauroyl lysine (AcLys(C$_{10}$)OH) have been characterized by means of critical aggregation concentration, size distribution and zeta-potential measurements. The CAC values obtained for the DMHNHC$_{14}$/C$_{13}$COOH and DMHNHC$_{14}$/AcLys(C$_{10}$)OH mixtures are much more lower than those showed by pure compounds. The structure of aggregates was studied using SAXS at Alba Synchrotron. The DMHNHC$_{14}$/C$_{13}$COOH mixtures with high content of the histidine derivative contain vesicles with a mean diameter of about 250 nm and positive z-potential values. The DMHNHC$_{14}$/AcLys(C$_{10}$)OH mixtures shows viscosity and aggregates of different size (vesicles and micelles) has been observed by DLS. These formulations showed good stability and no separation phases were observed during six weeks. Cytotoxicity assays have been also performed using representative cell lines: 3T3· fibroblast, HaCaT keratinocytes and HeLa tumoral cell line.

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4 FORCE PROFILE AND BACKSCATTERED LIGHT LOSS DETERMINATION IN AN OPTICAL TRAP USING MOMENTUM CHANGE METHOD

R. Bola[1,2], F. Català[1,2], R. Serrano[1], E. Martín-Badosa[1,2] and M. Montes-Usategui[1,2]

[1] *Optical Trapping Lab – Grup de Biofotònica, Departament de Física Aplicada, Universitat de Barcelona, 08028 Barcelona, Spain.*

[2] *Institut de Nanociència i Nanotecnologia (IN^{2}UB), 08028 Barcelona, Spain.*

The measurement of the light momentum of the trapping beam in an optical tweezers set-up allows for direct determination of optical forces. Under this scheme, the capture of most part of the photons interacting with the specimen is highly important and, in a certain way, indicates the precision of the force measurements, being the fraction of non-collected photons the major source of error. In single-beam optical traps, all the forward-scattered light is collected by considering the proper design for the detection set-up. Nevertheless, there is always a small fraction of light that is back-scattered and thereby never reaches the detection part.

In this work we quantify, both experimentally and computationally, the backscattered portion of light in single-beam optical traps and study its effect on force measurements using different targets. For this, we developed a laser-scanning method using acousto-optic deflectors (AODs) to precisely and rapidly determine the complete force profile and loss of light of trapped objects of different size and refractive index. The results are then compared with finite-difference time-domain (FDTD) calculations, which allows us to separate the forward-scattered from the backward-scattered fields. We demonstrate that forces can be measured from light-momentum changes within a ±5% error for most used microspheres.

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5 NANOTOOLS TO ENGINEER INSTRUCTIVE BIOLOGICAL MICROENVIRONMENTS FOR TISSUE REGENERATION

O. Castaño[1,2,3,4], J. Martí-Muñoz[2,4], C. Ximenes[2,4], M. A. Mateos-Timoneda[4,2,5], S. Pérez-Amodio[4,2,5], S. Rey-Viñolas[2,4], C. Navarro-Requena[2,4], A. Canosa[2,4] and E. Engel[2,5,4]

[1] *Serra Hunter Fellow. Dept. of Electronics and Biomedical Engineering, Universitat de Barcelona (UB), Martí i Franquès 1, 08028, Barcelona, Spain*

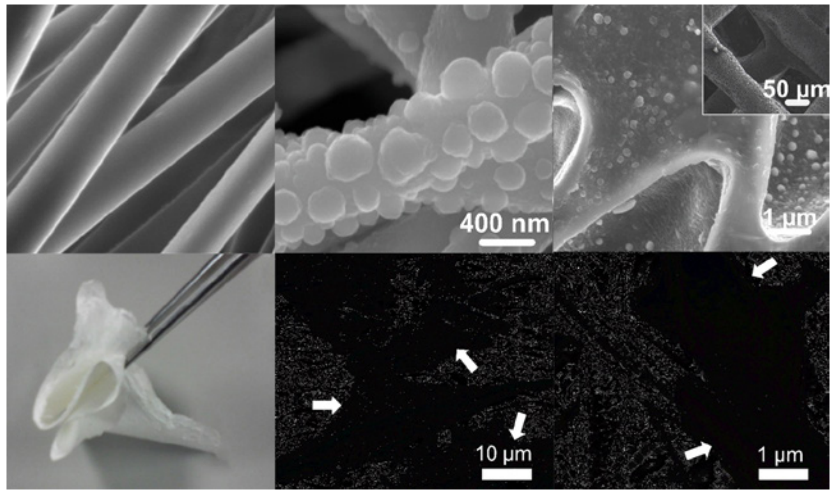
[2] *Institute for Bioengineering of Catalonia (IBEC), The Barcelona Institute of Science and Technology, Baldiri Reixac 10-12, 08028 Barcelona, Spain*

[3] *Institut de Nanociència i Nanotecnologia (IN2UB), 08028 Barcelona, Spain*

[4] *CIBER en Bioingeniería, Biomateriales y Nanomedicina, CIBER-BBN, Madrid, Spain*

[5] *Dept. of Materials Science & Metallurgical Engineering, Polytechnical University of Catalonia (UPC), Eduard Maristany 16, 08019, Barcelona, Spain.*

Currently in bone repair engineering, the extracellular matrix (ECM) is considered as an active architecture that can instruct cell functions through the introduction of different signals. Apart from mechanical and physical, chemical signals, such as growth factors and other biomolecules, have been validated with excellent results. However, they are controversial in terms of side effects, storage, cost-efficiency and regulation. In addition, bioactive metal ions have demonstrated to be a feasible tool to trigger signals produced by the own cells, which act as own signal regulators using natural mechanisms. Ca^{2+} are one of the most used ions to control cells fate by the creation of ion-rich microenvironments. Together with physical and/or mechanical stimuli can modulate the process of tissue healing. We have recently hypothesized and validated that calcium ions in the 3-10mM ranges is able to increase the expression of the vascular endothelial growth factor (VEGF) through the detection of calcium ions by the calcium sensing receptor (CaSR) actively present in mesenchymal progenitor cells. Nanotechnology is a useful tool to introduce Ca-signaling and other ions in biodegradable bone scaffolds[1]. Nanoparticles, electrospinning and surface engineering can be efficiently combined using calcium phosphate nanostructured biomaterials and electrospun ECM-like environments. Hence, several approaches are presented here involving nanostructured ion release platforms and electrospun polylactic acid nanofibers acting as temporary guiding templates. Results showed that these devices are not only a promising and low-cost tools for an efficient tissue vascularization, but also modulating the whole process of healing and tissue regeneration.



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6 OPTICAL TRAPPING AND LIGHT-MOMENTUM FORCE DETECTION IN EMBRYONIC TISSUE

Frederic Català[1,2], Mario Montes-Usategui[1,2], Timo Betz[3] and Arnau Farré[2,4]

[1] *Optical Trapping Lab – Grup de Biofotònica, Departament de Física Aplicada, Universitat de Barcelona*
[2] *Institut de Nanociència i Nanotecnologia (IN²UB), Barcelona*
[3] *Institute of Cell Biology, ZMBE, University of Münster, Münster, Germany*
[4] *Impetux Optics S.L., Trias i Giró 15 1-5, 08034 Barcelona*

Optical tweezers has found wide range of applications in biology, from studies on single-molecule physics, to redo-blood-cell transport in capillaries. Among these, optical trapping can be used for non-invasive quantitative studies on the biomechanics of developing embryos. Multiple processes, such as cell and tissue shaping, cell migration and morphogenesis, are driven by biomechanics, on which the ability of optical traps to measure forces with 100fN precision can be highly valuable. Here, we will review the main technical aspects to consider in experiments with 4-8 hours-post-fertilization zebrafish embryos, which are necessary for accurate optical trapping force detection.

Force measurement based on optical tweezers light momentum detection has been proven a robust scheme in a number of experimental situations, including *in vitro* and *in vivo*. Accurate measurement requires the trapping beam be entirely captured and conveyed appropriately to a position-sensing detector (PSD), which is not ensured *a priori* for thick and scattering samples, such as living embryos.

We have first analyzed the tolerance of the high-NA collecting lens and found that Abbe's sine condition is still valid up to 500-μm thick cambers, providing that the lens working plane is suitably reallocated, in order for its back focal plane (BFP) to contain the light momentum structure of the trapping beam. Second, we have studied the effect of light scattering through the embryo on the trapping force profiles of embedded polystyrene microbeads, and checked the validity of the light-momentum calibration within 20-30% reproducibility.

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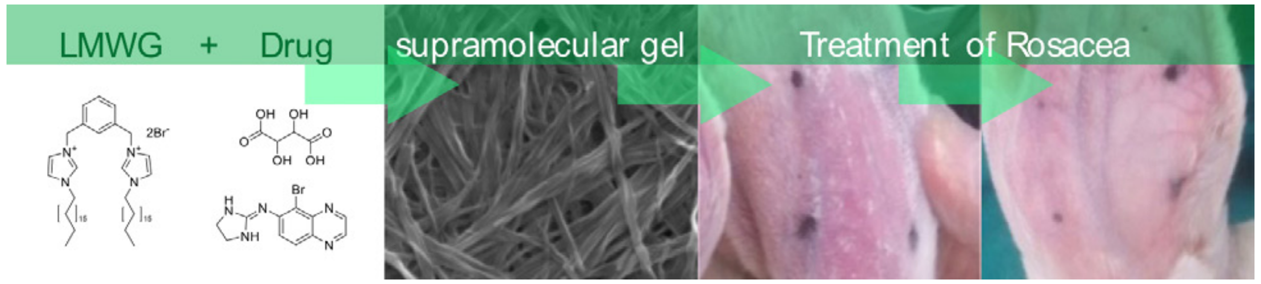
7 NANOSTRUCTURED SUPRAMOLECULAR HYDROGELS FOR THE EFFECTIVE DERMAL DELIVERY IN ROSACEA AND OTHER INFLAMMATORY SKIN DISEASES

David Limón[1,2], Claire Jiménez-Newman[1], Mafalda Rodrigues[1,2], Arántzazu González-Campo[3], David B. Amabilino[4,5], Ana C. Calpena[2,6] and Lluïsa Pérez-García[*,1,2,7]

[1] *Departament de Farmacologia, Toxicologia i Química Terapèutica, Universitat de Barcelona. Av. Joan XXIII 27-31, 08028 Barcelona (Spain).*
[2] *Institut de Nanociència i Nanotecnologia IN2UB, Universitat de Barcelona, 08028 Barcelona, (Spain).*
[3] *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC). Campus de la UAB, 08193, Bellaterra, Barcelona (Spain).*
[4] *School of Chemistry, The University of Nottingham, University Park, Nottingham NG7 2RD (United Kingdom).*
[5] *The GSK Carbon Neutral Laboratories for Sustainable Chemistry, The University of Nottingham, Triumph Road, Nottingham NG7 2TU (United Kingdom).*
[6] *Departament de Farmàcia, Tecnologia Farmacèutica i Fisicoquímica, Universitat de Barcelona. Av. Joan XXIII 27-31, 08028 Barcelona (Spain).*
[7] *Present address: School of Pharmacy, The University of Nottingham, University Park, Nottingham NG7 2RD, United Kingdom.*
[*] *Corresponding author. Email: mlperez@ub.edu*

A cationic gemini imidazolium-based amphiphile undergoes a self-assembly process to form thermoreversible nanostructured supramolecular hydrogels, which can also incorporate neutral (triamcinolone acetonide and betamethasone 17-valerate) and cationic drugs (brimonidine tartrate) for the topical treatment of Rosacea. The concentration of gelator and the type and concentration of drug incorporated strongly influence the gelling temperature, gel formation period, overall stability and morphology. NMR studies prove that these gels not only keep the drug at the interstitial space, but also within the fibers, opening perspectives for controlled release. Due to their specific design, this gel could importantly improve the efficacy in the dermal treatment of skin diseases such as Rosacea, as the drug release profile shows to be up to ten times faster, and the retention of the drug within the skin up to twenty times more effective as compared to the marketed products. *In-vivo* experiments demonstrate the rapid efficacy of these gels in reducing erythema, especially in the case of the gel with brimonidine.[1] All these results show that the properties of this novel nanostructured material point it as a great option for the dermal treatment not only of Rosacea, but of other skin diseases as well by the incorporation of other drugs.



Supramolecular gels spontaneously formed incorporating drugs useful in the dermal treatment of Rosacea, are effective both in vitro and in vivo.

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Acknowledgements

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8 INFLUENCE OF HYDROPHOBIC/SUPERHYDROPHOBIC MODIFICATION IN FABRICS ON VIABILITY OF MAMMALIAN CELLS

M.Carmen Morán[1,2], Guillem Ruano[1], Francesca Cirisano[3] and Michele Ferrari[3]

[1] Departament de Bioquímica i Fisiologia-Secció Fisiologia, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, 08028 Barcelona, Spain
[2] Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, 08028, Barcelona, Spain
[3] CNR-ICMATE Istituto di Chimica della Materia Condensata e di Tecnologie per l'Energia, 16149 Genova, Italy

Hydrophobic surfaces play an important role in biomedical engineering, especially tissue engineering. Tissue engineering is aiming to create biochemical and physico-chemical substitutes to improve or replace the biological functions of portions or the whole tissue of human body. In tissue engineering, a scaffold is required for the incorporation of living cells and to support the cells to adhere, grow, and differentiate. Cell adhesion, the binding of a cell to the extracellular matrix, other cells, or a specific surface, is essential for the growth and survival of the cell and also its communication with other cells. The hydrophobicity and roughness of the surface affect the cell attachment and growth [1]. Highly water repellent coatings with wettability properties known as superhydrophobicity are related to surfaces with contact angle above 150° and a very small hysteresis. The small area available for these surfaces when in contact with water address to be exploited in many applications where interactions with aqueous environment are usually strongly to be avoided. The combination of low surface energy and the existence of a specific surface morphology (micro/nano-roughness) coexist, lead to significantly less wettable surfaces [2].

In this work the influence of coatings at different degree of hydrophobicity has been investigated. 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 such as 3T3 fibroblasts, HaCaT keratinocytes and HeLa epithelial carcinoma cells. The obtained results suggested that, in addition to the chemistry and morphology of the coating, the characteristics of the substrate are important parameters on the final cell viabilities.

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9 ENGINEERING OF FRUSTRATION IN COLLOIDAL ARTIFICIAL ICES REALIZED ON MICROFEATURED GROOVED LATTICES

Antonio Ortiz-Ambriz[1], Johannes Loher[1] and Pietro Tierno[1,2,3]

[1] Departament de Física de la Matèria Condensada, Universitat de Barcelona, Av. Diagonal 647, 08028 Barcelona, Spain
[2] Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, 08028, Barcelona, Spain
[3] Universitat de Barcelona Institute of Complex Systems (UBICS), Universitat de Barcelona, Barcelona, Spain

Artificial spin-ice systems, namely lattices of interacting single domain ferromagnetic islands, have been used to date as microscopic models of frustration induced by lattice topology, allowing for the direct visualization of spin arrangements and textures. However, the engineering of frustrated ice states in which individual spins can be manipulated in situ and the real-time observation of their collective dynamics remain both challenging tasks. Inspired by recent theoretical advances, we realize a colloidal version of an artificial spin ice system using interacting polarizable particles confined to lattices of bistable gravitational traps. We show quantitatively that ice-selection rules emerge in this frustrated soft matter system by tuning the strength of the pair-interactions between the microscopic units. Via independent control of particle positioning and dipolar coupling, we introduce monopole-like defects and strings and use loops with defined chirality as an elementary unit to store binary information.

10 LIPOSOMES CONTAINING PAULLINIA CUPANA VAR. SORBILIS (GUARANA) FOR POTENTIAL TOPICAL APPLICATION: CYTOTOXICITY ASSESSMENT ON SKIN CELL LINES

Isabel Roggia[1], Montserrat Mitjans[2], Aline Ferreira[1], Patrícia Gomes[1] and Maria Pilar Vinardell[2]

[1] *Program Pós Graduate Studies in Nanosciences, University Franciscana, Santa Maria, Rio Grande do Sul, Brazil.*
[2] *Departament de Bioquímica i Fisiologia, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, Barcelona, Spain.*

The high content of alkaloids, mainly caffeine, present in guarana makes this compound a promising one for cosmetic use[1]. Its association with nanotechnology makes it possible to increase the permeability of the active substances until the dermis and release them directly into the lipid cells. Nevertheless, the safety of these formulations should be demonstrated. Thus, the objective of this work was to evaluate the *"in vitro"* cytotoxicity of liposomes containing guarana using different skin cells lines. The experiments were carried out for the liposome samples containing 1 mg.mL^{-1} guarana powder prepared by the reverse phase evaporation method (LFR)[2] for white liposomes (without guarana) (BFR) prepared by the same method and for guarana in free form (GL). The cell lines 3T3 murine fibroblasts, HaCaT spontaneously immortalized human keratinocyte and 1BR.3G human skin fibroblasts were used. Cells were seeded in 96 wells cell culture dishes. Cells were incubated for 24 h under 5% CO_2 at 37°C and the medium was then replaced with medium supplemented with 5% FBS containing the different treatments (GL, BFR and LFR) in a concentration range from 3.91 to 500 µg.mL^{-1} and incubated for 24h, 48h and 72h. Cytotoxicity was evaluated by the MTT[3] and NRU[4] assays. The results obtained show a significant reduction of the cell viability for the different cells tested at the maximum concentration for the different treatments, except for the BFR, which presented a reduction of viability at lower concentration of 31.25 µg.mL^{-1}. These results can indicate a potential damage induced by the liposomes and a protection of this damage in the presence of guarana, concluding that guarana-containing liposomes can be safe for topic applications.

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NANOPHARMACOTHERAPY [NPHARMA] RESEARCH AREA

11 DEVELOPMENT OF A DERMAL GEL OF PLURONIC® WITH LIPID NANOCARRIER (NLC) LOADED WITH A CORTICOSTEROID CLASS ONE

P. Carvajal-Vidal[1], C.L. Araya[1], A.C. Calpena[1,2] and M.L. García[1,2]

[1] *Department of Pharmacy, Pharmaceutical Technology and Physical Chemistry, University of Barcelona, Av. Joan XXIII 27-31, E-08028, Barcelona, Spain*
[2] *Institut de Nanociència i Nanotecnologia (IN^{2}UB), 08028 Barcelona, Spain*

Lipid nanocarriers (NLC) have been widely used for topical drug administration. They are characterized by being formed of a mixture of liquid and solid biocompatible lipids that must be compatible with each other, and be solids at room temperature. NLCs have the advantage of being able to incorporate large amounts of drug and improve its stability during storage. Corticosteroids are commonly used drugs for skin conditions such as rash, allergies, psoriasis and atopic dermatitis among others. The main problem presented by these lipophilic drugs is that due to their high permeability they can cause severe adverse systemic effects in the body.

A formulation of NLC with corticosteroid (class 1) was developed using the methodology of high pressure homogenization with hot temperature. The particles obtained had sizes smaller than 200nm with Polydispersity Index close to 0.2; suitable for skin application. Later and to improve its characteristics, from the formulation of NLC and directly a Pluronic® gel was developed. Both formulations were physicochemical characterized and their release profile was compared by Franz cells. The results show that the NLCs are stable when carrying out the in-situ polymer incorporation and that it is possible to modulate the release of this type of drug for topical administration.

12 DESIGN AND CHARACTERIZATION OF PIOGLITAZONE-LOADED MICROEMULSION FOR TREATMENT OF INFLAMMATORY DISEASES

Lupe Carolina Espinoza[1,2], Marcelle Silva-Abreu[1,3], Beatriz Clares[4] and Ana C. Calpena[1,3]

[1] Department of Pharmacy, Pharmaceutical Technology and Physical Chemistry, Faculty of Pharmacy and Food Sciences, University of Barcelona, 08028 Barcelona, Spain.
[2] Departamento de Química y Ciencias Exactas, Universidad Técnica Particular de Loja, Loja 1101608, Ecuador.
[3] Institute of Nanoscience and Nanotechnology (IN²UB), University of Barcelona, 08028 Barcelona, Spain
[4] Pharmacy and Pharmaceutical Technology Department, Faculty of Pharmacy, University of Granada, Granada, Spain.

Pioglitazone (PGZ) is a Peroxisome proliferator-activated receptor-gamma (PPAR-γ) agonist that is used to treat type 2 diabetes mellitus. PPAR-γ is a nuclear receptor that controls the expression of genes involved in glucose and lipid metabolism. Several studies have reported that PGZ inhibits proinflammatory cytokines and thus suggests that this drug could be used in the treatment of inflammatory processes. The purpose of this study was to develop and characterize a Pioglitazone-loaded microemulsion (PGZ-ME) in order to evaluate its anti-inflammatory activity. Solubility studies and six pseudoternary phase diagrams were carried out to determine the ME formulation. Physicochemical characterization included pH, droplet size, polydispersity index and morphological examination by transmission electron microscopy (TEM), viscosity and rheological behavior. The physical stability of the PGZ-ME was evaluated using the TurbiScanLab (Formulation, L'Union, France) of samples stored at 25°C for 60 days. The pharmacological efficacy of PGZ-ME was studied by a mouse ear edema model induced with 12-o-tetradecanoylphorbol 13-acetate (TPA) to determine the level of anti-inflammatory activity. The obtained result was a transparent and homogeneous PGZ-ME with spherical shape and lipid droplets of 250 nm. The rheogram showed Newtonian behavior with a linear relationship between shear stress and strain rate. The results of physical stability revealed that PGZ-ME is stable at 25°C during the time period studied since no sedimentation, creaming, flocculation or coalescence were observed. Efficacy studies revealed that topical treatment with PGZ-ME significantly inhibited inflammation by 43.9%. Consequently, these results lend credence to the possibility that PGZ-ME may be used as an alternative treatment for inflammatory diseases processes.

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13 STUDY OF TRANSMUCOSAL SWINE VAGINA PERMEATION OF CARPROFEN NANOPARTICLES

L. Gómez[1,2], A. Parra[1], A.C. Calpena[1,3], M. Rincón[1] and A.Gimeno[2]

[1] Department of Pharmacy and Pharmaceutical Technology and Physical Chemistry, Faculty of Pharmacy and Food Sciences, University of Barcelona, Spain.
[2] Department of Animal Research, Animal House of Bellvitge, University of Barcelona, CCiT-UB, Spain.
[3] Institute of Nanoscience and Nanotechnology (IN²UB), University of Barcelona. Spain

Introduction: Non-steroidal anti-inflammatory drugs (NSAIDs) include several drugs, such as ibuprofen, ketoprofen, carprofen (CP) and others. They are widely used in symptomatic pain treatment. Yet, they may also reduce the production of inflammatory effusion through, primarily, inhibition of cyclooxygenase-2 (COX-2) [1]. CP, (+)-6-Chloro-alpha-methylcarbazole-2-acetic-acid, is a racemic mixture of the R and S and it is extensively used in veterinary medicine, which has been investigating CP in several species [2]. No CP permeation work in swine's has been found among the consulted literature. The local administration of NSAIDs has been explored as a potential method in order to avoid the first pass effect and the gastrointestinal disorders that may occur when these drugs are administered orally. It is well known that the vehicle composition can affect both drug release and mucous membrane permeability properties. The use of polymeric nanospheres, such as poly (D,L-lactide-co-glycolide) (PLGA), could be considered nowadays 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 carprofen nanoparticles (NPs) in the swine vagina.

Methods: Nanoparticles with a matrix structure containing Carprofen were prepared by the solvent displacement technique described by Vega *et al.* [3] under optimized conditions previously determined. The transmucosal absorption parameters: permeability coefficient (Kp), lag time (Tl), flux (J), and the concentration in steady state (Css) of carprofen were estimated by means of an *ex vivo* permeation study using Franz Diffusion Cells and vaginal mucous (n=6) with an area of 0.64 cm². 500µL of NPs of carprofen was used as donor phase and the receptor phase was Phosphate Buffer Solution (PBS) pH 7.4 at 32ºC. Samples (300 µL) were withdrawn from the receptor compartment at prefixed times over 6 hours and replaced by an equivalent volume of fresh PBS at the same temperature. The amount of carprofen in the NPs and in the samples taken in the ex vivo permeation study was determined by a validated technique of high performance liquid chromatography with UV detection.

Results: Transmucosal absorption parameters were exposed in the next table expressed by median and range:

J	Kp*10³	Tl	Css
(mcg/h/cm²)	(cm/h)	(h)	(mcg/mL)
13.89	0.46	1.7	0.56
7.950-19.83	0.27-0.67	1.4-2.1	0.32-0.8

Conclusions: In base to the obtained results it can be concluded that NPs of carprofen are able to permeate the mucous membrane of swine vagina, thus suggesting a local antiinflamatory effect. In addition, in base of the Css results it can be concluded that NPs of carprofen are safe and non-toxic, since they are very far from the maximum concentration studied in other animal species (6.5-8 mcg /ml).

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14 SUITABILITY OF FUNCTIONALIZED LIPOSOMES AS VEHICLES FOR DRUGS: A PHYSICOCHEMICAL AND CYTOTOXIC STUDY

W. Kurniawan[1,2,3,*], Montserrat Mitjans Arnal[1,3], Mª Pilar Vinardell Martinez-Hidalgo[1,3], Joan Estelrich Latràs[2,3] and Mª. Antonia Busquets Viñas[2,3]

[1] CEREX Lab. Departament de Bioquimica i Fisiologia. Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona (UB), Avda. Joan XXIII, 27-31, 08028 Barcelona,
[2] COLLOID Lab. Departament de Farmàcia i Tecnologia Farmacèutica, i Fisicoquímica, Facultat de Farmàcia i Ciències de l'Alimentació, UB, Avda. Joan XXIII, 27-31, 08028 Barcelona
[3] IN²UB. Avda. Diagonal 645, 08028 Barcelona
** Correspondence: kurniachev@gmail.com*

Most of the efforts in the design of nanoparticles are focused on the attainment of a new generation of nanosystems for a variety of biomedical applications [1]. Several factors must match for the nanoparticles to be accepted as the alternative to the conventional medicines. In this sense, efficacy in drug encapsulation and targeting and, reduced side effects of both the vehicle and the drug are the main challenges involved in nanoparticles' production. Therefore, the physicochemical properties and the associated toxicity of these systems are the first steps to face in any synthesis strategy. On another hand, a common approach to overcome the limitations of the traditional pharmaceutical formulations consist on grafting the surface of the nanoparticles with molecules that confer a specific function. Taking into consideration these premises, we have synthesized and characterized liposomes with different surface properties aimed for anticancer therapy [2,3]. All preparations shared the lipid composition consisting on soy phosphatidylcholine and cholesterol at a molar ratio of 8:2 (mole ratio). Stealth® and peptide functionalized liposomes were obtained by adding to the basic composition DSPE-PEG (1,2 distearoyl - sn - glycero - 3 - phosphoethanolamine - N - [methoxy (polyethylene glycol)-2000] ammonium salt) or DSPE-PEG-Maleimido-Penetratin, respectively. Size, size distribution, stability in several media, cytotoxicity on Hela and 3T3 cells and hemolysis studies (Figure 1) indicated the feasibility of these structures for medical applications. Stealth® and functionalized liposomes were obtained by adding to the basic composition DSPE-PEG (1,2 distearoyl - sn - glycero - 3 - phosphoethanolamine - N - [methoxy(polyethylene glycol)-2000] ammonium salt) or DSPE-PEG-MAL-Penetratin, respectively.

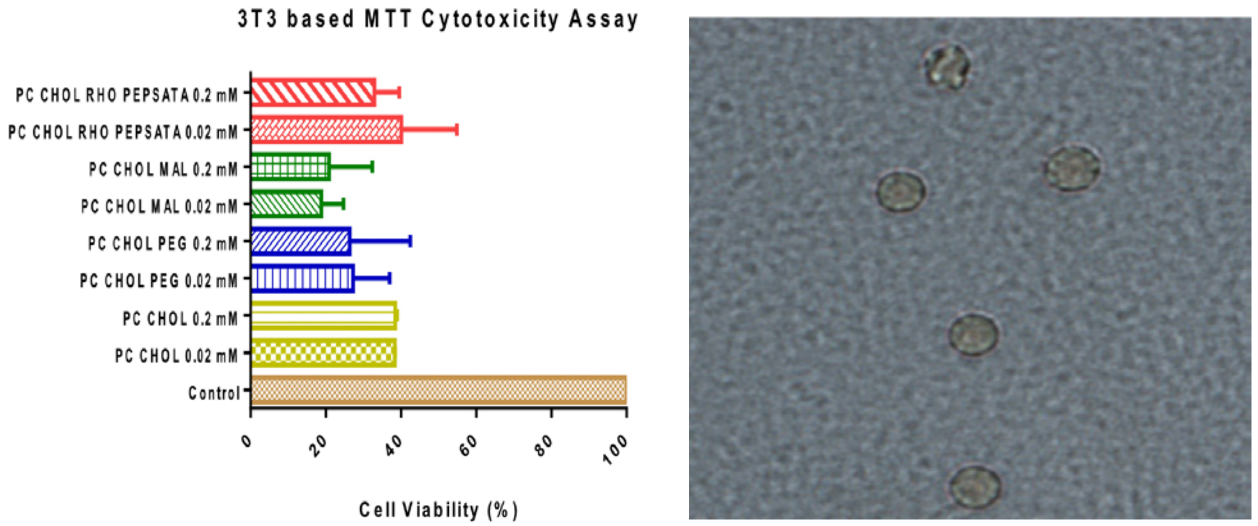

Figure 1. left) MTT cytotoxicitiy assay of the synthesized liposomes and, right) integrity of the red blood cells after incubation with functionalized liposomes.

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15 BEHAVIOURAL STUDY OF THIAZOLIDINEDIONE-LOADED NANOPARTICLES IN APP/PS1 TRANSGENIC MICE MODEL

M. Silva-Abreu[1,2], P. Andrés-Benito[3,4], E. Aso[3,4], A. C. Calpena[1,2], M. Espina[1,2], M. L. García[1,2]

[1] Department of Pharmacy, Pharmaceutical Technology and Physical Chemistry, Faculty of Pharmacy and Food Sciences, University of Barcelona, 08028 Barcelona, Spain.
[2] Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Spain.
[3] Servei d'Anatomia Patològica, IDIBELL-Hospital Universitari de Bellvitge, Universitat de Barcelona, L'Hospitalet de Llobregat, Spain.
[4] CIBERNED, Centro de Investigación Biomédica en Red de Enfermedades Neurodegenerativas, Instituto de Salud Carlos III, Spain.

Pioglitazone (PGZ) is a thiazolidinedione, an agonist of the peroxisome proliferator-activated receptor (PPARγ), used to treat type-2 diabetes. Several researchers have been reported the use of this drug for different functions such as anti-inflammatory, anti-angiogenic, antifibrotic, anti-tumor and neuroprotection effects. The main purpose of this study was to develop nanosystems of PGZ of a polymer nature in order to evaluate its effectiveness in the APP/PS1 transgenic mice model. The nanoparticles (NPs) were prepared by nanoprecipitation and physicochemical characterization included the droplet size, polydispersity index (PI), encapsulation efficiency (EE) and morphological examination by transmission electron microscopy (TEM) has been performed. Moreover, an *in vitro* release profile was carried out using Franz diffusion cells. The *in vivo* study was carried out on seven-month-old male APP/PS1 mice and wild-type-like (WT) littermates. Free-PGZ were dissolved in 5% DMSO and PGZ-NPs (10 mg/kg) were administered orally in a volume of 10 mL/kg body weight. Animals were treated for 5 days per week, during one month with the compounds or with the vehicle alone (n = 3-4). After a 3-day wash-out animals were subjected to behavioural evaluation with the two-object recognition test. APP/PS1 mice treated with the vehicle exhibited a memory impairment when compared to corresponding WT littermates ($p<0.01$) and that Free-PGZ ($p<0.05$) and PGZ-NPs ($p<0.01$) increased the recognition index in APP/PS1 mice when compared to the vehicle. No significant difference in the total exploration time during the memory acquisition session or the memory test was observed between the groups, discarding any possible impact of the treatments on the anxiety levels or the activity of the mice. The results showed an average size of particle of around 160 nm, PI 0.1 and EE approximately of 93 %. Moreover, the PGZ-NPs improved the cognitive deficit in APP/PS1 male mice in a similar way to Free-PGZ.

16 ACTIVITY LEISHMANICIDE OF A NANOSTRUCTURED GEL OF AMPHOTERICIN B (AMB)

Lilian Sosa[1], Magdalena Alcober[2], Diana Berenger[2], Beatriz Clares[3,4], Cristina Riera[2], Òscar Domènech[1,4] and Ana C. Calpena[1,4]

[1] Department of Pharmacy and Pharmaceutical and Physico-chemical Technology, Faculty of Pharmacy and Food Sciences, University of Barcelona, Barcelona Spain.
[2] Department of Biology, Healthcare and the Environment, School of Pharmacy and Food Sciences, University of Barcelona, Barcelona, Spain.
[3] Department of Pharmacy and Pharmaceutical Technology, School of Pharmacy, University of Granada, Granada, Spain.
[4] Institute of Nanoscience and Nanotechnology (IN²UB), University of Barcelona, Barcelona, Spain

The nanostructured gels of nonionic polyethylene copolymers (PEO) -polypropylene (PPO), have the property of being thermoreversible, capable of transporting drugs in addition to being administered topically, ocularly and intravenously (IV) without producing toxicity. AMB is a poorly soluble drug, administered via IV for the treatment of systemic mycosis and is the second therapeutic option for the treatment of visceral (VL) and cutaneous (CL) leishmaniasis. Currently there is no commercialized AMB topical formulation, only in India has the sale of FungisomeTM gel been allowed for this way. We have developed a nanostructured gel containing AMB and DMSO (5%) as a skin promoter to be administered via the cutaneous route as a possible CL treatment. Our formulation has been previously characterized and optimized, and we have also performed drug release, permeation and retention tests on human skin and cell viability respectively. In the present work we have determined the IC50 of our formulations with and without drug against promastigotes and amastigotes of the Leishmania genus. We will allow us to compare the values found (IC50) in both stages of the parasite with the amount of drug retained in the skin.

NANOMAGNETISM, NANOELECTRONICS AND NANOPHOTONICS [NELECTROMAGΦ] RESEARCH AREA

17 LANTHANIDE MOLECULAR SYSTEMS AS INFORMATION PROCESSING DEVICES FOR QUANTUM COMPUTING

David Aguilà[1], Leoní A. Barrios[1], Verónica Velasco[1], Olivier Roubeau[2], Fernando Luis[2], Simon J. Teat[3] and Guillem Aromí[1]

[1] Departament de Química Inorgànica i Orgànica, Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Spain
[2] Instituto de Ciencia de Materiales de Aragón (ICMA) and Departamento de Física de la Materia Condensada, CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain
[3] Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720, United States

The development of physical systems for implementing quantum bits (qubits) and gates (qugates) is nowadays one of the keys to achieve the realization of quantum computation. In this regard, electronic spins embedded in magnetic molecules have emerged as promising candidates due to their easy manipulation and high scalability.[1] In particular, complexes featuring lanthanide ions (Ln) have a vast potential to be used as molecular quantum gates, since each Ln can be exploited as a qubit. Following this proposal, we have designed a ligand-based strategy to obtain pure heterometallic complexes featuring more than one type of lanthanide ion. Depending on the ligand, dinuclear[2,3] [LnLn'] or trinuclear [LnLn'Ln] complexes can be deliberately obtained (Figure 1). The purity of the systems has been evaluated and confirmed by crystallographic and spectrometric measurements. Magnetic and EPR studies have been carried out to show that each Ln fulfills the requirements to be used as qubits, and that the derived molecular systems can perform successfully quantum logical operations.

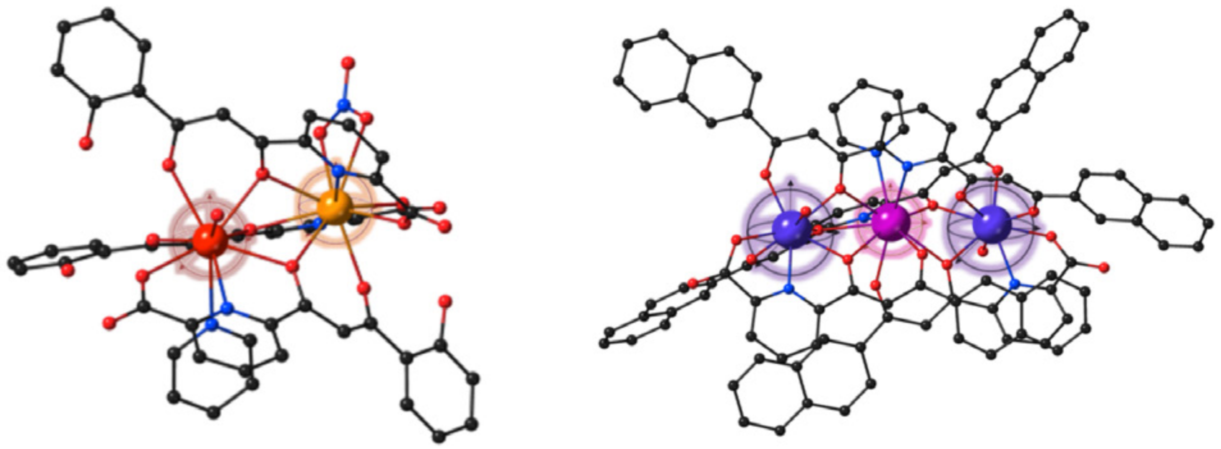

Figure 1 Molecular structure of the desgined [LnLn'] (left) and [LnLn'Ln] (right) systems

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18 MACHINE-READABLE PATTERN FOR COLORIMETRIC SENSOR INTERROGATION

I. Benito-Altamirano[1,2], P. Pfeiffer[1,2], O. Cusola[3] and J. D. Prades[1,2]

[1] MIND, Department of Electronic & Biomedical Engineering, Universitat de Barcelona, Spain
[2] Institut de Nanociència i Nanotecnologia (IN²UB), 08028 Barcelona, Spain
[3] CELBIOTECH - Paper Engineering Research Group. Universitat Politècnica de Catalunya, Spain

Colorimetric sensor interrogation using digital cameras is a convenient way to obtain quantitative measurement from colorimetric indicators for manifold applications, like gases or temperature sensing. However, the method is very sensitive to external factors like ambient light, camera setup, etc. To achieve accurate, reliable, and reproducible measurements, it is necessary to accompany the colorimetric indicators with a set of color references capable of correcting most of these effects. Also, to make possible automatic readout, such elements must be arranged in a machine-readable configuration. We propose here the following procedure to design a machine-readable pattern optimized for the measurement of a certain colorimetric indicator. We illustrate this with a NH_3 colorimetric indicator. We have successfully applied this methodology to other colorimetric indicators, like NO_2 or CO_2.

First, we exposed the colorimetric indicator to different NH3 concentrations (0–100 ppm in humid air, 50%RH), and acquired the colors developed at the indicator with a camera, always under a reference white light at 5500K. To obtain a finite set of reference colors, we applied a K-Means clustering method. Then, this reduced set of reference colors was used to build a machine-readable pattern that could be found by means of computer vision methods in any context and scene. We choose to work with the geometric elements of the QR-Codes, which offer proven elements for finding, positioning, and aligning the pattern in the image. Thus, the previous color references were spread over the QR-Code regions that usually accommodate digital data. Also, some regions in the QR-Code were reserved to allocate spots containing the colorimetric indicator. This design was printed using conventional techniques: ink-jet printing to produce the color references and screen-printing to transfer the functional NH_3 sensing-ink.

Without any correction, the color curves of the NH_3 indicator observed in images acquired at different ambient lights -white light sources of temperatures from 4500K to 6000K- were not coincident, and unsuitable for quantitative measurements. In contrast, after correcting the color curves of the indicators, by using the color references as landmarks to stablish a correspondence between apparent and real colors by means of a thin-plate spline, the color measurements obtained at different light temperatures were fully consistent, and suitable for quantitative measurement with an error of less than 5%.

19 HIGH-RESOLUTION ELECTRON MICROSCOPY AND HIGH-ANGLE ANNULAR DARK-FIELD IMAGE SIMULATION OF CEO$_2$ NANOPARTICLES

J. Blanco-Portals[1,2], T. Berestok[1,2,3], P. Torruella[1,2], C. Coll[1,2], L. López-Conesa[1,2,6], P. Guardia[3,4], E. Coy[5], A. Cabot[3,7], S. Estradé[1,2] and F. Peiró[1,2]

[1] *LENS-MIND, Departament d'Enginyeries i Electrònica, Universitat de Barcelona, 08028, Spain*
[2] *Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Barcelona, Spain*
[3] *Catalonia Institute for Energy Research – IREC, 08930 Sant Adrià de Besòs, Barcelona, Spain.*
[4] *Centre de Tecnologia Química de Catalunya and Universitat Rovira i Virgili, Tarragona, 43007 Spain*
[5] *NanoBioMedical Centre, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland.*
[6] *Centres Científics i Tecnològics (CCiT-UB), Universitat de Barcelona, 08028, Barcelona, Spain.*
[7] *ICREA, Pg. Lluís Companys 23, 08010 Barcelona, Spain.*

In cerium oxide nanoparticles, the facets exposed control the reactivity and the catalytic behavior, hence the precise characterization of the 3D geometry is crucial. We present a method to resolve the morphology of branched cerium oxide NPs, through the comparison between HRTEM experimental and simulated images. Octapod and tetrapod atomic models, suggested from a preliminary examination of the experimental HRTEM images, were constructed by assembling a cube-octahedral central body and truncated pyramidal arms pointing to the vertices of a cube. A comparative analysis of the intensity profiles of the simulated and experimental HRTEM images was then performed. This proved capable of discriminating between the two proposed geometries, showing CeO$_2$ NPs to be octapods. The obtained results were further confirmed by comparing High Angular Dark Field experimental and simulated images of the nanoparticles. The method can be suitable whenever 3D-Tomographic reconstruction is not feasible in TEM, for instance in the case of highly beam sensitive materials.

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20 DEPOSITION OF SIZE-CONTROLLED SI NANOCRYSTRALS BY ELECTRON BEAM EVAPORATION

O. Blázquez[1,2], J. López-Vidrier[3], J.L. Frieiro[1,2], L. López-Conesa[1,2,4], S. Estradé[1,2], F. Peiró[1,2], J. Ibáñez[5], S. Hernández[1,2], B. Garrido[1,2]

[1] *MIND, Department of Electronics and Biomedical Engineering, Universitat de Barcelona, Martí i Franquès 1, E-08028 Barcelona (Spain).*
[2] *Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Av. Joan XXIII S/N, E-08028 Barcelona (Spain).*
[3] *Laboratory for Nanotechnology, Dept. of Microsystems Engineering (IMTEK), University of Freiburg, Albert-Ludwigs-University Freiburg, Georges-Köhler-Allee 103, D–79110 Freiburg (Germany).*
[4] *TEM-MAT Unit, Scientific and Technological Centers, Universitat de Barcelona. C/Lluís Solé i Sabarís 1, E-08028 Barcelona (Spain).*
[5] *Institute of Earth Sciences Jaume Almera, ICTJA-CSIC, Lluís Solé i Sabarís s/n, 08028 Barcelona (Spain).*

Band gap energy of different materials can be tuned when nanostructured. Such is the case of Si nanocrystals, whose size directly modifies the band gap due to the quantum confinement effect, making them a promising material for applications in photovoltaics and light-emitting devices. Their fabrication is usually done by embedding them within a proper matrix, performing the deposition via chemical processes that employ harmful precursors. Physical deposition methods, like electron beam evaporation (EBE), allow the usage of safer materials, which is highly desirable aiming at mass production.

In this work, deposition of alternative layers of SiO$_2$ and Si onto Si and fused silica substrates has been performed in oxygen-rich atmosphere by EBE, modifying the thickness of the Si layers. X-ray spectroscopy was employed to determine the stoichiometry of the layers, showing the desired controlled oxidation of silicon-rich oxide (SRO) layers. Annealing at different temperatures resulted in the precipitation of Si in the form of nanocrystals, later confirmed by transmission electron microscopy (TEM) and Raman scattering measurements. Emission spectra obtained by photoluminescence (PL) of the samples showed two different contributions from different luminescent centers, as they could be deconvolved and had different dynamics when studied separately. Discussion on the origin of both luminescent centers has been done by comparing EBE-grown Si nanocrystals with high-quality ones obtained through chemical methods.

21 INKJET-PRINTED GOLD-ELECTRODES ONTO GLASS SUBSTRATES FOR ELECTROPHYSIOLOGIC RESEARCH ON NEURONS

A. Cabal[1], S. Teller[1], A. Cirera[1]
[1] *Departament d'Enginyeria Electrònica i Biomèdica, Facultat de Física*

Inkjet Printing (IP) is a low-cost, low-waste and contactless technique which allows the easy fabrication of electronic devices at a micrometer scale, with no need for masks. In addition, inkjet printing is a versatile tool, capable of depositing a huge variety of biocompatible printable materials (such as metals [1] or polymers [1, 2]) and hence, its interest for biological systems interfacing. Our aim is to provide a neural activity monitoring system [Figure 1a], by simultaneously employing inkjet-printed gold-electrodes onto glass for electrical measurement [4-7] and calcium imaging [7]. The transparency of the used materials enables the use of high resolution optical microscope for fluorescence imaging. In this way, neural electrical spikes can be correlated with fluorescence recordings. First of all, an experimental organometallic gold ink is rheologically studied for printing suitability. The deposit optimization is achieved by varying the different printer parameters, in order to obtain homogeneous gold tracks that become conductive after a thermal sintering process. Properties of the electrodes such as porosity (scanning electron microscopy), thickness (profilometer) and conductivity (2-probe method) are determined. A PDMS layer is attached to the samples, and erased in those areas (windows) where neuron culture takes place, in order to enclose the liquid medium [Figure 1b]. Several functionalization strategies are being employed and studied, including Poly-L-Lysine (PLL) or Polyethylene glycol (PEG), in order to obtain selective neuroadhesive or neurorepulsive properties over the substrate. This allows us to control the spatial distribution of rat cortical neurons. In conclusion, such an operational device could manage to dynamically analyse neuron populations and their connections, giving insight on the functions of the existent communication.

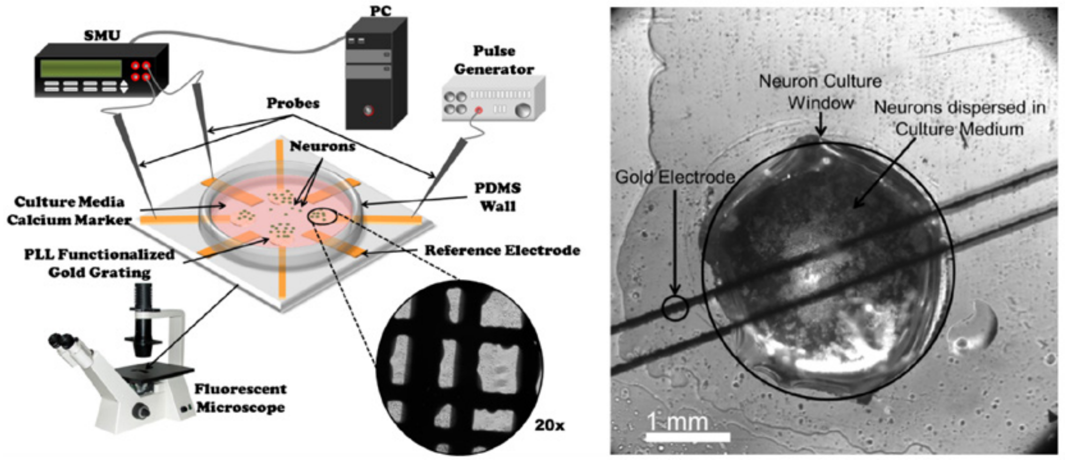

Figure 1. left) Monitoring system scheme; right) an example of a neuron culture performed inside a PDMS window.

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22 THE PLASMONIC RESPONSE OF A HEXAGONAL ARRAY OF NANOGAPS

A. Conde-Rubio[1,2], A. Fraile Rodríguez[1,2], F. Pérez-Murano[3], X. Batlle[1,2] and A. Labarta[1,2]
[1] *Departament de Física de la Matèria Condensada, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain*
[2] *Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Spain*
[3] *Institut de Microelectrónica de Barcelona (IMB-CNM, CSIC), Bellaterra, 08193, Spain*

The plasmon response of individual noble metal nanostructures is well known to be dependent on their size, geometry, composition, or surrounding medium. However, when these structures are arranged into arrays, its collective response can be strikingly different. On the one side, when nanostructures are very close, near field interactions hybridize the plasmonic modes. On the other side, the lattice distribution of plasmonic elements can give rise to long-range interactions that support collective modes. The optimization of these two related aspects gives rise to much more intense resonances than those of the single particles.

We have investigated the plasmonic response of a novel morphology of metal nanostructures consisting in triangular lattices of asterisk-shaped gold nano-elements of 300 to 500 nm separated by gaps ranging from 20 to 100 nm. The lattices have been simulated using Finite Difference Time Domain (FDTD) simulations. A metal-insulator-metal (MIM) configuration, in particular $Au-SiO_2-Au$, has been used to optimize the system response. FDTD simulations have shown two interesting features: first, a narrow peak in the visible region of the extinction spectrum corresponding to an almost complete absorption, shown in Fig. 1(a), and second, the fluctuation of the system between two geometrical configurations of the excitation modes that lingers for a remarkably longer time than the excitation pulse length.

A set of samples has been fabricated by electron beam lithography (EBL) on glass substrates and with a MIM configuration (see Fig.1(c)). To characterize the plasmonic response, Fourier Transform Infrared (FTIR) spectroscopy measurements have been performed, confirming the intense absorption of the system in the visible range. By using EBL as the lithography method, the resonances can be easily engineered to match the desired wavelength. These structures could therefore be of interest for SERS or applications based on light absorption such as photovoltaics.

This work was supported by Spanish MINECO (MAT2015-68772- P), Catalan DURSI (2014SGR220), and European Union FEDER funds (Una manera de hacer Europa). A. Conde-Rubio acknowledges Spanish MINECO for a Ph.D. contract (BES-2013-065377).

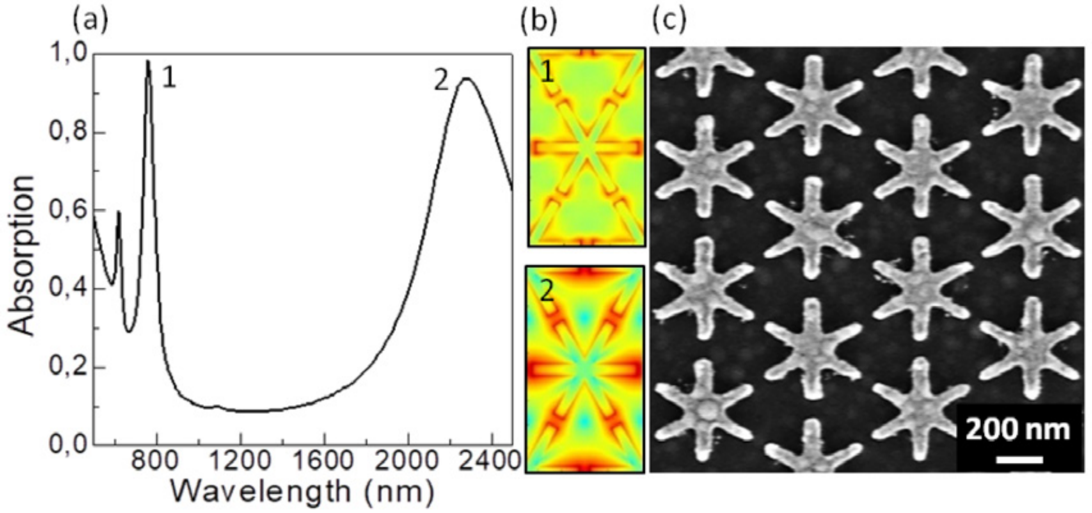

Figure 1. a) Absorption spectrum for an array of nanoasterisks of 500 nm pitch, 50 nm gap, 45 nm width and 0.5 Cr + 30 nm Au thickness. b) Log ($|E|^2/|E_0|^2$) for the maxima in (a). SEM micrograph of the array.

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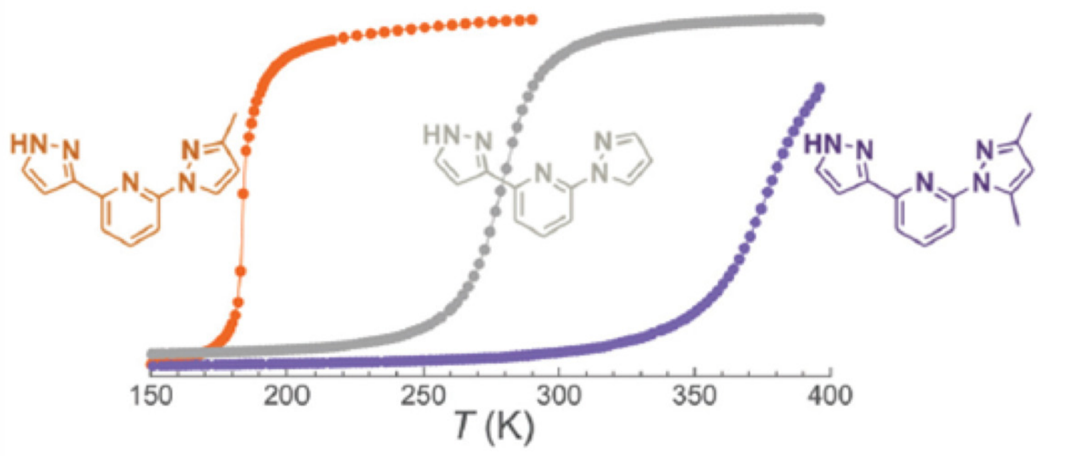
A PROBE OF STERIC LIGAND SUBSTITUENT EFFECTS ON THE SPIN CROSSOVER OF FE (II) COMPLEXES

R. Diego[1], C. Bartual-Murgui[1], S. Vela[2], M. Darawsheh[1], S.J. Teat[3], O. Roubeau[4] and G. Aromí[1]

[1] Departament de Química Inorgànica i Orgànica i IN2UB (Universitat de Barcelona, Diagonal 645, 08028 Barcelona, Espanya).
[2] Laboratoire de Chimie Quantique (Université de Strasbourg, 4 rue Blaise Pascal, F-67000 Strasbourg, France).
[3] Advanced Light Source (Berkeley Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, U.S.A).
[4] Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC i Universidad de Zaragoza (Plaza San Francisco s/n, 50009 Zaragoza, Espanya).

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 SCO is accompanied by changes to the magnetic and physical properties. Ergo, those materials characterized by this behaviour have been fashioned into molecule-based switching materials for potential applications in nanotechnology.[2] Identifying the individual factors affecting the temperature of the SCO is a challenging task since many variables are involved.[3] We present a series of three Fe(II) derivatives of 1,3-bpp of (2-(pyrazol-1-yl)-6-(1H-pyrazol-3-yl)pyridine: $[Fe(1,3\text{-}bpp)_2](ClO_4)_2$ **(1)**, $[Fe(met1,3\text{-}bpp)_2](ClO_4)_2$ **(2)**, $[Fe(dimet1,3\text{-}bpp)_2](ClO_4)_2$ **(3)**, unveiling how the ligand substituents (containing none, one or two methyl) can modulate drastically the SCO temperature through intramolecular non-covalent interactions as the main factor.[4] This modulation of the SCO temperature was observed in solid state and in solution (with T_{SCO} **(3)** > T_{SCO} **(1)** > T_{SCO} **(2)**) which allows to quantify the influence of the methyl substituents on the SCO temperature. The origin of these effects were demonstrated by DFT calculations, excluding the crystal packing effects and laying on the intramolecular non-covalent or steric interactions preferably.



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24

GAS SENSORS BASED ON NANOSTRUCTURED METAL OXIDES

Guillem Domènech-Gil[1,2], Lukas Hrachowina[3], Elena López-Aymerich[1,2], Irmina Peiró[2], Antonio Pardo[2], Michael S. Seifner[3], Isabel Gràcia[4], Carles Cané[4], Mauricio Moreno[1,2], Sven Barth[3] and Albert Romano-Rodríguez[1,2]

[1] Institute of Nanoscience and Nanotechnology (IN^{2}UB), Universitat de Barcelona (UB), 08028 Barcelona, Spain
[2] Department of Electronic and Biomedical Engineering, Universitat de Barcelona (UB), 08028 Barcelona, Spain
[3] Institute of Materials Chemistry, TU Wien, 1060 Vienna, Austria
[4] Institut de Microelectrònica de Barcelona-Centre Nacional de Microelectrònica, Consejo Superior de Investigaciones Científicas (CSIC), 08193 Bellaterra, Spain.

There is an increasing concern about toxic and potentially harmful gases present in the atmosphere, both for outdoor and indoor environments. To monitor them, gas sensor systems are required. Semiconducting nanowires, presenting high surface to volume ratios, have demonstrated remarkable performances in terms of sensitivity and response time working as gas sensing material. With this aim different types of gas sensors based on nanostructured material were fabricated.

In this work we are going to review some of the activities we have been carrying out to develop different gas sensors based on nanomaterials.

Single β-Ga_2O_3 nanowire-based sensors, fabricated from Vapour-Liquid-Solid (VLS) synthesized nanowires, showed fast, stable and reproducible response towards water vapor at room temperature with very low power consumptions (0.25 to 250 nW). The response measured increased with concentration up to 97 % and the response time lasted between 7 and 2 minutes when exposed from 40 to 80 % of relative humidity (RH), respectively.

In_2O_3 octahedral microstructures, synthesized using a Vapour-Solid method, were aligned into chains between electrodes inducing DEP forces to fabricate gas sensors. These devices, working between 200 and 300 ºC, showed relevant response towards variable concentrations of oxygen, RH, nitrogen dioxide (NO_2) and ethanol (EtOH). The considerable high response to NO_2 increased when RH was added, reaching response values up to 250 % with response times < 12 min.

The response of a gas sensor array based on SnO_2, WO_3 and Ge nanowires, grown on-chip using the VLS method, towards atmospheres containing known harmful gases such as CO and NO_2, and at different levels of relative humidity have been measured. The discrimination between all the three analytes in the environment has been achieved by the well-known Principal Component Analysis representation.

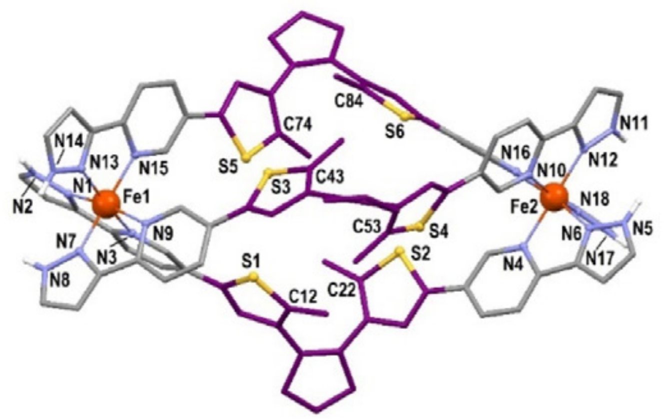
All these results will be discussed with the aim of developing advanced gas sensing devices and systems for environmental applications.

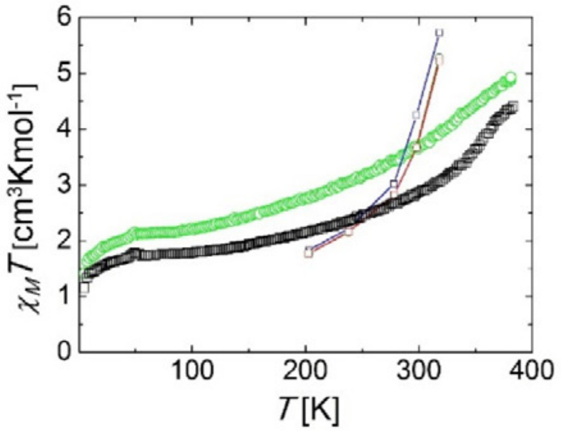
25 MAGNETO-OPTICAL MOLECULAR DEVICE: ENTANGLEMENT OF SPIN CROSSOVER, LUMINISCENCE, LIESST EFFECT AND PHOTOCHROMISM

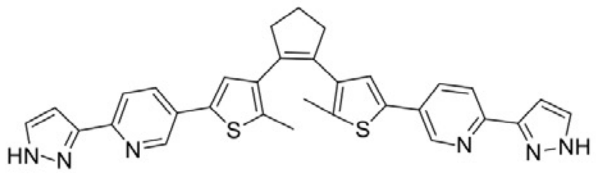
Marta Estrader[1], Jorge Salinas Uber[1], Leoni A. Barrios[1], Jorge García[1,3], Paul Lloyd-Williams[1,3], Olivier Roubeau[4], Simon J. Teat[5], and Guillem Aromí[1,2]

[1] Departament de Química Inorgànica i Orgànica, Universitat de Barcelona, Spain
[2] Institut de Nanociència i Nanotecnologia (IN^{2}UB), Universitat de Barcelona, Spain.
[3] Institute of Biomedicine of the University of Barcelona, Universitat de Barcelona, Spain
[4] ICMA, CSIC, Universidad de Zaragoza, Spain
[5] Advanced Light Source, Berkeley Laboratory, USA

The synthesis of a new ligand L which is designed to link two Fe(II) ions in form of the molecular triple stranded helicate [Fe$_2$L3]$^{4+}$ (cation of 1), which exhibits SCO in the solid state and in solution. In the solid state, the system can be addressed by irradiation at low temperature through the LIESST effect, resulting in the photogeneration of metastable HS Fe(II) centers that relax thermally to the LS upon warming. Irradiation of solid 1 with UV light produces a sizable change to the magnetic response of the material that is not reversible. In solution, the reversible full photo-conversion of the complex occurs thanks to the photo-cyclable moieties incorporated into L, as can be probed through absorption and 1H-NMR spectroscopy. The Evans method unveils the thermal SCO of 1 in solution and its dependence on the cyclization state, which can be manipulated externally through light irradiation. The fluorescence response of 1 in solution is also reversibly photo-switchable and in turn, is dependent on the spin state of the complex. The functional properties in solution are strictly of molecular origin and therefore, this assembly is a potential prototype of an externally addressable molecular device for spintronic applications.







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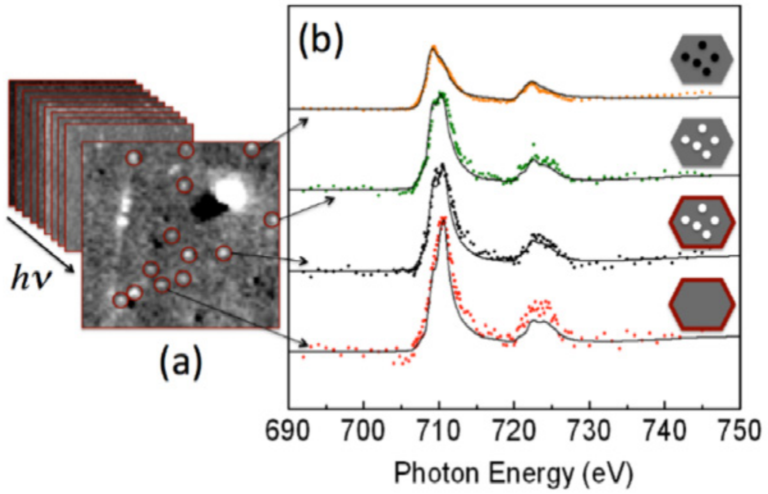
26 PROBING THE VARIABILITY IN OXIDATION STATES OF MAGNETITE NANOPARTICLES BY SINGLE-PARTICLE SPECTROSCOPY

A. Fraile Rodríguez[1,2], M. Escoda-Torroella[1,2], C. Moya[1,2], A. Romero[1,2], A. Labarta[1,2], X. Batlle[1,2]

[1] Departament de Física de la Matèria Condensada, Universitat de Barcelona, Av. Diagonal 647, 08028 Barcelona, Spain
[2] Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, 08028, Barcelona, Spain

Magnetite (Fe_3O_4) nanoparticles (NP) are versatile building blocks in a variety of applications due to its good magnetic performance, ease of production and functionalization by chemical routes, and low toxicity. However, controlling the electronic and magnetic properties of iron oxide NP remain a challenge because of their crucial dependence on composition, structure, surface chemistry, and interparticle interactions. The difficulty to disentangle these factors limits the ability to quantify their actual effects on the functional response of the NP.

In this work, we tackle this issue by studying the electronic and chemical properties of size- and shape-selected Fe_3O_4 NP with single particle sensitivity using synchrotron-based X-ray photoemission electron microscopy. The local X-ray absorption spectra reveal that the oxidation states and the amount and type of cations within the individual nanoparticles can show a striking local variability even when the average structural and magnetic parameters of the NP ensembles are homogeneous, and size-and sample-independent [1]. Our results show the key role of the oleic acid concentration during the synthesis reaction on the formation and distribution of the Fe phases within the individual NP. When the concentration of oleic acid is high enough, NP are composed of a Fe_3O_4 core surrounded by a γ-Fe_2O_3 shell. However, at low concentration of the fatty acid, the Fe_3O_4 NP are inhomogeneous with small inclusions of FeO and Fe phases, due to an uncontrolled reduction of Fe^{3+} cations [1]. Our results underline the importance of combining advanced synthesis techniques with single-particle investigations so as to improve the understanding and control over the electronic and magnetic phenomena at the nanoscale.



This work was supported by the Spanish MINECO (MAT201568772-P), Catalan DURSI (2014SGR220) and European Union FEDER funds.

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27 STRESS-INDUCED NANOSCALE MAGNETIC DOMAIN CONFIGURATIONS IMPRINTED IN Ni THIN FILMS BY PROXIMITY TO V_2O_3

A. Fraile Rodríguez[1,2], I. Valmianski[3], M. García del Muro[1,2], J. G. Ramírez[4], F. Kronast[5], I. Schuller[3], A. Labarta[1,2] and X. Batlle[1,2]

[1] *Departament de Física de la Matèria Condensada, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain*
[2] *Institut de Nanociència i Nanotecnologia (IN²UB), Universitat de Barcelona, Spain*
[3] *Department of Physics, University of California San Diego, La Jolla 92093, United States*
[4] *Department of Physics, Universidad de los Andes, Bogotá 111711, Colombia*
[5] *Helmholtz-Zentrum Berlin für Materialien und Energie, 12489 Berlin, Germany*

Nanoscale manipulation of magnetic thin films can be achieved through proximity effects in bilayer or multilayer structures. In particular, the proximity of a ferromagnetic (FM) thin film to a vanadium oxide results in a reversible modification of the magnetic properties due to the magnetoelastic anisotropy caused by the interfacial stress. However, it remains to be proven if the recently reported nanoscale phase coexistence in V_2O_3 yields a nanoscale magnetic domain pattern in the Ni layer.

In this work, we combine photoemission electron microscopy (PEEM) with X-ray magnetic circular dichroism (XMCD) to map the temperature-driven variation of the Ni domain configuration across the SPT of V_2O_3, in Ni (10 nm)/V_2O_3 (100 nm) bilayers. The histograms of the Ni magnetization orientations indicate sharp distributions around two different directions corresponding to the low-T and high-T states, respectively, and a broad distribution of intermediate orientations across the SPT, suggesting that the magnetization rotation is induced by the SPT. Thus, the fraction of the reoriented spins monotonically increases with the predominance of one of the coexisting V_2O_3 structural phases, in agreement with the evolution of the metal-insulator (MI) transition in the V_2O_3 thin film [3]. Furthermore, below the SPT, the Ni domains form stripe patterns with length (100s of nm) and periodicity matching the MI striped pattern in V_2O_3 [3]. More importantly, an in-plane reorientation of the Ni magnetization is observed, likely due to the rotation of the stress anisotropy axis associated with the SPT in V_2O_3 from the monoclinic low-Tto the rhombohedral high-T phases. This in agreement with in-plane ferromagnetic resonance experiments. Finally, the spatial-resolved map of the SPT transition temperatures across the sample obtained from the Ni domain pattern at each temperature is consistent with the nanoscale phase coexistence in V_2O_3 [3].

This work was supported by the Spanish MINECO MAT2015-68772- P project, European Union FEDER funds and the US-DOE DE-FG02-87ER-45332 grant.

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28 ENHANCEMENT OF THE RESISTIVE SWITCHING PROPERTIES OF SiAlO BY INTRODUCING Tb NANO-BARRIERS

J. L. Frieiro[1,2], O. Blázquez[1,2], J. López-Vidrier[3], S. Hernández[1,2] and B. Garrido[1,2]

[1] *MIND, Department of Electronics and Biomedical Engineering, Universitat de Barcelona, Martí i Franquès 1, E-08028 Barcelona (Spain)*
[2] *Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Av. Joan XXIII S/N, E-08028 Barcelona (Spain)*
[3] *Laboratory for Nanotechnology, Dept. of Microsystems Engineering (IMTEK), University of Freiburg, Albert-Ludwigs-University Freiburg, Georges-Köhler-Allee 103, D–79110 Freiburg (Germany)*

Resistive switching has recently drawn attention due to its possibilities to be employed as the future technology for optically-readable electronic memories. Materials showing this behavior can switch between high and low resistance states through voltage application. Diffusion of oxygen ions, responsible for this characteristic behavior, can also originate problems after a large number of cycles due to out-diffusion processes. Si-based oxides have already proved to be good candidates as active layers for this technology, and the introduction of additional materials may help improving the device operation.

In this work, electron beam evaporation has been employed to fabricate Al/SiO_2 nanomultilayer (NML) devices that exhibit resistive switching behavior. Despite the mentioned properties, the number of cycles the devices could withstand was very small, which is inferred to be caused by the degradation of the Al/SiO_2 bilayer (out-diffusion of oxygen from the active layer). Including nanolayers of a rare earth element, such as Tb in this case, resistive switching properties are enhanced, achieving longer endurance and larger difference between high and low resistance states. The large size of Tb ions, their clustering and electronegativity, make them suitable for limiting the oxygen out-diffusion. This idea is supported by the study of charge transport mechanisms within the different resistance states.

29 TAILORING FERROMAGNETIC ORDER IN COBALT FERRITE NANOPARTICLES THROUGH CRYSTALLINE NANOSTRUCTURE

A. Fraile Rodríguez[1,2], M. García del Muro[1,2], C. Moya[1,2], C. Piamonteze[3], X. Batlle[1,2], A. Labarta[1,2]
[1] Departament de Física de la Matèria Condensada, Universitat de Barcelona, 08028 Barcelona (Spain)
[2] Institut de Nanociència i Nanotecnologia (IN²UB), 08028 Barcelona (Spain)
[3] Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI (Switzerland)

Cobalt ferrite nanoparticles (NP), CoFe$_2$O$_4$, are attracting a lot of attention due to their potential applications, e.g. as permanent magnets, as a result of their high values of the magnetocrystalline anisotropy, saturation magnetization, and magneto-optical coefficients. However, in NP with spinel structure such as CoFe$_2$O$_4$, structural modifications at the grain boundaries and other crystallographic defects within each nanoparticle may provoke destabilization of the ferrimagnetic order due to the magnetic frustration arising from the competition between the inter- and intra-sublattice interactions. Recently we showed that monodisperse, stoichiometric CoFe$_2$O$_4$ NP, chemically synthesized with a controlled, progressive degree of structural disorder, can exhibit a wide variety of magnetic phenomena ranging from bulk-like ferrimagnetic order with high coercive fields for NP nearly free from structural imperfections, to glassy magnetic behaviour for the most structurally defective samples [1,2].

In this work, we deepen our understanding of this issue by studying the samples using complementary local probes: element- and site-specific X-Ray Magnetic Circular Dichroism (XMCD) measurements on ensembles of monodisperse NP combined with a structural characterization of a representative selection of individual NP by high-resolution transmission electron microscopy. By comparison of the experimental XMCD spectra to a linear combination of ligand field multiplet simulated spectra, the cation occupancies for each site are quantified. For the structurally defective samples, the Fe^{3+} cations occupy about 33% tetrahedral (Td) sites and 54% octahedral (Oh) sites, whereas Co2+ ions occupy 60% Td and 40% Oh sites, whereas a 10% increase (decrease) of the Co^{2+} (Fe^{2+}) ions in Oh sites is found for the highly crystalline sample. The XMCD loops show a progressive opening and squareness of the loops at all sites as the particles become less structurally defective. However, the Co^{2+} (Oh) sites are significantly more affected by the magnetic frustration associated to the structural defects than the Fe^{3+} and Fe^{2+} cations. Measurements with different probing depths yield to similar results indicating an homogeneous cationic and magnetic order within the whole volume of the nanoparticle.

This work was supported by MINECO (MAT2015-68772-P), DURSI (2009SGR856, 2014SGR220), and European Union FEDER funds.

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30 EFFECT OF PROCESSING METHODS ON THE STRUCTURE AND ELECTRONIC PROPERTIES OF PEDOT:PSS FILMS

I. Gabaldón-Saucedo[1,*], E. Gutiérrez[2], M. C. García-Guitérrez[2], A. Varea[1], A. Rodríguez-Rodríguez[2], A. Nogales[2], E. Rebollar[3], A. Vilà[1], T. Ezquerra[2], A. Cirera[1]
[1] Departament d'Enginyeries Electrònica, IN²UB-Universitat de Barcelona, 08028, Barcelona, Spain.
[2] Instituto de Estructura de la Materia (IEM-CSIC), Serrano 121, 28006, Madrid, Spain.
[3] Instituto de Química Física Rocasolano (IQFR-CSIC), Serrano 119, 28006, Madrid, Spain.
** igabaldon@el.ub.edu*

Conducting polymers are materials known by their lack of structural arrangement, which is a limiting factor for their electrical properties [1]. For many years, the focus of research has pointed out to enhance the molecular packing of polymers by employing distinct additives [2], thermal treatments [3], and different kinds of dopant species [4]. In energy applications, poly-3,4-ethylenedioxythiophene (PEDOT) doped with polystyrene sulfonate (PSS) has been particularly used to take the positive charges outside circuit in organic solar cells. The electronic transport of this compound material is intrinsically related to the nature of packing between quite long PSS chains and smaller segments of PEDOT chains [1-4]. Though researchers have a closer understanding about how PEDOT:PSS structures are, there is still question about how to modify the spatial distribution of polymer chains in order to transport charges through the material as fast as possible. In this research, PEDOT:PSS pristine was processed into thin films by employing several deposition methods (Electrospray Deposition, Spin Coating and Drop Casting) and different substrate treatments in order to study the relationship between the structure and electronic properties. Crystalline structures of these films were analyzed by Wide-Angle X-Ray Scattering (WAXS) using the synchrotron radiation. Raman Spectroscopy was employed to study aspects related to the molecular configuration of PEDOT in PSS environment. Electrical properties of thin films were measured by using an Atomic Force Microscope in Conductive mode (C-AFM) in order to observe the impact of the deposition method impact on the electrical current. Influence of physical deposition methods on PEDOT:PSS arrangement provide a route towards the development of electronic devices with enhanced properties.

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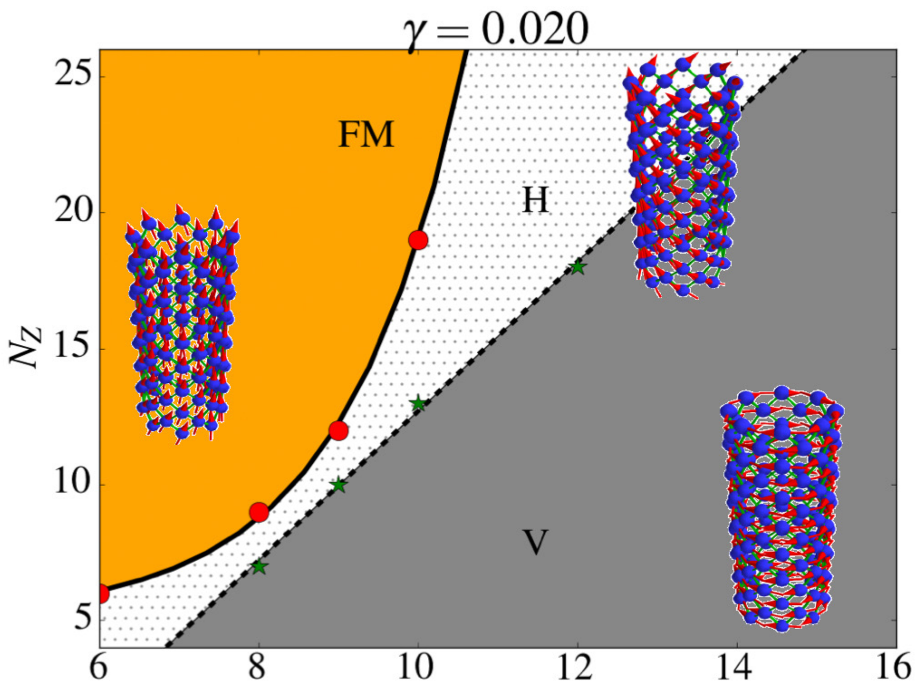
31 EFFECT OF DIPOLAR INTERACTION ON THE MAGNETIC PROPERTIES OF TUBULAR NANOSTRUCTURES

Òscar Iglesias[1], Hernán Salinas[2], Johans Restrepo[2]

[1] *Dpt. de Física de la Matèria Condensada and IN²UB, UB, Av. Diagonal 647, 08028 Barcelona, Spain*
[2] *Grupo de Magnetismo y Simulación G+ y Grupo de Instrumentación Científica y Microelectrónica, Instituto de Física, Universidad de Antioquia. A.A. 1226, Medellín, (Colombia)*

We have studied the low temperature magnetic equilibrium configurations and hysteretic properties of magnetic nanotubes. The results have been obtained by atomistic Monte Carlo simulations of a lattice of Heisenberg magnetic moments residing on the cylindrical lattice of single-wall zigzag nanotubes which interact via competing short-range exchange (J) and long-range dipolar interactions (D). In order to ensure that the low temperature magnetic states correspond to the true ground states, a simulated annealing protocol was followed. Results reveal the occurrence of different low-temperature magnetic states depending of the degree of competition between the exchange and dipolar energies given by the parameter $\gamma = D/J$: collinear FM states at low γ, vortex states above a certain threshold γ^*, and interesting non-collinear helical states for intermediate values of γ. We introduce a new order parameter related to the curl of the magnetization, which allows us to characterize the transition between these states and the appearance of helical structures. Stability of helical states are analyzed through analytical calculations. Finally, ground state phase diagrams of the states observed via simulation have been obtained for different aspect ratios of the nanotubes and values of γ.

(Work supported by Spanish MINECO (MAT2015-68772-P), Catalan DURSI (2014SGR220) and EU FEDER funds (Una manera de hacer Europa) also CSUC for supercomputer facilities.



Phase diagram for nanotubes having N spins per ring and Nz layers of length, showing stability regoins for FM (orange), Helical (white) and Vortex (grey) states.

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32 DESIGN, FABRICATION AND CHARACTERISATION OF Si NANOPILLARS-BASED PHOTONIC CRYSTALS FOR MECHANICAL SENSING

E. López-Aymerich[1,2,*], M. Dimaki[3], W. Svendsen[3], M. Moreno[1,2], F. Serras[4], A. Romano-Rodríguez[1,2]

[1] *Institute of Nanoscience an Nanotechnology (IN²UB), Universitat de Barcelona (UB), c/Martí i Franquès 1, E-08028 Barcelona,Spain*
[2] *MIND-Department of Electronics, Universitat de Barcelona (UB), c/Martí i Franquès 1, E-08028 Barcelona,Spain*
[3] *Department Nanotech, Technical University of Denmark (DTU), Ørsteds Plads 345, DK-2800 Kongens Lyngby, Dennmark*
[4] *Departmen of Genetics, Microbiology and Statistics and Institute of Biomedicine (IBUB), University of Barcelona, Spain*
* *e-mail: elopez@el.ub.edu; Tel.: +34-934-034-804*

Photonic device and system development is a fast growing field of basic and translational research because of the vast number of potential applications. Their use and study represent a challenge due to the difficulty of their fabrication at the nanoscale. Despite of that, different basic photonic devices have been developed thanks to the advanced knowledge on the silicon nanofabrication technologies [1]. Photonic crystals are defined as periodic arrangements of dielectric nanostructures inside a dielectric environment, both with quite different refraction indexes. Depending on the number of directions in which the structure is periodic, one can distinguish between one, two or three dimensional photonic crystals. The behavior of photons in a photonic crystal can be explained analogously as electrons do in a solid-ionic crystal. Moreover, if the dielectrics forming the photonic crystal show low light absorption, reflections and refractions within the dielectric material's interfaces would promote interferences between them, permitting the propagation of only certain wavelengths. Those which are allowed by the structure are known as light modes, while those which are not, are called forbidden modes. Tuning in the proper way the photonic crystal geometry and material configuration, one would have control over these permitted and non-permitted propagation wavelengths giving rise to the appearance of photonic bandgaps. They are described as a set of frequencies at which photons are forbidden to propagate in the crystal structure and thus, produce their complete absorption [2].

One potential application of photonic crystals would be their use as sensors since the bands of electromagnetic wave propagation are strongly susceptible to changes in the geometry of the crystal. Accordingly, a deformation would produce a change in the photonic band gap energy and/or spread. This deformation can be originated by, for example, the mechanical stresses produced during the growth and regeneration of living tissues. Evaluating these changes would allow the elucidation of the stopping mechanisms of this growth, as well as the investigation, for instance, whether cancer cells suffer less stresses than healthy cells.

This work summarizes the results obtained in our group and showed the potential capability of hexagonal arrays of silicon nanopillars to operate as photonic crystals and, thus, to act as mechanical sensors. One of the main conclusions of these works was the suitability of using silicon for the fabrication of the nanostructures due to its high refraction index value (3.42), and since the silicon technology is advanced enough for the implementation and development of the fabrication process. Moreover, simulations have shown that using a hexagonal lattice of nanopillars gives rise to a photonic band gap in the Near-Infrared range of the electromagnetic spectrum, around 1.5 µm, for horizontal light incidence [3], which is the most used wavelength range in optical fiber communications.

On the other hand, the deflection capability of the nanostructure arrangement was also simulated. The results reveal that the deflection is higher in pillars with smaller radii for a range of forces between 1-20 nN [4].

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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 plasma etching. This fabrication has been optimized and the last experiments have resulted in structures consisting on a 660x660 μm^2 nanopillars zone, enclosed by a 20µm-wide wall, and with 4 square-shaped grating structures, attached to the centre of each wall side, of 150x150 μm^2 [5]. Both the nanopillars and the fabricated zone are shown in Figure 1.

The morphological characterisation of the nanostructure has been carried out via scanning electron microscopy (SEM) and hyperspectral near infrared (HS-NIR). SEM shows the correct pattern fabrication and the almost perfect cylindrical shape of the 2 micrometres-tall pillars. Vertical illumination in the HS-NIR system both in air and water environments confirm the appearance of absorption peaks in the NIR range of wavelengths and their shift among different nanopillars radii and spacing. Finally, first compatibility tests with living cells have been recently performed successfully.

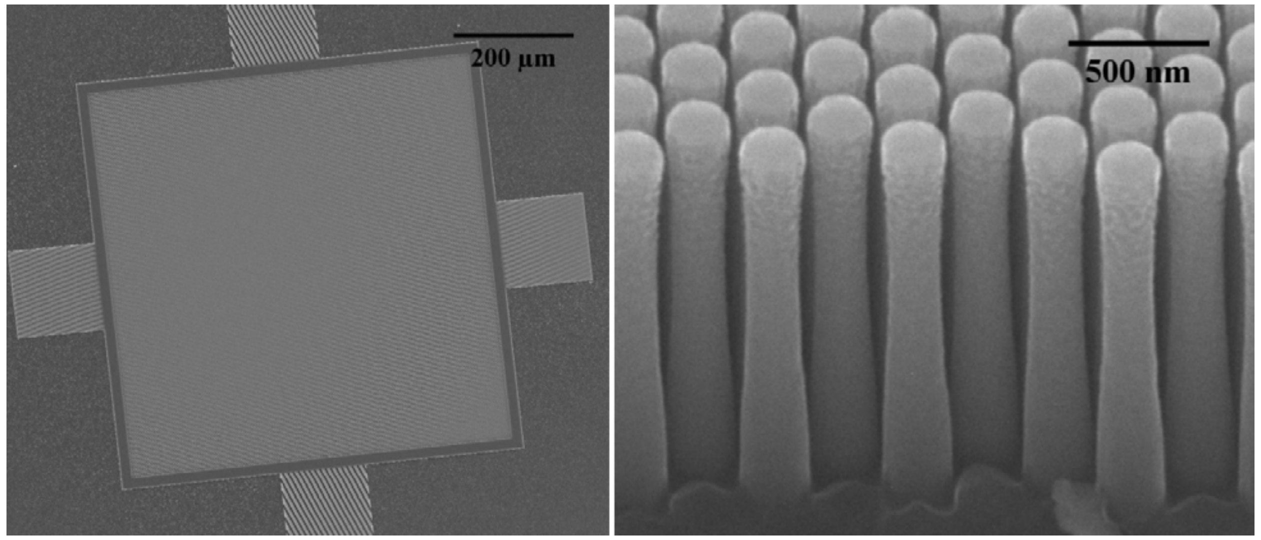

Figure 1. Overview of the fabricated zone (left); Nanopillar's seen in almost in cross-section (30°) (right).

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33 ELECTRICAL MEASUREMENTS OF NANOMATERIALS USING IN-SITU TEM: FROM 2D STRUCTURES TO FUNCTIONAL DEVICES

Gemma Martín[1,2], Sònia Estradé[1,2], Francesca Peiró[1,2] and Albert Cornet[1,2]
[1] LENS/MIND, Department of Engineering: Electronics, Universitat de Barcelona, Barcelona, Spain.
[2] Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Barcelona, Spain.

In-situ Transmission Electron Microscopy (TEM) techniques are becoming more and more relevant, as they allow a direct observation of the dynamic behavior at nanoscale level through imaging, diffraction and quantitative measurement of some properties transforming a standard TEM into a nano-lab.

Recently, *in-situ* TEM biasing is becoming one of the most important in-situ technique because it allows to obtain high-resolution, real-time dynamic thermal and electrical analysis of the specimen in multiple application topics: ferroelectric materials [1], characterization of low-dimensional structures (such as graphene [2] and molybdenum disulphide [3]), lithium-ion batteries[4] or study the evolution of filament formation in Resistive Random Access Memories (ReRAM) devices [5], among others.

In this work, different experiments carried out using *in-situ* TEM biasing in combination with structural and analytical characterizations are exposed. Figure 1(a) shows a picture of the TEM-STM holder with the Scanning Tunneling Microscope (STM) platinum tip on the right hand side and a wire as a sample support on the left hand side. The STM tip is used as an *in-situ* TEM electrical probe and can be positioned in a millimeter-scale workspace with subnanometer resolution, enabling the selection of a specific nanostructure, picking it up and applying a voltage to perform electrical measurements.

First of all, to better understand the behavior of Graphene Oxide (GO) in electronic nano-devices, the elucidation of the effects of electrical current through a single graphene oxide sheet have been studied by *in-situ* TEM. The reduction of GO has been measured qualitatively from the comparison of conductivity of the sample before and after the reduction, all in the same experiment. Besides, with this technique it is possible to control the reduction from the measure of the conductivity of the sample and also characterize the sample during the experiment (both through TEM observation and through current-voltage characteristic). Besides, the combination with other techniques like Raman spectroscopy or Electron Energy Loss Spectroscopy (EELS) give us a quantitative measure of the reduction of the sample with the TEM-STM system.

Secondly, ferroelectric and piezoelectric structures based on La_2WO_6 have been characterized by *in-situ* TEM. An I-V characteristic has been taken for each step of the tip controlled with the piezoelectrics of the holder. During the experiment a decrease of the resistance is observed while more pressure is applied from the tip. Besides, ferroelectricity characterization has been carried out from the cycle of the hysteresis switching current using the I-V method. The measured current is maximum when the applied voltage is close to the coercive voltage of the ferroelectric films and these current maxima correspond to the dipole reorientation contribution of the ferroelectric material.

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Finally, the study of the Conductive Filament (CF) formation mechanism in ReRAM devices has been addressed by *in-situ* TEM analysis of the structure and composition of the CF. Several samples have been characterized in order to study all the different states of the ReRAM device: pristine state, HRS (High Resistance State), LRS (Low Resistance State) and HBD (Hard Breakdown) at the nanoscale by High Resolution TEM (HRTEM), EELS and Energy-Dispersive X-ray Spectroscopy (EDX) techniques. Moreover, in-situ TEM biasing experiments have been performed to observe the formation of the CF in real time and to understand the physical mechanism behind the CF formation in ReRAM devices.

In conclusion, *in-situ* microscopy expands the horizons of the characterization and study of materials and, in particular, *in-situ* TEM-STM is a very useful and versatile tool to electrically characterize samples from nanomaterials to functional devices.

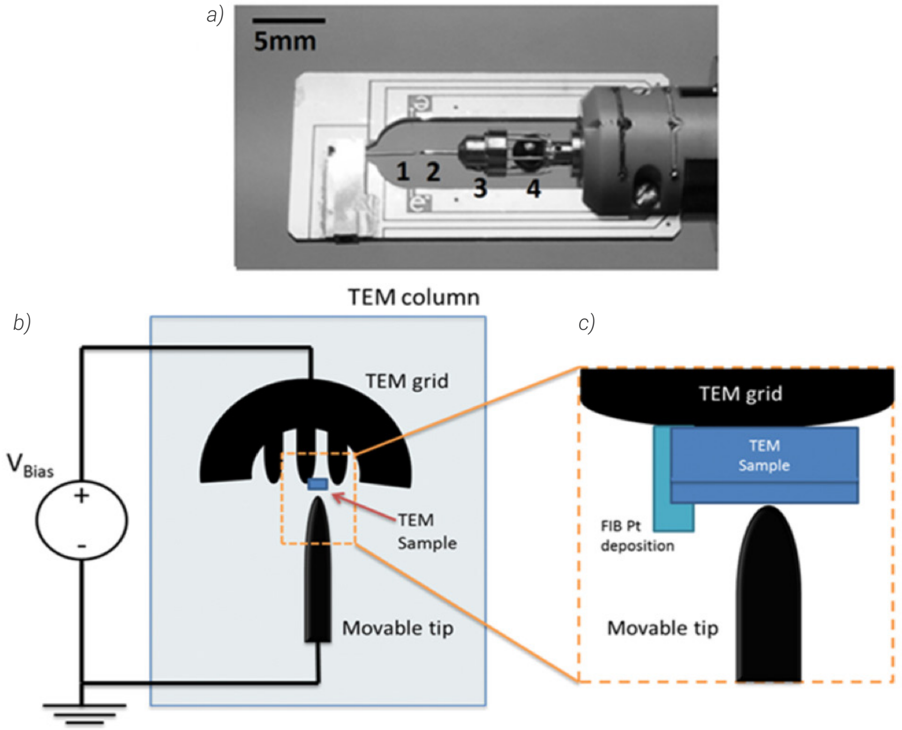

Figure 1: a) The TEM-STM holder used for the simultaneous observation and electrical measurements. The image shows the different parts of the TEM-STM holder: the platinum wire with the GO sheet attached (1); the STM movable tip (2); the hat (3) and the sapphire ball (4), b) schematic representation of in situ TEM-STM system and c) zoom on the tip of in situ TEM-STM system.

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34 SIMPLE AND DIRECT SYNTHETIC METHODS TO PRODUCE COLLOIDAL NOBLE METAL HYBRID AND TERNARY CHALCOGENIDE SYSTEMS USING NANOPARTICLES AS PRECURSORS

Guillem Montañá-Mora[1,2], Mariona Dalmases[1,2] and Albert Figuerola[1,2]
[1] *Departament de Química Inorgànica i Orgànica, Secció de Química Inorgànica, Universitat de Barcelona.*
E-mail: guillemonmora@gmail.com
[2] *Institut de Nanociència i Nanotecnologia, IN²UB, Universitat de Barcelona*

Recently, nanostructured semiconductor materials have been widely investigated due to the possibility of modifying their properties with a compositional or structural variation as well as with a morphologic change [1]. In particular, ternary and hybrid materials have stand out for many applications such as optoelectronics, photovoltaics, thermoelectricity and catalysis [2]. However, their synthesis is not always straightforward, and finding precursor species that are able to react under the same conditions is not an easy task. Developing a simple, cheap and flexible method[3] for their synthesis would be highly desirable.

In this poster, two different room temperature solution methods are assessed for the formation of 0D hybrid and ternary metal chalcogenides of the group 11 (Cu, Ag and Au). The first one entails the reaction between presynthesized nanoparticles and a molecular metallic precursor, while the second consists on the simple mixing of two different colloidal suspensions. As a result, Au-Cu-Se, Au-Cu-S, Au-Ag-Se and Au-Ag-S systems were obtained and structurally, compositionally and morphologically characterized. The suitability of the two methods is evaluated for each ternary system.

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35 HYBRID MOLECULAR-INORGANIC MATERIALS: HETEROMETALLIC CO$_4$DY COMPLEX GRAFTED ON IRON OXIDE NANOPARTICLES

Lidia Rosado Piquer[1], Jan H-G. Dreiser[2] and E. Carolina Sañudo[1]

[1] Inorganic Chemistry Department, Institute of Nanoscience and Nanotechnology (IN²UB), University of Barcelona, Av. Diagonal, 645, 08028, Barcelona, Spain
[2] Swiss Light Source, Paul Scherrer Institut, WSLA/106, CH-5232 Villigen PSI, Switzerland

Solvent free microwave assisted synthesis has been used for the synthesis of M$_4$Ln complexes (Fig. 1) (M = Ni, Co; Ln = Tb, Dy, Gd, La). It is proposed as a new and green synthetic tool, with low temperatures and short reaction times. We have achieved a controlled synthesis with the possibility of tuning the magnetic properties of the complexes by introducing the desired metal.

These metalorganic structures present characteristic cores that provide them with interesting magnetic properties. Such complexes are called molecular nanomagnets (MNMs) and have been investigated due to their possible application in fields like magnetic coolers or information storage and processing. In order to fabricate devices for this aim, deposition and nanostructuration of these complexes on surfaces is required.

We report one of the complexes of the M$_4$Ln family: [Co$_4$Dy(OH)$_2$(chp)$_4$(tBuSALOH)$_5$(H2O)$_2$(MeCN)]. It has been characterized and grafted onto iron oxide nanoparticles (NPs) in order to obtain the nanostructured material. The hybrid system NP-Co$_4$Dy (Fig. 2) has been characterized by element specific XMCD with the aim of studying the coupling between Co, Dy and Fe. Moreover, other characterization techniques like XPS, TEM, EDX and SQUID magnetometry have been used.

Previous studies have been done in the group with a very similar system using the analogous complex Ni$_4$Tb[1].

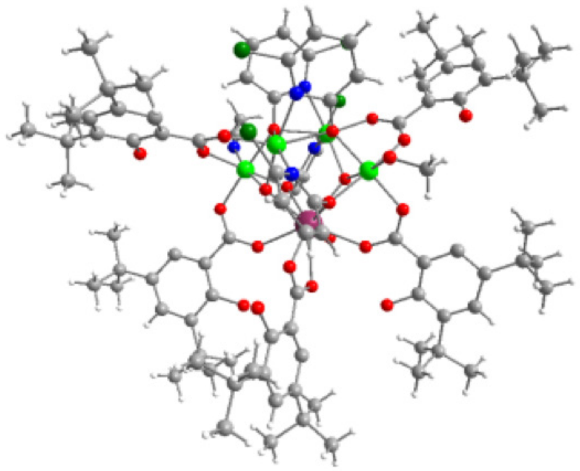

Figure 1: Structure of the M$_4$Ln complexes with the general formula: [M$_4$Ln(OH)$_2$(chp)$_4$(tBuSALOH)$_5$(H$_2$O)(MeCN)(Solv)].

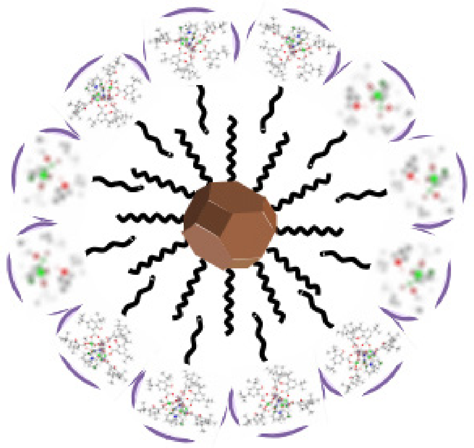

Figure 2: Schematic representation of the hybrid system NP-Co$_4$Dy

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36 STUDY OF OXYGEN DEFICIENT ALPHA-BI$_2$O$_3$ COMBING EELS + DFT

P. Torruella[1,2], C. Coll[1,2], G. Martín[1,2], L. López-Conesa[1,2,3], M. Vila[4,5], C. Díaz-Guerra[4], M. Varela[4], M.L.Ruiz-González[6], J. Piqueras[4], S. Estradé[1,2] and F. Peiró[1,2]

[1] LENS-MIND, Departament d'Enginyeria Electrònica i Biomèdica, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain.
[2] IN²UB - Institute of Nanoscience and Nanotechnology, Universitat de Barcelona, 08028 Barcelona, Spain
[3] Unitat TEM-MAT, Centres Científics i Tecnològics de la Universitat de Barcelona (CCiTUB), Lluís Solé i Sabarís 1, 08028 Barcelona
[4] Departamento de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, 28040 Madrid, Spain.
[5] IMDEA Materials Institute, c/Eric Kandel 2, Getafe, 28960, Madrid, Spain
[6] Departamento de Química Inorgánica, Facultad de Químicas, Universidad Complutense de Madrid, 28040 Madrid, Spain.

Density Functional Theory (DFT) calculations are widely used in the understanding of the electronic structure of the materials. Combined with Electron Energy Loss Spectroscopy (EELS) it is a powerful tool to elucidate all the features which appear in the experimental spectra [1]. In the present work we address the characterization of bismuth oxide, an interesting material with potential applications in the fields of optics, electrochemistry and in fuel cells, using EELS and DFT [2]. One the most promising properties of Bi$_2$O$_3$ is its abnormally high oxygen conductivity, which is normally discussed in terms of oxygen vacancy generation and transport [3]. However, most of the literature about this material are studies performed at the macroscopic level and even though local properties such as the electronic environment of the oxygen would be highly interesting, little experimental work has been done in this matter [4]. We have performed pioneering core and low-loss EELS studies in three different α- Bi$_2$O$_3$ samples which exhibit different oxygen conductivity values. These are the first reported core-loss EELS measurements of this material to our knowledge and as such, how spectral features relate to structural and electronic properties remains unclear.

Detailed EELS measurements have revealed significant differences in the Electron energy-loss near-edge structure (ELNES) of the respective oxygen K edges. Since there are not reported EEL spectra of α-Bi$_2$O$_3$ the interpretation of the ELNES features required DFT calculations. First, the bulk α-Bi$_2$O$_3$ ELNES (without oxygen vacancies) was simulated using WIEN2k [5]. Then DFT simulations of oxygen deficient Bi$_2$O$_3$ were carried out. The theoretical data obtained from DFT was compared to the experimental data. Several simulations were performed considering a different fraction of oxygen deficiency. The results showed a shift of the O K edge depending on the amount of vacancies. Furthermore, EELS analysis together with DFT enabled to discern, from the non equivalent O crystallographic sites in the unit cell, which was the site where the oxygen vacancies appear, in addition to establishing a relationship between the fraction of oxygen vacancies and the shift of the O K edge.

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NANOSTRUCTURED MATERIALS [NMATERIALS] RESEARCH AREA

37 AGGREGATION STUDY OF GOLD (I) COMPLEXES USING SAXS TECHNIQUE

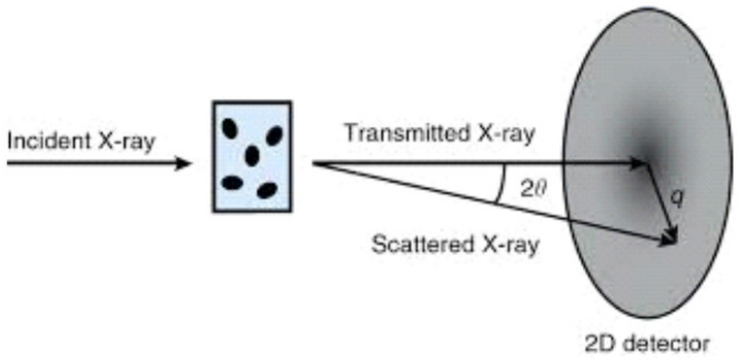
Alejandro Llanos Montetes[1], Andrea Pinto Martínez[1,2] and Laura Rodríguez Raurell[1,2]

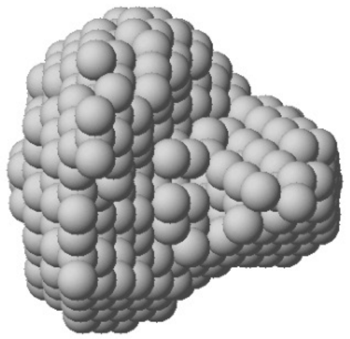
[1] *Departament de Química Inorgànica i Orgànica, Universitat de Barcelona, Martí i Franqués 1-11, 08028 Barcelona, Spain*

[2] *Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, 08028, Barcelona, Spain*

Gold (I) compounds are in focus of many chemistry researches due to their potential applications in different areas such as luminescence, molecular recognition, optical switches, electronics and catalysis. The capability of establishing weak Au(I)···Au(I) aurophilic contacts together with the classical interactions (e.g. π-π stacking or hydrogen bonding) can modulate the resulting assemblies and properties. [1,2]

In this work, we are interested in the level of aggregation in their very early state. A good technique for that purpose is SAXS (Small Angle X-Ray Scattering) which we can determine the size of these aggregates by measuring density differences with nanoscale precision. [3] In this way, we can determine the shape and size of the primary aggregates and understand the first steps of the aggregation that will give rise to the formation of more complex structures.





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38 HYBRID CARBON NANOTUBES AND GRAPHENE NANOWALLS ELECTRODES FOR SUPERCAPACITOR APPLICATIONS

J. Martí-González[1,2], F. Pantoja[1,2], A. Musheghyan-Avetisyan[1,2], I. Alshaikh[1,2], R. Amade[1,2], J.L. Andújar[1,2], E. Pascual[1,2] and E. Bertran-Serra[1,2]

[1] *FEMAN-ENPHOCAMAT Group, Dep. Applied Physics, Universitat de Barcelona, C/ Martí i Franquès, 1, 08028 Barcelona*

[2] *Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona*

Electrochemical double layer capacitors (EDLC), also known as supercapacitors, are one of the most promising electrochemical energy storage devices for high power delivery applications due to its high power density, high energy density and fast charging rate [1-3]. The use of high surface area electrodes is critical in order to maximize these properties. We propose a new method to obtain hybrid electrodes of carbon nanotubes (CNTs) and graphene nanowalls (GNWs). Both are carbon-based nanostructures that present high specific surface, high electric conductivity, chemical inertness thermal and mechanical stability, so they are suitable candidates in order to use them as electrodes in supercapacitors [4, 5]. CNTs are obtained directly on stainless steel surface by plasma enhanced chemical vapor deposition (PECVD), without use of diffusion barrier and using the internal alloys elements of the substrate as a catalyst. With this approach is possible to obtain low resistance contact between the CNTs and the substrate [6]. GNWs obtained by inductively coupled plasma chemical vapor deposition (ICP-CVD) present catalyst free growth, so virtually they can be grown on every substrate that withstands the synthesis temperature. As a result, hybrid structures of GNWs-CNTs can be synthetized. The aim of the present work is to obtain different types of carbon-nanostructured electrodes by combining GNWs and CNTs in order to maximize their capacitance. Raman and SEM characterization shows that various samples of independently CNTs, GNWs, and combination of CNTs-GNWs morphologies have been obtained.

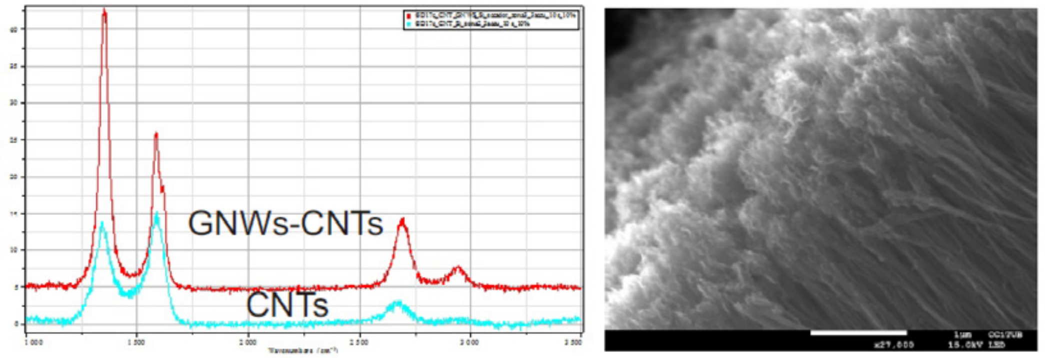

Figure 1: On left, Raman spectra of CNTs and GNWs-CNTs samples. On right, SEM image of GNWs-CNTs sample.

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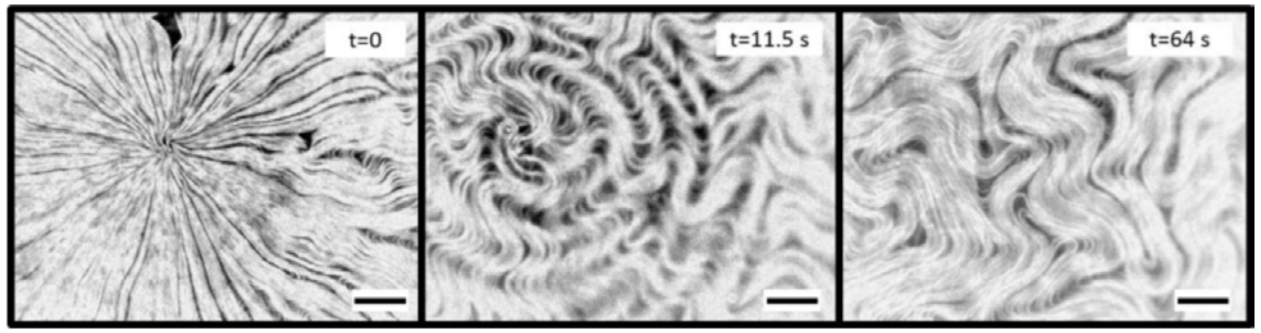
39 DETECTING THE BEND INSTABILITY OF EXTENSILE ACTIVE NEMATICS

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

[1] *Departament de Ciència de Materials i Química Física, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain*
[2] *Institute of Nanoscience and Nanotechnology (IN^{2}UB), Universitat de Barcelona, Spain*

Active matter embraces systems composed of particles that harness energy to produce motion, driving the system far from equilibrium [1]. The interactions between the constituting units give rise to a wealth of collective dynamical behaviors qualitatively different from that expected of an individual particle. For example, active systems at a low Reynolds number, like bacterial suspensions, show chaotic flows characterized by patterns of jets and swirls [2]. This flow regime is known as active turbulence. Some active systems present a nematic order, which is why they are referred to as active nematics. Many theoretical studies have dealt with the elucidation of the origin of active turbulence in aligned active nematics. So far, there is an ongoing consensus that this turbulent regime arises from a first instability which is intrinsic to the material [1, 3, 4]. However, to the best of our knowledge, nobody has reported the observation of the primary instability of an aligned active nematic which is at the origin of such turbulent states. Here, we report and characterize such instability, in particular the bend instability, in an in-vitro reconstitution of the cytoskeletal network, which has shown to organize as an extensile active nematic when condensed at a soft interface. This preparation was originally proposed by the group of Dogic at Brandeis University [5] and it consists of PEG-depeleted bundles of micrometer-sized microtubules continuously stirred by clusters of kinesin fueled with ATP. We have succeeded at aligning the material by means of a local aspiration and we have followed the onset of the instability. Specifically, we have measured its intrinsic wavelength and time-scale. We have seen that from this first relaxation, the instability repeats in cascade until arriving to the turbulent regime. Tuning the composition of the material we have obtained the most unstable modes of the instability and its associated time-scale.



Fluorescence micrographs of successive states of the bend instability occurring in the AN. (Scale bar: 100 μm).

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40 TRANSPORT AND ASSEMBLY OF COLLOIDS IN LIQUID CRYSTALS

Josep M. Pagès[1,4], Arthur. V. Straube[2,3], Pietro Tierno[3,4,5], Jordi Ignés-Mullol[1,4] and Francesc Sagués[1,4]

[1] *Departament de Ciència de Materials i Química Física, Universitat de Barcelona, Catalonia*
[2] *Department of Mathematics and Computer Science, Freie Universität Berlin, Berlin, Germany*
[3] *Departament de Física de la Matèria Condensada, Universitat de Barcelona, Catalonia*
[4] *Institut de Nanociència i Nanotecnologia (IN^{2}UB), Universitat de Barcelona, Catalonia*
[5] *Universitat de Barcelona Institute of Complex Systems (UBICS), Universitat de Barcelona, Catalonia*

Colloidal microparticles dispersed in a liquid medium present a rich variety of interactions, even more when an external field is applied [1]. When the host is a nematic liquid crystal (NLC), inclusions can be driven by means of liquid crystal-enabled electrosmosis (LCEEO) [2]. This process is based on the unbalanced ionic flows at both sides of the inclusions coupled to the local orientational distortions of the nematic matrix. Peanut-shaped colloidal inclusions guarantee a dipolar component in the defect configuration of the local director field. The use of alternating current (AC) is of special interest in this case because ion migration is avoided, while enabling not only solid particle transport but water-based cargoes as well [3].

Experimentally, we prepared hybrid LC cells with plates coated with a transparent electrode, ITO. One plate was functionalized with a photosensitive self-assembled monolayer, which can turn the local director field from homeotropic to planar anchoring of the NLC under UV forcing. The reverse modulation is achieved with blue light. The counterplate was treated with a polyimide resin to obtain a strong homeotropic anchoring of the mesogen. The anchoring was controlled by using a custom LED EPI-illumination system which features a Gaussian profile. Under UV light, LC molecules develop an in-plane radial pattern (pure splay texture) expanding from the centre of the light spot where anisometric particles will assemble in a circular cluster [4].

In this contribution, we address a circular colloidal assembly above a topological defect in a LC which presents three different states as shown in Fig.1. As time proceed, a solidified central core (I) ,where the area fraction occupied by particles (φ) remains mostly constant, is followed by a liquid-like corona (II) ending in a dispersed, gas-like phase (III). Directly, from φ we can determine the mechanical pressure of the system. We also develop a model which captures the basic physics of the process. Further simulations are in complete qualitative agreement.

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41 TAILORING PLASMONIC RESPONSE BY LANGMUIR–BLODGETT GOLD NANOPARTICLE TEMPLATING FOR THE FABRICATION OF SERS SUBSTRATES

M. Tahghighi[1,2], I. Mannelli[1], D. Janner[3,4] and J. Ignés-Mullol[1,2]

[1] *Departament de Ciència de Materials i Química Física, Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain*
[2] *Institute of Nanoscience and Nanotechnology (IN²UB), Universitat de Barcelona, Spain*
[3] *Politecnico di Torino, Dipartimento di Scienza Applicata e Tecnologia (DISAT), Italy.*
[4] *INSTM UdR Torino Politecnico, Corso Duca degli Abruzzi 24, Torino 10129, Italy.*

Nanoparticle self-assembly is a robust and versatile strategy for the development of functional nanostructured materials, offering low-cost and scalable methods that can be fine-tuned for many different specific applications. In this work, we demonstrate a pathway for the fabrication of tailorable two- dimensional lattices of gold nanoparticles to be used in Surface Enhanced Raman Scattering (SERS) detection of biomolecules. As a first step, nanoparticles are spread as a monolayer at the water/air interface, compressed to a target lateral density in a Langmuir–Blodgett technique, and transferred to a properly functionalized substrate 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 nanoparticle grow thus tuning the plasmonic response and SERS enhancement. Compared to direct deposition or self-assembly methods, our protocol enables to obtain consistent results and much higher coverage of Au nanoparticles thanks to the active control of the surface pressure of the spread monolayer.

NANOENERGY: PRODUCTION, STORAGE AND ENVIRONMENT (NENERGY) RESEARCH AREA

42 STUDY OF NEW NANOSTRUCTURED CATALYSTS FOR SELECTIVE PROCESSES IN THE REDUCTION OF CO_2

A. Pajares[1,2], X. Liu[1], Y. Wang[1], P. Ramírez de la Piscina[1] and N. Homs[1,2]

[1] *Departament de Química Inorgànica i Orgànica, secció de Química Inorgànica & Institut de Nanociència i Nanotecnología (IN²UB), Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain.*
[2] *Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, 08930 Barcelona, Spain.*

The accumulation of CO_2 in the atmosphere has increased significantly in the last century and its rising concentration in the atmosphere plays a significant role in the climate of our planet through the greenhouse effect. Thus, the mitigation of atmospheric CO_2 becomes more and more crucial. Today, the reuse of CO_2 through its chemical recycling is a promising route, which could contribute to the decrease of globally emitted CO_2; nowadays we can consider CO_2 as a truly key molecule in an energy-sustainable development.

A particular approach to the use of CO_2 consists of its reduction to CO, by using H_2 as a reducing agent, through the reverse water gas shift reaction (RWGS). This reaction has been studied over metal-based (Cu, Pt) catalysts. Transition metal carbides (TMCs) have received interest because of their similar properties to noble metals in different aspects, and recently were reported to be useful for the activation of CO_2. The most studied TMCs as catalysts are probably those of Mo. We have recently proposed new strategies for the synthesis of Mo_xC-based catalysts. In our group, we continue to develop new routes for the synthesis of transition metal carbides such as those of group 5 elements, which can be useful for RWGS application. Moreover, along the different pathways to achieve CO_2 conversion, the photocatalytic reduction of CO_2 is one of the most attractive method. Mesoporous silicas with immobilized organic donor–acceptor molecules have been reported to exhibit long-lived charge separation. Periodic mesoporous organosilicas (PMOs) are organic-inorganic materials, which can be suitable for the construction of organic donor–acceptor systems useful in photocatalysis. However, PMOs materials have not high photo-efficient active sites. The introduction of TiO_2 moieties immobilized in the silica framework can help to improve the photocatalytic efficiency for reduction of CO_2. Actually, we are developing new Ti-PMOs materials by introduction of different amounts of TiO_2 into the framework of mesoscopic ordered biphenyl-PMOs to be used in the photocatalytic reduction of CO_2. In the present work, a summary of the activities of the MATCAT group on this will be presented.

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IN²

Institut de Nanociència
i Nanotecnologia

UNIVERSITAT DE
BARCELONA

IN^{2}UB
Universitat de Barcelona
Facultat de Química
Av. Diagonal 645
08028 Barcelona
+34 93 402 12 66
in2ub@ub.edu

IN^2 Institut de Nanociència i Nanotecnologia
UNIVERSITAT DE BARCELONA