SCIENCE • INDUSTRY • SOCIETY

2021 IMAGINENANO

NanoSpain Conf 2021

November 23-25, 2021 • Bilbao (Spain)

www.imaginenano.com

ABSTRACTS BOOK

• ORGANISER

BILBAO EXHIBITION CENTRE

EXPOSSIBLE!

PHANTOMS foundation

Your Qubits Characterized & Measured with One Integrated Control Stack Solution

QBLOX

1 qubit

20 qubits

Shorten Setup Time
Quick Calibration
Advanced Sequencing

Fully-integrated
Quantum Control Stacks
Ultrastable DC to 18.5 GHz
Synchronized <<1 ns
Dedicated Qubit OS

100s qubits

Contact us via **sales@qblox.com** for a personalized demo or visit **qblox.com** >

On behalf of the International, Scientific and Technical Committees we take great pleasure in welcoming you to Bilbao for the fifth edition of **ImagineNano**.
Since 2011 **ImagineNano** has strengthened its position as one of the main events dedicated to Nanoscience and Nanotechnology (N&N) in Europe. The outstanding results of participation that have been reached and the interest created by the discussions, have laid the foundations for the upcoming edition.

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

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

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

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

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

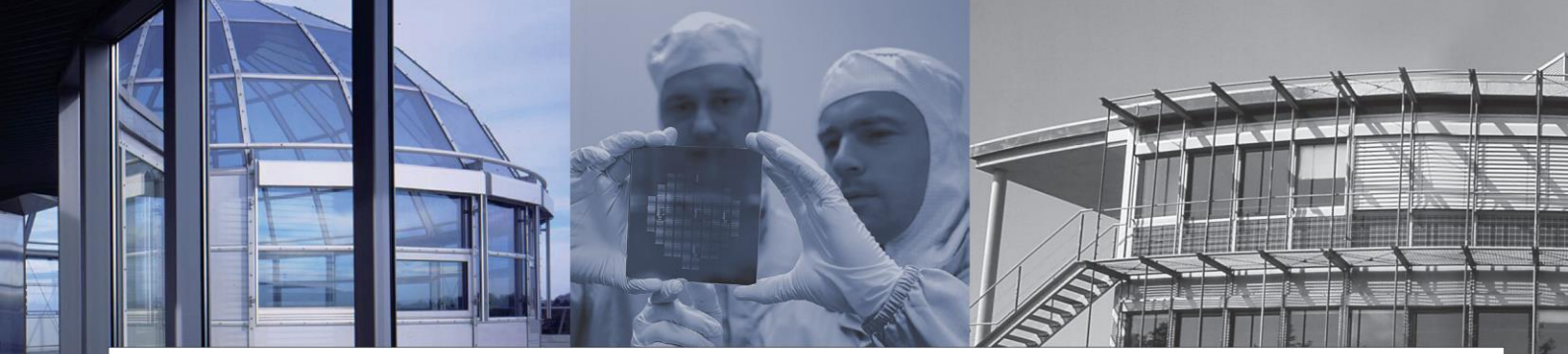
The Basque Country demonstrates its strengths in nanoscience, micro and nanotechnology, and positions itself as a major player in the "nano" world, reason why **ImagineNano** is organized for the 5th time in Bilbao.

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

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

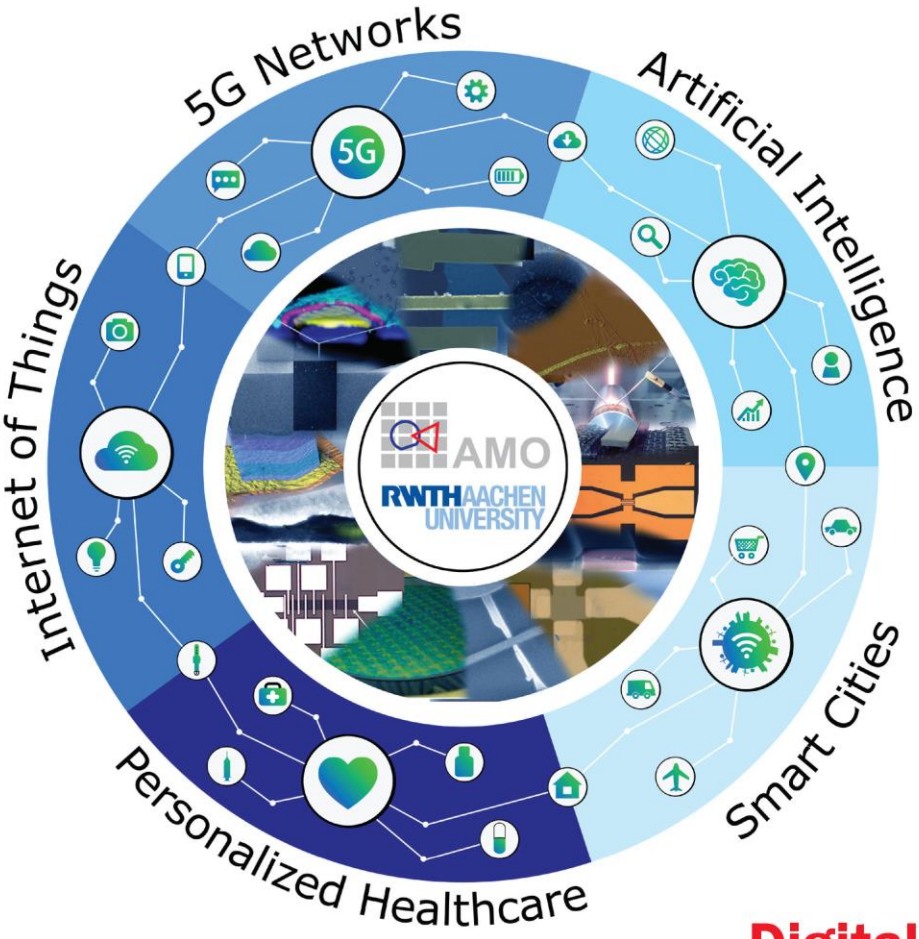
ORGANISER

PHANTOMS foundation



Aachen Graphene & 2D-Materials Center

From basic research to innovation



Digital Hardware

- Electronics for neuromorphic computing
- Sensor technology for autonomous driving and IoT
- Optoelectronics for high speed data communication
- Electronics for wearables and implantables

AMO

AMO GmbH
Otto-Blumenthal-Straße 25 ■ D-52074 Aachen ■ Germany
Phone +49 241 88 67-125 ■ Fax +49 241 88 67-571
services@amo.de ■ www.amo.de

INDEX

COMMITTEES

IMAGINENANO 2021 MAIN ORGANISERS

Antonio Correia (Phantoms Foundation, Spain)
Ricardo Muiño (DIPC, Spain)

QUANTUM2021 MAIN ORGANISERS

Antonio Correia (Phantoms Foundation, Spain)
Ricardo Muiño (DIPC, Spain)
Pablo Ordejon (ICN2, Spain)
Valerio Pruneri (ICFO, Spain)
Stephan Roche (ICREA/ICN2, Spain)
Daniel Sanchez Portal (CFM - CSIC - UPV/EHU – DIPC, Spain)

GRAPHENE & 2DM SCIENCE & INDUSTRY (GSI) ORGANISING COMMITTEE

Antonio Correia (Phantoms Foundation, Spain)
Stephan Roche (ICREA/ICN2, Spain)

3PM 2021 ORGANISING COMMITTEE

Andreas Berger (CIC nanoGUNE, Spain)
Antonio Correia (Phantoms Foundation, Spain)
David García (ICN2, Spain)
Antonio García Martín (IMN – CNM / CSIC, Spain)
Lluis F. Marsal (Universitat Rovira i Virgili, Spain)
Hernan Miguez (IMSC-CSIC, Spain)
Fernando Moreno (Universidad de Cantabria, Spain)
Juan José Saenz (DIPC, Spain) *In memoriam*

IC2 - NANOCOMPOSITES 20121 ORGANISING COMMITTEE

Eric Anglaret (Université Montpellier, France)
Antonio Correia (Phantoms Foundation, Spain)
Ignacio Dancausa (APTIE, Spain)
Alfonso López (APTIE, Spain)

NANOSPAIN 2021 ORGANISING COMMITTEE

Xavier Bouju (CEMES-CNRS & C'Nano Grand Sud-Ouest, France)
Fernando Briones (IMN –CNM / CSIC, Spain)
Antonio Correia (Phantoms Foundation, Spain)
Pedro Echenique (DIPC, Spain)
Lars Montelius (INL, Portugal)
José Manuel Perlado Martín (IFN-ETSII / UPM, Spain)
Emilio Prieto (Centro Español de Metrologia – CEM, Spain)
Juan José Saenz (DIPC, Spain) *In memoriam*
Josep Samitier (IBEC/Universidad de Barcelona, Spain)
Daniel Sánchez Portal (CFM - CSIC - UPV/EHU – DIPC, Spain)

3D PRINTING SPAIN 2021 – BEYOND NANO ORGANISING COMMITTEE

Antonio Correia (Phantoms Foundation, Spain)
Shlomo Magdassi (The Hebrew University of Jerusalem, Israe))
Josep Samitier (IBEC/UB, Spain)

ABSTRACTS BOOKS

QUANTUM NANOSPAIN 3PM 3D PRINTING GSI IC2

SPONSORS

MAIN SPONSOR

PROVINCIAL GOVERNMENT OF BIZKAIA

The Regional Government is the executive body that, within its area of competence, assumes the government and administration of Bizkaia. The historical figure of the Deputy General heads the Regional Government. The latter is elected by the Provincial Parliament of Bizkaia. The Deputy General elects, in turn, the Regional Deputies, who head the various departments that make up the Regional Government. Currently, this is formed by the following Regional Departments: Agriculture / Culture / Economic Promotion / Environment / General Deputy / Presidency / Public Works and Transport / Social Action / Treasury and Finance

More info: https://web.bizkaia.eus/

PLATINUM SPONSOR

IKUR is the Basque strategy promoted by the Education Department of the Basque Government to boost the Scientific Research in specific strategical areas and to position them at international level. Although its first focus is to enhance the generation of knowledge of excellence, in the medium and long term, it also seeks the technological development in these fields.

More info: www.science.eus/en/ikur

GOLD SPONSORS

With a dedicated team of scientists, engineers and developers we are pushing quantum technology to support scientists worldwide with our scalable qubit control and readout equipment from ultrastable DC to 18.5 GHz for academic and industrial quantum labs. The Qblox control stack combines unlevelled noise performance, low-latency arbitrary control flows and can be scaled up to 100s of qubits. Our company is based in the Netherlands as a spinoff of QuTech, which enables us to implement the latest scientific insights and take a position upfront in the worldwide race towards quantum advantage. Using the technology developed at QuTech as a springboard, the Qblox team has fundamentally reimagined the architecture of quantum control to create a single integrated control stack that provides all the functionality needed to manipulate and measure quantum computers. The Qblox architecture speeds up calibration routines by orders of magnitude, saving research teams significant amounts of time and money. The Qblox team is interested in meeting experiment quantum physicists to learn about their applications and how Qblox could support their scaling needs.

More info: www.qblox.com

GOLD SPONSORS

AMOs mission as a research oriented company is to efficiently close the gap between university research and industrial application. For this purpose AMO identifies those topics from basic research that seem particularly suitable for industrial implementation and demonstrates these in application-oriented technology. In joint projects and bilateral cooperation, research and development results are transferred to industry for maintenance and creation of jobs. Thus nanotechnology is expected to provide considerable potential for application areas such as information technology, biotechnology and environmental technology. Headed by Prof. Max Lemme, AMO operates a high level 400 m² cleanroom. Furthermore AMO offers a range of services from consulting to prototype development.

More info: www.amo.de

We provide ready-to-use nanomaterials, including functionalized nanoparticles, quantum dots, carbon nanomaterials, boron nitride nanotubes, perovskites, and OLED materials. Our biomedical materials comprise degradable polymers, natural polymers, block copolymers, hydrogels, and PEGs. Our high-performance energy materials and electronics materials have advanced semiconducting capacity and power density. Our high-purity metal salts, deposition precursors, metals, alloys, oxides, monomers, polymers, initiators, and additional polymerization tools ensure the synthesis of high-quality materials.

More info: www.sigmaaldrich.com/ES/en/products/materials-science

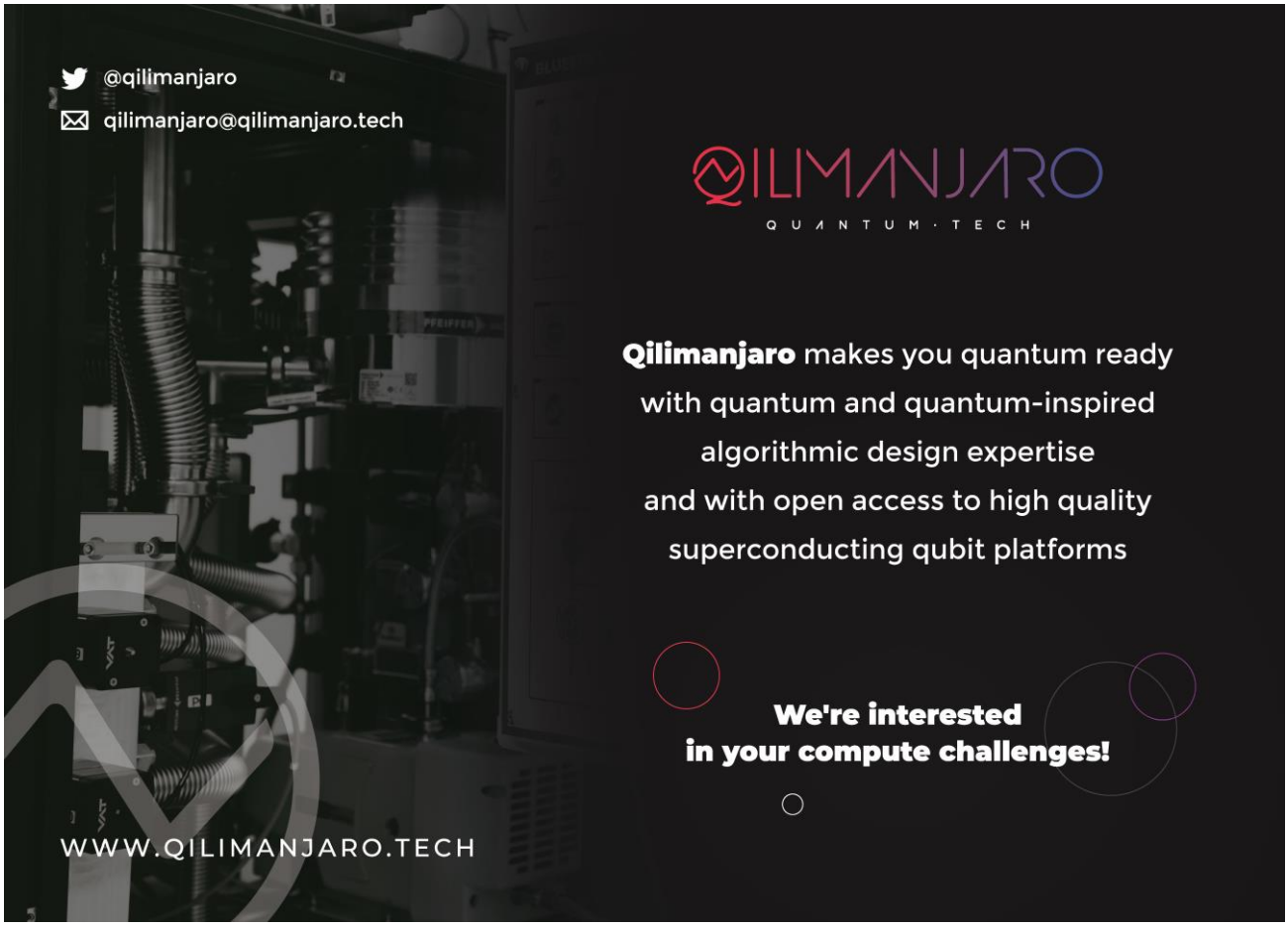
SILVER SPONSORS

Born in 1999 as a joint initiative between Consejo Superior de Investigaciones Científicas (CSIC) and Universidad del Pais Vasco – Euskal Herriko Unibertsitatea (UPV/EHU), the long-term aim of CFM is to push forward the frontiers of knowledge on advanced materials science research, by putting together stable teams with a record of excellence in scientific research. CFM quality work has been recognized by the Basque Government acknowledging its instrumental body MPC as a Basic Excellence Research Center (BERC).

More info: **https://cfm.ehu.es/**

Qilimanjaro Quantum Tech (www.qilimanjaro.tech) is a quantum computing company that began operations in 2020 as a spin-off of the Barcelona Supercomputing Center - Spanish Supercomputing Center (BSC, https://www.bsc.es), of the Institute High Energy Physics (IFAE, www.ifae.es) and the University of Barcelona (UB, www.ub.edu). It develops algorithmic and cloud access services as well as quantum platforms aimed at optimization, simulation and Machine Learning problems for use cases in sectors such as logistics, chemistry and finance. Qilimanjaro participates in the direction of the European Innovation Council Horizon2020 project on "Coherent Quantum Annealing". It is a member of the European Quantum Industry Consortium (QuIC) since its creation in 2021. It has been awarded as "Exponential Leader 2021" by the Generalitat de Catalunya.

More info: www.qilimanjaro.tech



SILVER SPONSORS

Donostia International Physics Center

DIPC (Donostia International Physics Center) was created in April 2000 to promote scientific research in the area of basic and applied Physics, focusing both on the particular interest and needs of the Basque Society and of the international scientific community. The DIPC was created as an intellectual centre whose main aim is to promote and catalyse the development of basic research and basic research oriented towards material science to reach the highest level. Since its creation, the DIPC has been an open institution, linked to the University of the Basque Country, serving as a platform for the internationalising of basic science in the Basque Country in the field of materials.

More info: http://dipc.org/index.php

MULTIVERSE COMPUTING

Multiverse Computing provides software for companies from the financial industry wanting to gain an edge with quantum computing. Their fields of expertise are portfolio optimization problems, risk analysis, and market simulation.
Digital methods usually fail at efficiently tackling these problems. Quantum computing, however, provides a powerful toolbox to tackle these complex problems, such as outstanding optimization methods, software for quantum machine learning, and quantum enhanced Monte Carlo algorithms.
Multiverse Computing applies these cutting edge methods to provide software which is customized to needs, giving companies a chance to derive value from the second quantum revolution.

More info: www.multiversecomputing.com

BRONZE SPONSORS

Materials for Quantum Technology (MQT) is a multidisciplinary, open access journal devoted to publishing cutting-edge research on the development and application of materials for all quantum-enabled technologies and devices. IOP Publishing is currently covering all article publication costs, so the journal is free for authors to publish in until 2023. Discover more about the journal and the research published at iopscience.org/mqt.

More info: https:// iopscience.org/mqt

BRONZE SPONSORS

OXFORD INSTRUMENTS NANOSCIENCE

Oxford Instruments Nanoscience is part of the Research and Discovery Sector at Oxford Instruments, providing advanced solutions that create unique environments and enable analytical measurements down to the molecular and atomic level, predominantly used in scientific research and applied R&D. At Oxford Instruments Nanoscience, we design, supply and support market-leading research tools that enable quantum technologies, nano technology research, advanced materials and nano device development in the physical sciences. Our tools support research to the atomic scale through creation of high performance, cryogen free, low temperature, and magnetic environments. This is based upon our core technologies in low and ultra-low temperatures, high magnetic fields and system integration with increasing levels of experimental and measurement readiness

More info: https://nanoscience.oxinst.com/

BRONZE SPONSORS

TECNALIA is the largest centre of applied research and technological development in Spain, a benchmark in Europe and a member of the Basque Research and Technology Alliance. TECNALIA collaborates with companies and institutions to improve their competitiveness, people's quality of life and achieve sustainable growth.
Its Mission: To transform technological research into prosperity.
Its Vision: To be agents of transformation of companies and society for their adaptation to the challenges of a changing future.

More info: www.tecnalia.com

OTHER SPONSOR

American Elements' catalog of more than 35,000 products makes it the world's largest manufacturer devoted exclusively to advanced materials in both industrial bulk and laboratory/research quantities. And the company's materials science research & development programs have been a key resource for corporate, government & academic new product development for over two decades. Our ability to cost-effectively scale lab top successes to industrial scale production has been instrumental to ushering in many of the fundamental technological breakthroughs since 1990 including LED lighting, smartphones, and electric cars.

More info: www.americanelements.com

Spanish Nanomedicine Platform (nanoMED Spain) aims to bring together the most important Spanish researchers, industries and administrations, in order to promote a common strategy in such a multidisciplinary field as nanomedicine.

More info: http://nanomedspain.net/

EXHIBITORS

EXHIBITORS

CIC biomaGUNE
MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

izasa scientific
a werfen company

CIC bioGUNE
MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

attocube
WITTENSTEIN Group

AMO

HIDEN ANALYTICAL

ScienTec Ibérica
La solución a su medida

CSI Concept Scientific Instruments
Atomic Force Microscopes

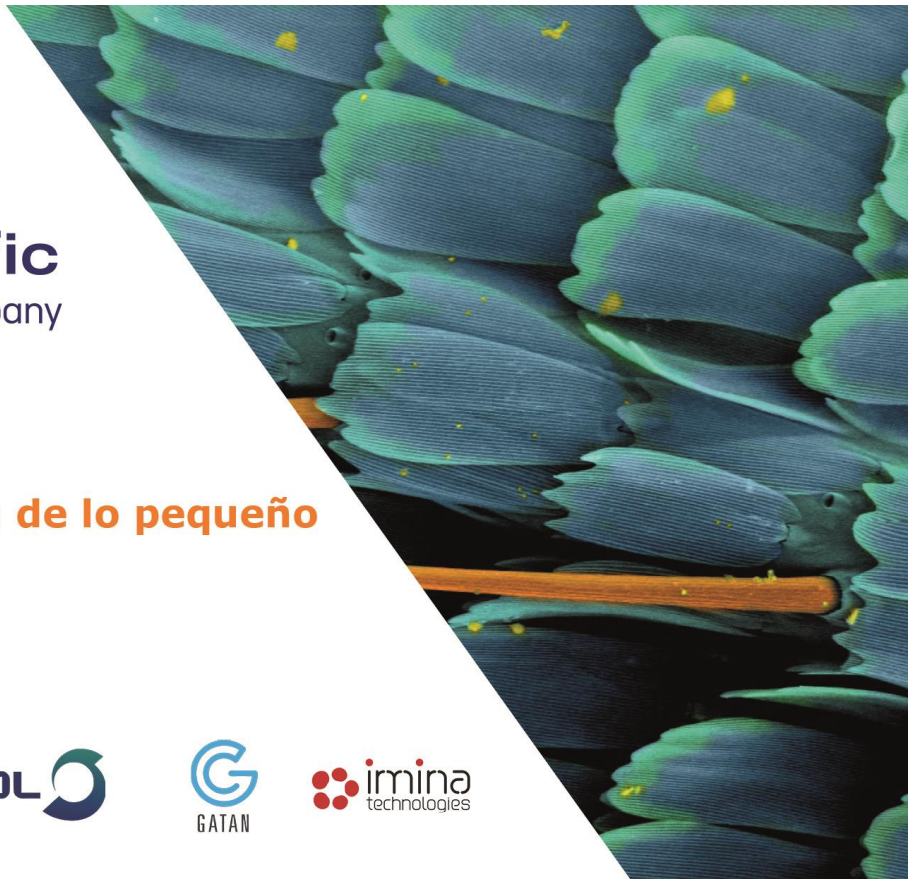
EXADDON

NANOMED
SPAIN

KILIMANJARO
QUANTUM · TECH

QBLOX

Advertisement



SPEAKERS

Communication at the nanoscale. Nanoparticles that "talk" to one another.

Elena Aznar

Instituto Interuniversitario de Investigación de Reconocimiento Molecular y Desarrollo Tecnológico (IDM) Universitat Politècnica de València, Universitat de València, Camino de Vera s/n, 46022 Valencia, Spain

elazgi@upvnet.upv.es

Chemical communication is based on the exchange of molecular messengers between different entities. Communication networks enable a group to share information and act together towards the achievement of a common goal. Considering this aim, coordinated communication displays an essential role as it is necessary to organize the collective behaviour in a defined order to assure efficiency and productivity. In fact, nature life is based on communication processes developed in coordinated communities at the molecular scale involving the use of chemical messengers. [1-2] Transferring communication capabilities to human-made nanoscale systems has attracted significant attention in recent years due to potential applications in areas such as biomedicine or ICT (Information and Communication Technologies). Compared to traditional telecommunication technologies, chemical communication offers interesting features such as the reduced size of molecular transceivers and receivers, minimal power consumption and the ability to operate in biological and physiological environments. Some micro- and nanovehicles capable of interacting with living systems by means of sending or receiving chemical messengers have been developed.[3] Linear communication between particles or feedback between two particles have also been reported. [4-7] However, the field is still in its infancy and more complex communication communities should be demonstrated with the future aim to integrate coordinated multicomponent communities of nanodevices with advanced capabilities. Strategies of cooperation and coordination between different nanoparticles enable sophisticated functionalities that go beyond those carried out by individual agents. However, regardless of the aforementioned advancements made in the last years, the definition of technologies to support practical and useful applications of communication at nanoscale, while essential to motivate further growth of this field in the research community, is still very limited and still scarcely explored.

References

[1] D. Malak, O.B. Akan, Nano Commun Netw, 3 (2012) 19

[2] J. T. Hancock, Cell Signalling; Oxford University Press, Oxford (2016)

[3] M. de Luis, A. Llopis-Lorente, P. Rincón, J. Gadea, F. Sancenón, E. Aznar, R. Villalonga, J.R. Murguía, R. Martínez-Máñez, Angew. Chem. Int. Ed., 58 (2019) 14986

[4] A. Llopis- Lorente, P. Díez, A. Sánchez, M.D. Marcos, F. Sancenón, P. Martínez-Ruiz, R. Villalonga, R. Martínez-Máñez, Nano Today, 18 (2018) 8

[5] P. Díez, A. Sánchez, M. Gamella, P. Martínez-Ruíz, E. Aznar, C. de la Torre, J.R. Murguía, R. Martínez-Máñez, R. Villalonga, J.M. Pingarrón, J. Am. Chem. Soc., 136 (2014) 9116

[6] C. Giménez, E. Climent, E. Aznar, R. Martínez-Máñez, F. Sancenón, M.D. Marcos, P. Amorós, K. Rurack, Angew. Chem. Int. Ed., 53 (2014) 1262

[7] A. Llopis-Lorente, P. Díez, A. Sánchez, M.D. Marcos, F. Sancenón, P. Martínez-Ruiz, R. Villalonga, R. Martínez-Máñez, Nat. Commun., 8 (2017) 15511

Colloidal nanomaterials for life science: tailoring surface chemistry for old, new and emerging functions

M. Lucia Curri

Department of Chemistry University of Bari and Italian National Research Council CNR IPCF, via Orabona 4, 70126 Bari, Italy.

marialucia.curri@uniba.it

In the last years, the extraordinary advances in the field of nanomaterial science have resulted in a great potential for applications in life science.
A variety of preparative and post-preparative colloidal routes have demonstrated able to obtain a wide choice of inorganic nanoparticles (NPs) and nanocrystals (NCs), with different compositions, that can be achieved with a high control on size, shape and surface chemistry, ultimately tailoring their electronic, optical, magnetic, thermal and chemical size dependent properties. A range of functionalization strategies have been developed to suitably engineer the surface of NPs and NCs and tune their specific chemical reactivity towards the surrounding environment. The control of nano-bio interfaces has demonstrate essential to enable nanomaterials conjugation and combination with biologically relevant entities, thus producing advanced materials for diagnostics and therapy. The ability of engineering the surface of specialized nanomaterials, such as semiconductors, plasmonic and magnetic nanostructures, with tailored procedures, allowing to ingeniously combine NPs and NCs with peptides, drugs and other significant biological systems, is decisive for their application in diagnosis and treatment of different diseases, including cancer and neurodegenerative disorders. In particular, examples of drug delivery, labelling, diagnostic and theranostics systems, based on NIR photoactive nanomaterials, plasmonic nanostructures and magnetic NPs will be reported.

References

[1] F. Vischio, E. Fanizza et al J. Phys. Chem. C, 124 (2019) 23205.
[2] N. Depalo, M. Corricelli et al ACS Applied Materials and Interfaces, 9 (2017) 43113.
[3] G. Valente, N. Depalo et al Nano Research, 9 (2016) 644.
[4] C. Ingrosso, M. Corricelli et al J. Mater. Chem. B., 7 (2019) 768.

Figures

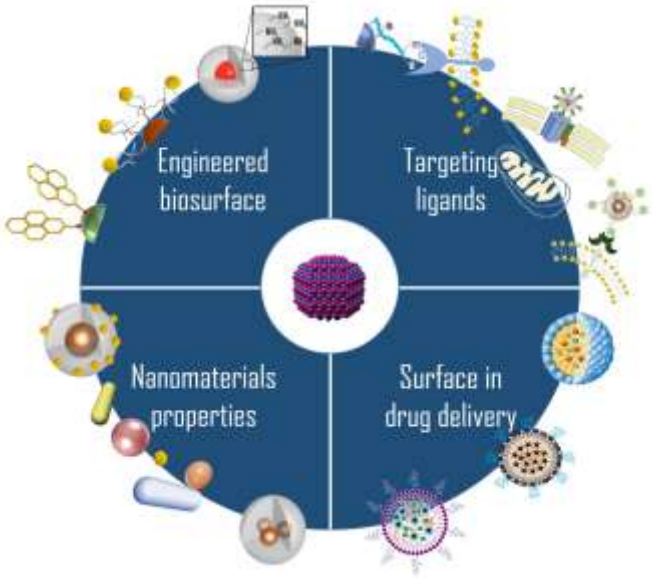


Figure 1: Engineering bio-interface in colloidal nanomaterials for diagnosis and therapy

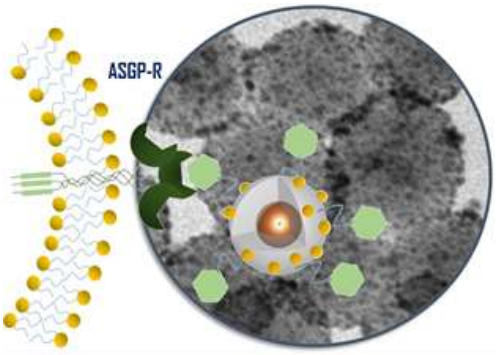


Figure 2: Carbohydrate bioconjugated magnetic/plasmonic Au NPs decorated $Fe_2O_3@SiO_2$ nanostructures for targeting

Strong interactions in functional organic materials and devices - a curse or a blessing?

Frank Ortmann

TU Munich, Germany

frank.ortmann@tu-dresden.de

Electronic or excitonic transfer processes are central to the operation of any electronic or optoelectronic device and need to be understood at the nanoscale. In organic molecular materials, they are affected by strong interactions. Electron-phonon coupling is an essential ingredient for understanding electronic and optical properties. In addition, the Coulomb interaction is greatly enhanced by the low dielectric constants of these materials and can surpass the electronvolt energy scale. This however opens interesting perspectives to using strong interactions as a design tool for band structure engineering, doping or tuning of optical and excitonic properties in OLEDs, photovoltaics or photodetectors.
In my talk I will discuss how to describe these strong interactions in organic semiconductors and how to explore them for devices. Besides applications, this renders these materials an intriguing platform for fundamental studies.

References

[1] K. Ortstein et al. "Band gap engineering in blended organic semiconductor films based on dielectric interactions" Nat. Mater. 20, 1407 (2021).
[2] N. Shin et al. "Electronic Doping and Enhancement of n-Channel Polycrystalline OFET Performance through Gate Oxide Modifications with Aminosilanes" Adv. Mater. Interfaces 8, 2100320 (2021).
[3] M. Panhans et al. "Molecular vibrations reduce the maximum achievable photovoltage in organic solar cells" Nat. Commun. 11, 1488 (2020).
[4] K. Ortstein et al. "Energy Level Engineering in Organic Thin Films by Tailored Halogenation" Adv. Funct. Mater. 30, 2002987 (2020).
[5] M. Schwarze et al. "Molecular Parameters Responsible for Thermally Activated Transport in Doped Organic Semiconductors" Nat. Mater. 18, 242 (2019).
[6] M. Schwarze et al. "Impact of molecular quadrupole moments on the energy levels at organic heterojunctions" Nat. Commun. 10, 2466 (2019).
[7] C. Gaul et al. "Insight into doping efficiency of organic semiconductors from the analysis of the density of states in n-doped C60 and ZnPc" Nat. Mater. 17, 439 (2018).

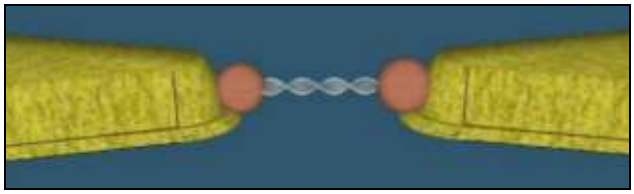
Surprising Charge Transport in DNA

Danny Porath

[1] *Institute of Chemistry and Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, 91904 Israel*

danny.porath@mail.huji.ac.il

Figures



Charge transport through molecular structures is interesting both scientifically and technologically. To date, DNA is the only type of polymer that transports significant current over distances of more than a few nanometers in individual molecules. Nevertheless, and in spite of large efforts to elucidate the charge transport mechanism through DNA a satisfying characterization and mechanistic description has not been provided yet. Measuring the charge transport in DNA was elusive due to great technical difficulties leading to various results. We recently devised an experiment in which double-stranded DNA is well positioned between metal electrodes. Electrical measurements give surprisingly high currents, up to tens of nA, over 100 base-pairs (~30 nm) elevated from the surface. We further found that homogeneous and non-homogeneous sequences transport charge similarly and that at least one continuous backbone is essential to enable transport. The theoretical calculations and the temperature dependence suggest resonant hopping through the backbone as the charge transport mechanism.

References

[1] "Backbone Charge Transport in Double Stranded DNA", Roman Zhuravel et. Al., Nature Nanotechnology 9, 836 (2020)

Functional Coatings for Sterile Surfaces

Meital Reches

Institute of Chemistry and the Center for Nanoscience and Nanotechnology, Jerusalem, Israel

Meital.reches@mail.huji.ac.il

Abstract

The lecture will present bio-inspired functional coatings that are spontaneously formed by short peptides. These peptide-based coatings self-assemble on metals, oxides and polymers under mild conditions without any need for a curing step. The coating can serve in many functions. One application is preventing biofouling - the undesirable adhesion of biomolecules and organisms to surfaces. (1,2) This process leads to numerous adverse phenomenon including hospital-acquired infection, blockage of water desalination facilities and food contamination. We showed that this coating prevents the first step of biofouling, which involves the adsorption of bioorganic molecules to the substrate. Moreover, the coating significantly reduces the attachment of various organisms such as bacteria and fungi to surfaces. Another function that these peptide-based coatings can mediate is the adhesion of mammalian cells to implants. (3) This function is important for the integrating of implants into the human body. Finally, we showed that these peptides self-assemble in solution into particles that adsorb and release active compound that synergistically reduce the amount of bacteria and viruses on the surface. (4,5)

References

[1] Maity, S., Nir,S., Zada, T.,Reches, M., Chem. Commun., 50 (2014) 11154
[2] Nir, S. & Reches, M. (2016) Curr. Opin. Biotechnol., 39 (2016) 48
[3] Yuran, S., Dolid, A. & Reches, M., ACS Biomater. Eng. 4, (2018), 4051.
[4] Nir, S., Zanuy, D., Zada, T., Agazani, O., Aleman, C., Shalev, D. E., & Reches, M., Nanoscale, 11 (2019) 8752
[5] Hu, T., Agazani, O., Nir, S., Cohen, M., Pan, S., & Reches, M., ACS Appl. Mater. Interfaces, 13 (2021) 48469

Figures

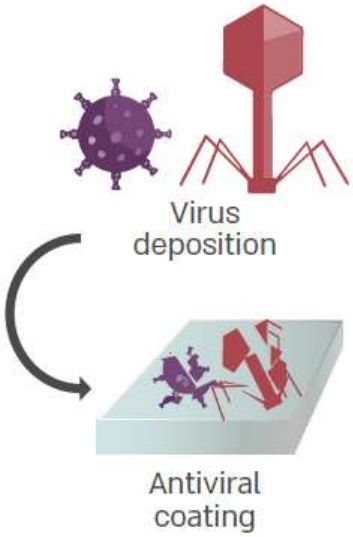


Figure 1: A peptide-based coating disrupts the supramolecular structure of both bacteriophages and corona virus and act as an antiviral coating.

Order from the disorder with intrinsically disordered peptide amphiphiles

Roy Beck

Tel Aviv University, Tel Aviv, Israel

Roy@tauex.tau.ac.il

The concept that a given amino-acid sequence will not form a 3D folded structure but still have biological functionality has developed only in the last ~15 years. The discovery rate and characterization of intrinsically disordered proteins have been increasing continually, becoming one of the fastest-growing areas of proteomics [1]. It is now estimated that over 50% of eukaryotic proteins contain large intrinsically disordered regions involved in a wide range of cellular functions, including transcription, translation, signaling, and regulation of protein assembly. Structural flexibility and plasticity originating from the lack of an ordered structure suggest a significant functional advantage for these proteins, enabling them to interact with a broad range of binding partners.

Amphiphilic molecules and their self-assembled structures have long been the target of extensive research due to their potential applications in materials design to biomedical fields. An emerging class of molecules, namely, peptide amphiphiles, combines key advantages and circumvents some disadvantages of conventional phospholipids and block copolymers.

In this talk, I present new peptide amphiphiles composed of an intrinsically disordered peptide conjugated to variants of hydrophobic domains [2]. These molecules termed intrinsically disordered peptide amphiphiles, exhibit a sharp pH-induced micellar phase-transition from low-dispersity spheres to extremely elongated worm-like micelles. I will present various experimental characterizations of the transition and propose a theoretical model to describe the pH response [Fig. 1]. I will also show the potential of the shape transition to serve as a mechanism for the design of a cargo hold-and-release application. Such amphiphilic systems demonstrate the power of tailoring the interactions between disordered peptides for various stimuli-responsive biomedical applications.

References

[1] T. Ehm, H. Shinar, S. Meir, A. Sekhon, V. Sethi, I. L. Morgan, G. Rahamim, O. A. Saleh, and R. Beck, *Intrinsically Disordered Proteins at the Nano-Scale*, Nano Future. **5**, (2021) 022501.

[2] G. Jacoby, M. Segal Asher, T. Ehm, I. Abutbul Ionita, H. Shinar, S. Azoulay-Ginsburg, I. Zemach, G. Koren, D. Danino, M. M. Kozlov, R. J. Amir, and R. Beck, *Order from Disorder with Intrinsically Disordered Peptide Amphiphiles*, J. Am. Chem. Soc. **143**, (2021) 11879.

Figures

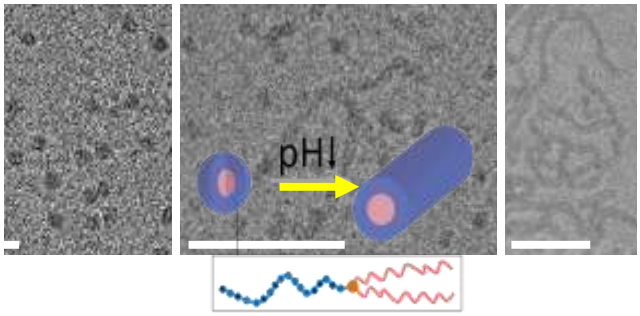


Figure 1: Cryogenic TEM of intrinsically disordered peptide amphiphiles transitioning via alternation of pH between isolated nanoscopic micelles to worm-like micelles.

Mechanically stable graphene with quadratic out-of-plane acoustic modes

Ion Errea

University of the Basque Country (UPV/EHU), San Sebastian, Spain
Centro de Física de Materiales (CSIC-UPV/EHU), San Sebastian, Spain
Donostia International Physics Center (DIPC), San Sebastian, Spain

ion.errea@ehu.eus

The phonon properties of 2D materials are far from trivial as the harmonic approximation predicts fast diverging atomic displacements as a function of the sample size and finite linewidths of the longitudinal and transverse in-plane acoustic phonon modes at small momenta. These problems arise due to the quadratic dispersion of the acoustic out-of-plane phonon frequencies obtained in the harmonic approximation. By including anharmonicity within the self-consistent harmonic approximation (SCHA) we show that the divergences in the atomic displacements are suppressed and the linewidths of in-plane acoustic phonons vanish at low momenta, recovering the physical picture. By calculating the phonon spectra from the Hessian of the anharmonic free energy, we conclude that the physical dispersion expected experimentally for the acoustic out-of-plane mode should be quadratic (see Figure 1). We verify this result both using atomistic simulations and using a membrane model for graphene. Our conclusions [1] have a crucial role in the understanding of the mechanical and thermal properties of graphene and other strictly two-dimensional material.

References

[1] U. Aseginolaza *et al.* in preparation.

Figures

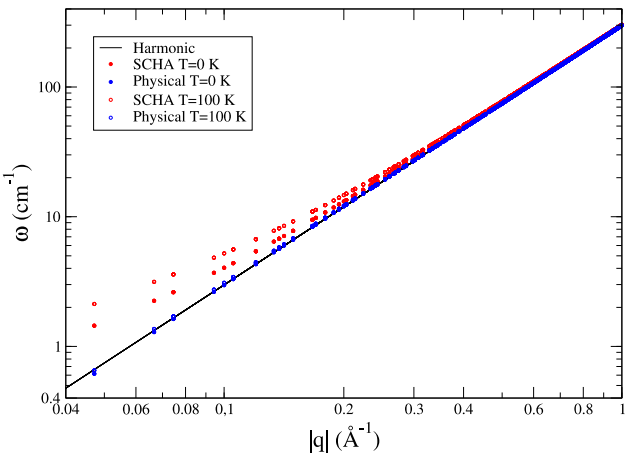


Figure 1: Frequency of the ZA mode in the harmonic approximation, within the SCHA and obtained from the Hessian of the SCHA (labeled as "Physical") both at 0 K and 100K using the membrane model. The physical phonons recover the quadratic dispersion of the harmonic solution.

Graphene nanoarchitectures: insights from theory and experiments

Aran Garcia-Lekue

Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastian (Spain)

Ikerbasque, Basque Foundation for Science, 48013 Bilbao (Spain)

wmbgalea@ehu.eus

Graphene-based materials *are* promising units for the development of novel electronic, spintronic or optoelectronic devices. For *their true potential to be realized, a precise* atomic-level *control and understanding of the conformational or chemistry related electronic signatures in these systems is* crucial. *By using state-of-the-art experimental techniques,* graphene nanoarchitectures *can now be built with atomic precision, which has opened the door to exploring their electronic properties at the nanoscale.*

In this talk, I will review some of our works on graphene nanoarchitectures, performed in close collaboration with our experimental colleagues. Using density-functional theory (DFT), we have investigated the electronic, magnetic and transport properties of graphene nanoribbons and nanoporous graphene, with special focus on the role of chemical doping and the creation of tunable pores in the carbon backbone. Our findings are compared with scanning tunneling microscopy (STM) and angle-resolved photoemission (ARPES).

Depending on the conformational details and the doping mechanism, various effects are observed and explained, such as semiconductor-to-metal transition, energy gap modification, tuning of topological properties, emergence of magnetism and control of electron confinement.[1-4]

References

[1] J. Li *et al.*, ACS Nano 14, 1895 (2020)
[2] M. Panighel *et al.,* ACS Nano 14, 11120 (2020)
[3] N. Friedrich *et al.,* Phys. Rev. Lett. 125, 146801(2020)
[4] J. Li *et al.,* Nat. Commun. 12, 5538 (2021)

Figures

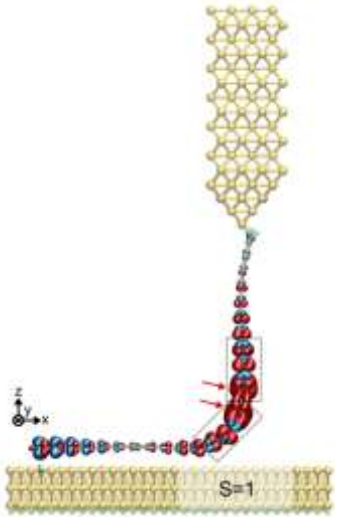


Figure 1: DFT optimized structure of a graphene nanoribbon doped with a pair of boron atoms, and contacted by a scanning tunneling microscope (STM) tip. Magnetization isosurfaces are shown over the atomic structure. Figure adapted from Ref. [3].

Labelled Self-propelled nanosystems: towards improved (nano)theragnostic agents

Jordi Llop
A. C. Hortelao, C. Simó, M. Guix, S. Guallar-Garrido, E. Julián, D. Vilela, L. Rejc, P. Ramos-Cabrer, U. Cossío, V. Gómez-Vallejo, T. Patiño, S. Sánchez.

CIC biomaGUNE, Basque Research and Technology Alliance, Paseo Miramon 182, San Sebastian, Spain

jllop@cicbiomagune.es

Abstract

Nanoparticles have been widely investigated in the biomedical field: They are small-sized, their surface composition and properties can be easily tuned, and they have the capacity to carry large amounts of cargoes. Additionally, they can be provided with imaging capabilities, enabling their non-invasive in vivo tracking. These properties position nanoparticles as promising therapeutic, diagnostic or even theragnostic agents. However, recent studies have demonstrated that only a small fraction of the nanoparticles typically reach the target site, resulting in insufficient accumulation to guarantee diagnostic or therapeutic efficacy. Moreover, distribution within the targeted tissue or organ is often heterogeneous.

Micro- and nanomotors, which are micro- and nanodevices capable to self-propel in different media, have proven to overcome a number of limitations of classical nanomedicines, by enhancing targeting properties and penetration capacity in complex structures. Still, the design of biocompatible motors capable to self-propel in biological fluids remains challenging, and their control and in vivo visualization to aid in the evaluation of motile nanomedicines and facilitate the eventual translation into the clinics remains unresolved.

In this talk, recent works related to the radiolabelling and subsequent investigation of micro- and nanomotors carried out in collaboration with Prof. Samuel Sánchez (IBEC, Barcelona) will be discussed. The discussion will include labelling strategies and pioneering in vitro PET studies to evaluate motile properties of tubular micromotors at the macroscopic level [1], as well as recent results covering the radiolabelling and in vitro/in vivo evaluation of biocompatible, enzyme-powered nanobots [2]. Finally, currently ongoing applications of the nanobots as theragnostic agents in a mouse cancer model will be presented.

References

[1] D. Vilela, U. Cossío, J. Parmar, A.M. Martínez-Villacorta, V. Gómez-Vallejo, J. Llop, S. Sánchez. ACS Nano, 12 (2018) 1220-1227.

[2] A. C. Hortelao, C. Simó, M. Guix, S. Guallar-Garrido, E. Julián, D. Vilela, L. Rejc, P. Ramos-Cabrer, U. Cossío, V. Gómez-Vallejo, T. Patiño, J. Llop, S. Sánchez., Science Robotics, 6 (2021) eabd2823.

Synthesis and Colloidal Properties of Gold Nanoparticles Functionalized with Cyclic Poly(ethylene oxide)s

M. Ali Aboudzadeh [a,b]
Marek Grzelczak [a]
Fabienne Barroso-Bujans [a,c]

[a] *Donostia International Physics Center (DIPC), Paseo Manuel Lardizábal 4, San Sebastian, Spain*
[b] *CNRS, University Pau & Pays Adour, E2S UPPA, Institut des Sciences Analytiques et de Physico-Chimie pour l'Environnement et les Matériaux, IPREM, UMR5254, PAU, France*
[c] *IKERBASQUE - Basque Foundation for Science, María Díaz de Haro 3, Bilbao, Spain*
mohammadali.aboudzadeh@ehu.eus
m.aboudzadeh-barihi@univ-pau.fr

Abstract

Particular polymer topologies such as cyclic polymers, beyond linearity, have been shown to alter significantly the properties of diverse polymer preparations in both bulk and solutions, when compared to their linear counterparts.[1] Click chemistry and in particular, copper-catalyzed alkyne−azide cycloaddition (CuAAC) has allowed access to a variety of cyclic architectures.[2] On the other hand, gold nanoparticles (AuNPs) continue to attract much attention across a wide range of fields due to their optical properties and biocompatibility. [3]

In this work, we explore the possibility of applying cyclic polyethylene oxide (PEO) on inorganic AuNPs, with particular attention to how this polymer topology might affect the colloidal stability. The exchange of citrate ligand (used in the synthesis of AuNPs) with thiol functional group of cyclic PEO will allow to form a strong covalent bond with the gold surface. Thiolated cyclic polymers were obtained by performing CuAAC between a PEO bis(azide) of Mn = 2, 6 or 11 kg/mol and a previously synthesized thiolated di-alkyne molecule.

Purity and mono-dispersity of synthesized thiolated cyclic polymer were confirmed by MALDI-ToF MS, NMR and SEC techniques. [4] UV-Vis-NIR spectra of initially stabilized AuNPs exhibits a maximum of localized surface plasmon band at 517 nm. Upon addition of cyclic PEO, the plasmon band shifted to 522 nm, suggesting the ligand exchange. The width of the plasmon band remained constant after washing confirming the colloidal stability of AuNPs.

To conclude, macrocyclic PEOs containing a pendant thiol group have been synthesized by the click reaction between PEO bis(azide) and a previously-synthesized bis(alkyne) linker. We used this system to decorate gold nanoparticles with potential applications in biomedical devices.

References

[1] T. Yamamoto, Y. Tezuka, Soft Matter, 11 (2015) 7458.
[2] B. A. Laurent, S. M. Grayson, J. Am. Chem. Soc., 128 (2006) 4238.
[3] L. A. Dykman, N. G. Khlebtsov, Chem. Rev., 114 (2014) 1258.
[4] M. Ali Aboudzadeh *et al.*, Polym. Chem., 10 (2019) 6495.

Figures

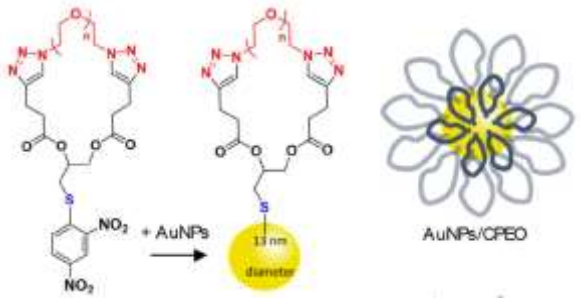


Figure 1: Synthesized AuNP@CPEO samples by ligand exchange of AuNP@citrate against cyclic PEO samples.

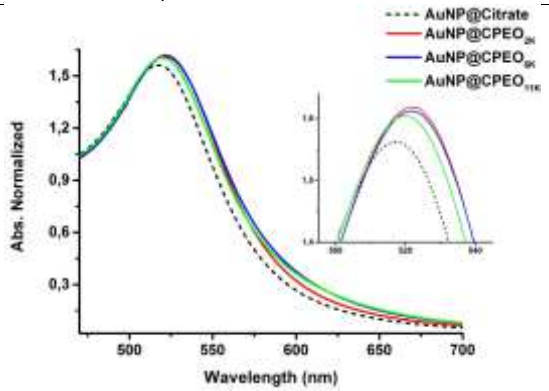


Figure 2: Normalized UV-Vis absorbance spectra of AuNP@CPEO conjugates in water.

Nano in 3D: CNT and Conjugated Polymers for Electrosensitive Tissue Regeneration

Núria Alegret[1,2,3]
Antonio Dominguez-Alfaro,[1,2] Blanca Arnaiz,[2] Luisa Mestroni,[3] David Mecerreyes[1] and Maurizio Prato.[2]

[1] *POLYMAT University of the Basque Country UPV/EHU, Avenida de Tolosa 72, 20018 Donostia-San Sebastián, Spain*

[2] *CIC biomaGUNE, Paseo de Miramón 182, 2014 Donostia-San Sebastián, Spain*

[3] *Cardiovascular Institute, University of Colorado Denver, 12700 E. 19th Avenue, Aurora, Colorado 80045, United States*

nuria.alegret@ehu.eus

Three-dimensional cellular organization was demonstrated to be able to induce cellular network outputs that strongly differ from the 2D constructs. The morphology, shape and porosity are critical parameters, and electrical conductivity is an important asset when dealing with electroactive cells, such as neurons or cardiac cells.

Carbon nanotubes (CNTs) are one of the most promising materials to interface with electrically active tissues.[1] Their combination with polymers has been extensively studied, and the materials produced showed a great potential in tissue regeneration.[2] On the other side, the design of electrodes based on conductive polymers (CPs) in brain-machine interface technology offers the opportunity to reduce gliosis, improve adaptability and increased charge-transfer efficiency.[3] However, very little is reported about the combination of CPs and CNTs, and only 2D films have been synthesized and tested *in vitro*.

Here, we construct 3D porous and conductive composites, composed exclusively of CNTs and or PEDOT.[4] We developed new and easy strategies, based on chemical and electrochemical polymerizations. The resulting materials are very promising scaffolds with low density, high and homogeneous porosity, electrical conductivity and Young Modulus similar to the *in vivo* tissue. Its high biocompatibility was demonstrated by incubation of astrocytic, neuroblastoma-derived SH-SY5Y and cardiac cells. Interestingly, we also found that our scaffolds are *per se* able to induce neuron-like differentiation of the SH-SY5Y cells. Overall, we demonstrated that the hereby presented scaffolds fulfill all the requirements for the successful growth, development and regeneration of conductive cells.

References

[1] a) Usmani, S. *et al.* (2016). *Sci. Adv.*, 2 : e1600087 b) Fabbro, A. *et al.* (2012). *ACS Nano,* 6: 2041

[2] Mohanty, F. and S. K. Swain 2017 *Curr. Org. Synth.,* 14: 249

[3] Bosi, S. *et al.* (2015) *Sci. Rep.,* 5: 9562

[4] Dominguez-Alfaro *et al.* (2019), *ACS Bimater. Sci. Eng.*

Figures

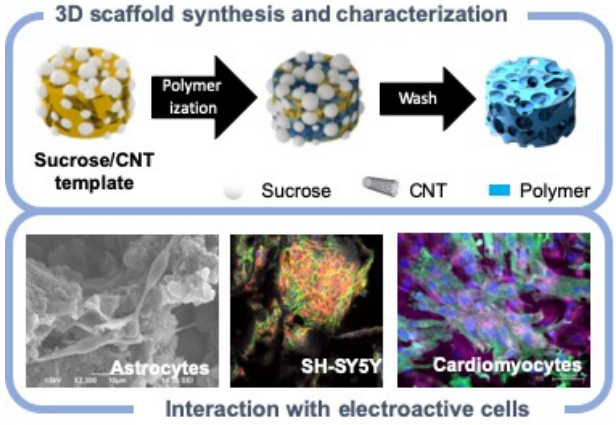


Figure 1: (Top) Schematic representation of the development of 3D scaffolds composed of CNT and PEDOT. (Bottom, from left to right) SEM image of the incubation of astrocytes; confocal image of the differentiated SH-SY5Y cells cultured (red: tubulin, green: cytoesqueleton); confocal image of primary co-cultureof cardiac myocytes (green) and fibroblasts (pink).

Functionalized Biomimetic Nanohydroxyapatite as Ingredient for 3D Bioinks

José María Alonso[1]
Virginia Sáez-Martínez,[1] Africa García-Barrientos,[1] Nagore Martínez de Cestafe,[2] Sara Mchichou,[1,3] Raúl Pérez-González.[1]

[1]*I+Med S. Coop, Parque Tecnológico de Alava. C/Albert Einstein 15, nave 15, 01510, Vitoria-Gasteiz, Spain.*
[2]*Unikare Bioscience, Parque Tecnológico de Alava. C/Albert Einstein 15, 01510, Vitoria-Gasteiz, Spain.*
[3]*Dpto. Química Orgánica I, Centro Joxe Mari Korta. UPV/EHU. Avda. Tolosa 72, 20018, San Sebastián, Spain.*

jalonso@imasmed.com

i+Med is cooperative society of scientists established in 2014 and focused on the development and commercialization of biomedicine solutions for the controlled release of drugs, vitamins, growth factors and other active compounds.
i+Med develops own products as well as drug products and medical devices for third parties. The company holds two patents on nanogels with biomedical applications and manufactures medical devices with CE Marking.
The main research lines of the company include controlled release, functional coatings, active nanoparticles and biomaterials. In this regard i+Med produces biomimetic nanohydroxyapatite (nHAp) and functionalized nanohydroxyapatite for biomedical applications [1].
nHAp is a natural mineral produced by the organism. I+Med has applied a synthesis method that mimics the physiologic biosynthesis conditions to get biomimetic nanoparticles avoiding toxic residues. The main property, apart from the nanometric size that helps to get better into the inner layers of the tooth enamel, is their spheroidal shape that increases the biocompatibility (Figure 1).
An analogous approach has been employed for the synthesis of metals functionalized nHAps. This kind of nHAps display applications not only in Odontology but also in Prosthetics and Traumatology. The latter is due to their antibacterial properties which prevents infections in prosthesis implantation and their ability to promote (osteogenesis). Moreover, nHAp has been successfully incorporated by Unikare (i+Med´s sister company) to commercially available bioinks for processing by bioprinting technologies. Resulting bioinks are promising candidates as biomaterials additive manufacturing solutions for biomedical products and tissue engineering.

References

[1] K. Lin, J. Chang. Hydroxyapatite (HAp) for biomedical applications. Woodhead Publishing, 2015, 3.

Figures

Figure 1: TEM image of synthesized nHAp.

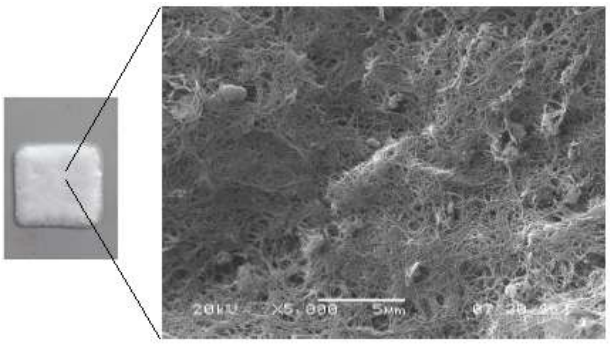


Figure 2: Collagen-nHAp Bioink

Controlled deposition and characterization of single bacteria using nanomechanical sensors in air

Alicia Aparicio-Millán
Eduardo Gil-Santos, Jose Jaime Ruz, Sergio García-López, Priscila Monteiro Kosaka, Montserrat Calleja, Javier Tamayo

Instituto de Micro y Nanotecnología (IMN-CNM, CSIC), C/ Isaac Newton 8 (PTM, Tres Cantos), Madrid, Spain

alicia.aparicio@csic.es

Abstract

Nanomechanical resonators have emerged as excellent tools in microbiology due to their extraordinary capability to characterize the mass and mechanical properties of a variety of microbiological entities [1]. These sensors have allowed to detect, characterize and identify individual bio-entities, such as human cells, bacteria, viruses and proteins. Meanwhile researchers have succeeded on characterizing individual cells in liquid environment, single viruses or proteins applications have been limited to vacuum condition, mainly due to their small sizes, thus, being far from their intrinsic conformation.

In this work, we present a novel technique based on the use of commercial microcapillaries, that allows to deposit individual bioentities on controlled positions of the sensors (Figure 1) with micrometric precision in air conditions [2]. We accurately characterize the mass and mechanical properties of different types of alive bacteria that are close to their intrinsic conformation. We achieve it by simultaneously tracking multiple mechanical resonance frequencies of the sensors and analysing the changes induced by bacteria adsorption (Figure 2).

Importantly, this technique may find applications for a great variety of analytes and wide diversity of sensors. In addition, besides being extremely useful for quick analyte characterization, it may offer a vast variety of applications, such as, accurate sensors calibration to increase their reliability or to test the sensors capabilities.

References

[1] J. Tamayo, et al. "Biosensors based on nanomechanical systems". Chemical Society Review, 42 (2013) 1287.

[2] A. Aparicio-Millan, et al. "Controlled deposition of individual and alive bacteria onto nanomechanical resonator sensors for their characterization in air". *In preparation.*

Figures

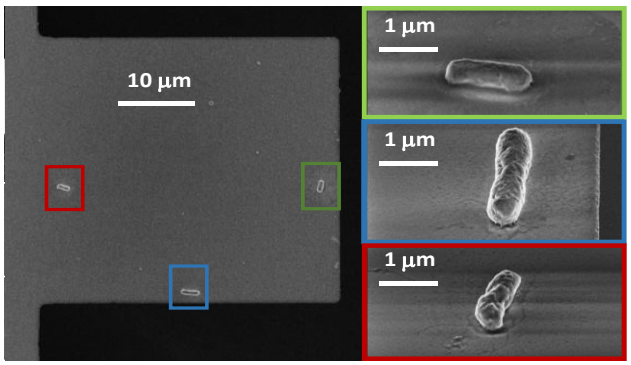


Figure 1: On the left: Scanning Electron Microscope (SEM) image of a squared resonator (40 µm length and width, 100 nm thickness) with three Escherichia Coli bacteria deposited on different targeted positions. On the right: Zoomed SEM images of each event.

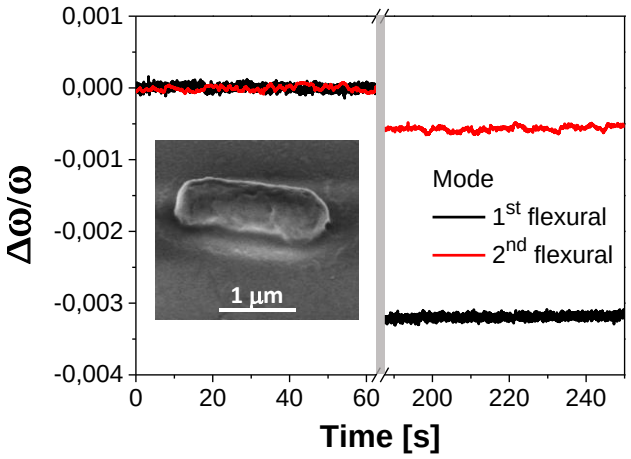


Figure 2: Relative frequency shift of the two first flexural modes of the squared resonator induced by the adsorption of an Escherichia Coli on the free end of the resonator.

Synthesis and characterization of amphiphilic fluorinated polymers for phase transfer solubilization of hydrophobic gold nanoparticles.

Juan Manuel Arango
Sónia Lopez-Fernandez, Jorge Blanco, Carolina Carrillo-Carrión, Mónica Carril.

Instituto Biofisika UPV/EHU, CSIC, Barrio Sarriena s/n, E-48940, Leioa, Bizkaia, Spain. Departamento de Bioquímica y Biología Molecular, UPV/EHU, 48940, Bilbao, Spain

jarango001@ikasle.ehu.eus

There are many synthetic protocols that produce nanoparticles (NPs) that are only dispersed in organic solvents [1]. Among the methods to transfer those NPs to water, the polymer coating strategy is one of the most popular ones. It is based on the use of an amphiphilic polymer that orients its hydrophobic side to the NPs and exposes a water-friendly side that allows water dispersibility [2]. In this context, herein we report a methodology for the encapsulation of hydrophobic NPs that takes advantage of the enhanced hydrophobicity of novel fluorinated amphiphilic polymers.

The synthesis of the fluorinated polymers was based on a ring opening reaction over poly (isobutylene-alt-maleic anhydride) polymer with a small fluorinated amino ending building block. The amount of fluorine present in such polymers was controlled by the reaction stoichiometry and confirmed by elemental analysis and ^{19}F NMR. Thus, a family of polymers with different degree of fluorination were synthetized to encapsulate hydrophobic Au NPs of gold core size of 4, 14 and 18 nm. The encapsulation process took place by a simple and straightforward phase transfer strategy and could be monitored by observing the transfer of colour from the organic phase to the aqueous phase, indicating that the red coloured Au NPs were eventually dispersed in water, as a result of the proper encapsulation with the amphiphilic fluorinated polymer (figure 1).

The colloidal stability of freshly encapsulated NPs was confirmed by ultraviolet-visible spectroscopy (UV-Vis) and the gold core size was analysed by transmission electronic microscopy (TEM). The colloidal stability over time was controlled by visual inspection of the formation of precipitates, by UV-Vis and by Dynamic Light Scattering (DLS). We observed that the highest colloidal stability was achieved with the polymer having the highest fluorination degree. Nonetheless, similar colloidal stability could be achieved with the rest of the polymers by increasing the amount of polymer around the NPs.

Furthermore, the so-obtained Au NPs were exposed to different pH conditions (pH =5, 6 and 7.4) and to the presence of different cations of biological interest such as Na^+, K^+, Ca^{2+} and Mg^{2+} at two ranges of concentration (20 and 100 mM). Accordingly, Dynamic Light Scattering (DLS) experiments allowed to determine how the hydrodynamic radii changed over these parameters. A raise in the pH value generated a slight increase in the radii of the Au NPs for every single sample. Also, divalent cations generated a dramatic increase in the radii observed compared to the monovalent ones leading to aggregation in some cases. These observations indicate that these amphiphilic polymers may be potentially used in the future to deliver hydrophobic cargoes.

References

[1]. S. Ashraf, B. Pelaz, P.del Pino, M. Carril, A. Escudero, W. J. Parak, M. G. Soliman, Q. Zhang, C. Carrillo-Carrion, Chem. Mater. 1 (2017), 411.

[2]. C.J. Lin, R.A. Sperling, J. K. Li, T. Yang, P. Li, M. Zanella, W. H. Chang, W. J. Parak. Small, 3 (2008), 335.

Figures

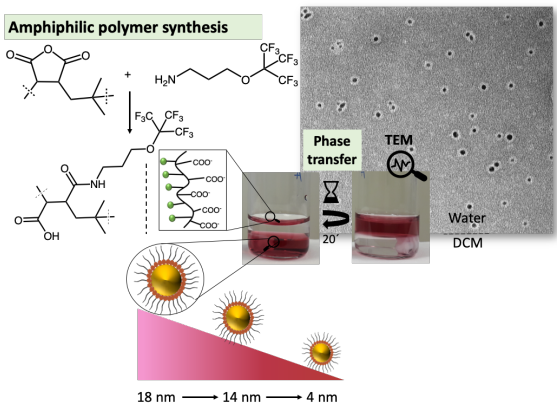


Figure 1: Encapsulation process of Au NPs with amphiphilic fluorinated polymers

Nanomed Spain, the Spanish Technological Platform for Nanomedicine: promoting public-private collaboration, innovation and clinical translation of nanomedicine in Spain

Cristina Arimany
Teresa Sanchis, Josep Samitier
Nanomed Spain, Institute for Bioengineering of Catalonia, Baldiri Reixac 10-12, 08028 Barcelona, Spain
carimany@ibecbarcelona.eu

Abstract

The Spanish Platform for Nanomedicine (NanoMed Spain - http://nanomedspain.net/) is a forum that brings together 170+ public research centres, hospitals, companies and government representatives active in nanomedicine. Nanomed Spain is an instrument to coordinate entities involved in research and innovation, fundamental to the transfer of results to industry and the health system in this highly multidisciplinary field. It is also a means of connection to facilitate the internationalization of initiatives and projects, with the aim of improving the competitiveness of Spain in this field. Industry in the biomedical and biotechnology sector plays a leading role in the Platform, very actively supported by technology centers, research organizations, universities and hospitals, as well as by the national public administration.

Nanomed Spain was created in 2005 based on the model of the European Technological Platforms and in particular, of the European Technology Platform on Nanomedicine (ETPN), also created in 2005 by the industrial partners of the area and the European Commission as a communication tool for all actors in the sector with the aim of contributing to the joint development of new and innovative medical products and applications.

The mission of Nanomed Spain is to promote and facilitate public-private partnerships in research and innovation in nanomedicine in Spain, with the aim of accelerating the development of innovative therapeutics and diagnostics based on the capabilities offered by nanotechnology applied to health care.

The important role of research and innovation and multidisciplinary and multisectoral collaboration has been stressed more than ever in the fight against COVID-19. Nanomedicine has proven to play a very important role, from diagnosis with the use of nanosensors to treatment with targeted therapies, through the design of vaccines using nanomaterials or the identification of new drugs through in vitro models of organoids.

It is necessary to continue advancing and generating knowledge in this field, as well as to continue working in the coordination of the healthcare sector with various industrial sectors (pharmaceutical, biotechnology, medical technologies) and research centers in order to face the new health challenges that may appear in the next few years in the most efficient way possible. In this talk we will review how Nanomed Spain contributes to this endeavor.

Unique Spin-orbit Properties of Magnetic Layered Bulk $CoTiO_3$

Mikel Arruabarrena[1]
A. Leonardo[2,3], M. Rodriguez-Vega[4], G. Fiete[5,6], A. Ayuela[1,3]

[1]*Centro de Física de Materiales, Paseo Manuel Lardizabal 5, Donostia-San Sebastián, Spain*
[2]*Department of Applied Physics II, University of the Basque Country UPV/ EHU, Bilbao, Spain*
[3]*Donostia International Physics Center (DIPC), Paseo Manuel Lardizabal 4, Donostia-San Sebastián, Spain*
[4]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA*
[5]*Department of Physics, Northeastern University, Boston, USA*
[6]*Department of Physics, Massachusetts Institute of Technology, Cambridge, USA*

marruabarrena001@ikasle.ehu.es

Cobalt titanate $CoTiO_3$ has currently attracted a lot of interest in condensed matter physics because of exhibiting unique magnetic and topological properties, like Dirac magnons[1],[2].
We present spin density functional calculations on this cobaltate, including spin-orbit interactions. We analyze the different magnetic configurations. There are two critical temperatures, related to the transition between the magnetic configurations shown in figure 1.
We also find that cobalt titanate presents out-of-plane magnetic anisotropy, a finding that seems to be in disagreement with previous experimental reports[3,4].
However, we observe that n-type doping in the form of Ti-Co anti-site ordering can switch the anisotropy in-plane[5].

References

[1] M. Elliot et al., Nat. Commun. **12**, 3936 (2021).
[2] B. Yuan et al., Phys. Rev. X **10**, 011062 (2020).
[3] H. Watanabe et. al, J. Magn. Magn. Mater, **15-18**, 549 (1980).
[4] R.E. Newnham et al., Acta Crystallographica **17**, 240 (1964).
[5] M. Arruabarrena et al., arXiv:2108.10847, (2021).

Figures

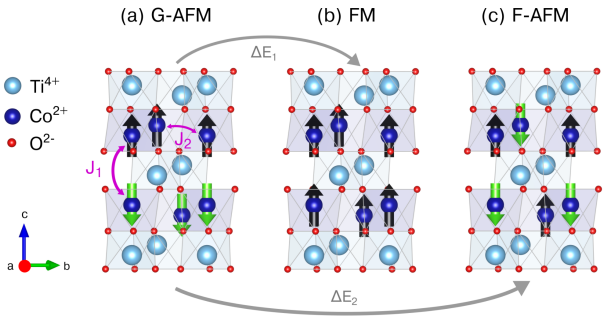


Figure 1: Magnetic configurations of cobalt titanate, presented in ascending energetic order: (a) antiferromagnetic between layers (G-AFM), (b) ferromagnetic (FM), and (c) fully antiferromagnetic (F-AFM).

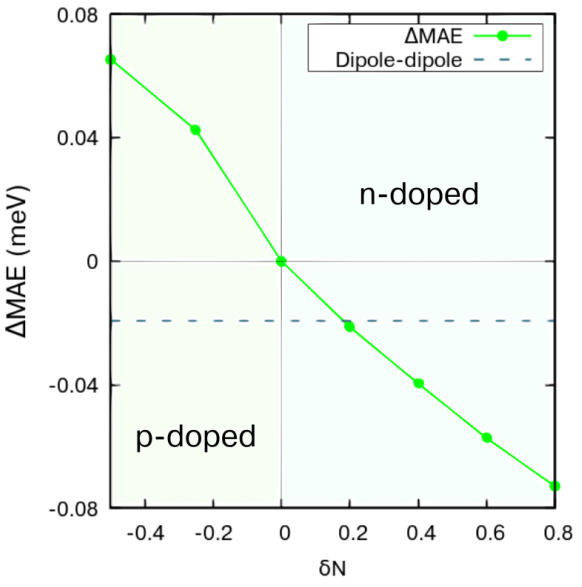


Figure 2: Change of the magnetocrystalline anisotropy energy (ΔMAE) with respect to the variation of the number of electrons in the unit cell (δN). In the n-doped region, for δN values larger than 0.2, the magnetocrystalline anisotropy energy becomes smaller than the magnetic dipole-dipole interaction, which switches the anisotropy in-plane.

Nanoengineered surfaces for modulating cell-surface interaction

Akash Bachhuka
Department of Electronics, Electric and Automatic Engineering, Rovira i Virgili University (URV), Tarragona, Spain

Akash.bachhuka@urv.cat

Abstract

The greatest challenge in the field of biomaterials is the understanding and the prediction of long-term biological responses in patients receiving implantable materials. Reconstructing and detailing these mechanisms may allow for more targeted approaches and highlights how immune processes are amenable to manipulation by synthetic biomaterials. The interplay between plasma polymerized thin films in combination with surface nanotopography proved to be an important factor in cell-surface interaction [1] (Figure 1). We demonstrated that the right combination of chemistry and nanotopography can be used to modulate cellular adhesion, collagen deposition [1] and the expression of pro-inflammatory signals [2-4] (Figure 2). We anticipate that future explorations in this field of research will facilitate the rational design of biomedical implants with physicochemical surface characteristics tailored at the nanoscale that will enhance utility and function and improve clinical outcomes.

References

[1] Bachhuka A, J. Hayball, L. E. Smith, K. Vasilev. ACS Applied Materials & Interfaces. 2015, 7, 23767-75

[2] Chen Z#, Bachhuka A#, Han S, Wei F, Lu S, Visalakshan R. M, Vasilev K, Xiao Y. ACS Nano, 2017, 11 (5), 4494-4506.

[3] Christo SN#, Bachhuka A#, Diener KR, Mierczynska A, Hayball JD, and Vasilev K. Advanced Healthcare Materials, 2016.

[4] Bachhuka A, Christo SN, Cavallaro A, Diener KR, Mierczynska A, Smith LE, Marian R, Manavis J, Hayball JD, Vasilev K. Journal of colloid and interface science. 2015, 457, 9-17.

Figures

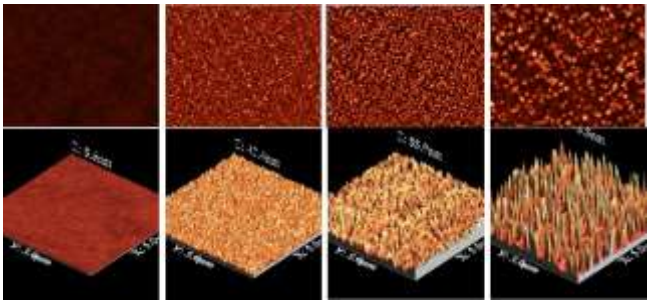


Figure 1: Atomic Force Microscopic images (2D and 3D) of surfaces modified with 16, 38 or 68 nm gold nanoparticles.

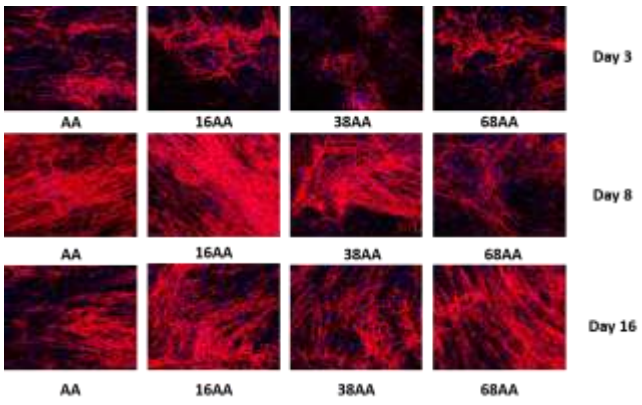


Figure 2: Representative laser scanning confocal microscopy images of human dermal fibroblasts and deposited collagen I on plasma polymerised allylamine (AApp) and nanotopographically modified surfaces (16AApp, 38AApp and 68AApp) at days 3, 8 and 16.(Blue: nucleus/DAPI; Pink/Red: collagen I).

Magnetic alginate hydrogels: the role of particles' surface functionalization

Mariusz Barczak[1]
Piotr Borowski[1], Cristina Gila-Vilchez[2,4], Miguel Alaminos[3,4], Fernando González-Caballero[2,4], Modesto T.López-López[2,4]

[1]*Department of Theoretical Chemistry, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie- Skłodowska University, 20031, Lublin, Poland*
[2]*Department of Applied Physics, Faculty of Sciences, University of Granada, 18071, Granada, Spain*
[3]*Tissue Engineering Group, Department of Histology, University of Granada, Granada, Spain*
[4]*Instituto de Investigación Biosanitaria ibs.GRANADA, Granada, Spain*

mariusz.barczak@mail.umcs.pl

Introduction

Hydrogels can be considered as three-dimensional, hydrophilic networks of flexible polymer chains swollen by water or other fluid. They are able to store a large amount of water (even up to thousands times their dry weight) while maintaining the structure that can be cast into practically any shape or form [1]. They are soft and capable of retaining large amounts of water thus closely resemble living tissues. Mainly for that reason hydrogels are considered as particularly promising materials in the rapidly developing field of tissue engineering as matrices for replacing and regenerating different tissues and organs [2-4].

There is a plethora of different hydrogelators which can be used to fabricate hydrogels; among them alginate-based hydrogels are considered as one of the preferred formulations, mainly due to low cost and excellent biocompatibility of alginate hydrogelators [5,6]. To fabricate "smart" materials, alginate hydrogels can be doped with magnetic particles. Incorporation of magnetically-susceptible species into hydrogel structure may provide additional features like, for example, stimuli-responsive action, improved thermal properties or tailorable rheological properties without affecting biocompatibility [7,8]. The rheological properties of the magnetic hydrogels (also called ferrogels) in the presence of magnetic field are then predominantly controlled by the factors related to the type, size, shape and concentration of the incorporated magnetic particles [9-11].

Functionalized magnetic particles can be used to modulate the interactions between them and the polymer filaments that form the hydrogels having a direct impact on the properties of the hydrogels, as has been recently shown [9]. However, apart from bulk iron providing magnetic field actuation, the surface of magnetic particles can be used to tune specific or nonspecific interactions with the hydrogelator moieties [12], which in turn can affect the final properties of resulting hydrogels and even provide more favorable features like better adhesion of biological species (e.g., cells).

Goal

The main objective of this work was to determine the role of surface functionalization of iron particles on the properties of the resulting alginate magnetic hydrogels [13]. We hypothesize that different surface chemistries of iron particles can affect chemical interactions between the both phases in a distinct way, and these changes will contribute to the different microstructure, mechanical properties, and biocompatibility of ferrogels. Alginate was chosen as a model matrix due to its high biocompatibility allowing its use in biomedical applications. A set of different surface functionalizations of iron/silica core-shell microparticles has been chosen. Interactions between specific surface groups and alginate chains have been elucidated with the aid of DFT quantum chemistry calculations to get a more detailed insight into those interactions.

Results

Iron microparticles were modified by introducing a number of functionalities on their surface, ranging from amine to phenyl groups. Although surface functionalizations have not significantly affected the properties of the microparticles themselves, they changed remarkably the final properties of magnetic hydrogels obtained by embedding the iron microparticles into the pre-polymerized alginate matrix (cf. Figure 1). Thus, the successful dispersion of functionalized microparticles was twofold beneficial [13]:

(i) magnetic activity was introduced in-situ,

(ii) enhancement of the macroscopic and mecha-nical properties was achieved thanks to the altered interactions of alginate with functionalized surface.

Among all the systems studied, amine functionalized IMP-based hydrogels (1-ALG, 2-ALG and 5-ALG) exhibited superior properties when compared with the hydrogel prepared with the use of their non-functionalized counterpart (R-ALG). Properties such as hydrogel integrity, water-holding capability, storage modulus of the amine-based hydrogels (1-ALG and 2-ALG) were significantly altered in comparison with pure hydrogel (R-ALG) or phenyl-

functionalized one (4-ALG). For example, storage moduli for the 1-ALG and 4-ALG are 410 and 483 Pa, respectively, while for the R-ALG and 4-ALG - 137 Pa and 141 Pa, respectively (cf. Figure 2). SEM images revealed that the lack of adequate surface chemistry limits the contact between both phases, which are connected only by limited number of anchoring points. In contrast, amination of the iron surface results in more tight covering of most of the microparticles' surface by multiple connections (cf. figure 1). Theoretical DFT calculations revealed that alginate chains are chemically active not only because of the presence of carboxyl groups but also other non-carboxylic oxygen arrangements which can interact with functionalities. Even blocking of all carboxyl groups by calcium cations during alginate crosslinking does not limit the possibility of tuning of alginate interactions with appropriately modified surfaces [13].
Biocompatibility *in vitro* of the obtained hydrogels depends on the surface chemistry of functionalized microparticles and thus, apart from the macroscopic and mechanical properties, also the cell viability depends on the functionalization (cf. Figure 3).

References

[1] D. Seliktar, Science, 336 (2012) 1124.
[2] J.L. Drury, D.J. Mooney, Biomaterials, 24 (2003) 4337.
[3] N.A. Peppas, et al., Advanced Materials, 18 (2006) 1345.
[4] H. Geckil, et al., Nanomedicine, 5 (2010) 469.
[5] A. Espona-Noguera et al., International Journal of Biological Macromolecules, 107 (2018) 1261.
[6] H. Wang et al., ACS Biomaterials Science & Engineering, 5 (2019) 3654.
[7] J. Supramaniam et al., International Journal of Biological Macromolecules, 118 (2018) 640.
[8] C. Gila-Vilchez et al., Smart Materials & Structures, 28 (2019) 035018.
[9] A.B. Bonhome-Espinosa et al., Soft Matter, 13 (2017) 2928.
[10] C. Gila-Vilchez et al., Journal of Rheology, 62 (2018) 1083.
[11] C. Gila-Vilchez et al., Philosophical Transactions Mathematical Physical and Engineering Sciences, 377 (2019) 20180217.
[12] E. Tanasa et al., Nanomaterials, 9 (2019) 1384.
[13] M. Barczak et al., Carbohydrate Polymers 247 (2020) 116747.

Acknowledgement

Mariusz Barczak thanks to Polish National Agency for Academic Exchange (NAWA) for supporting the research and his stay at the University of Granada in the frame of the Bekker programme fellowship no. PPN/BEK/2018/1/00235/U/00001.

This study was also supported by project FIS2017-85954-R (Ministerio de Economía, Industria y Competitividad, MINECO, and Agencia Estatal de Investigación, AEI, Spain, cofunded by Fondo Europeo de Desarrollo Regional, FEDER, European Union).

Figures

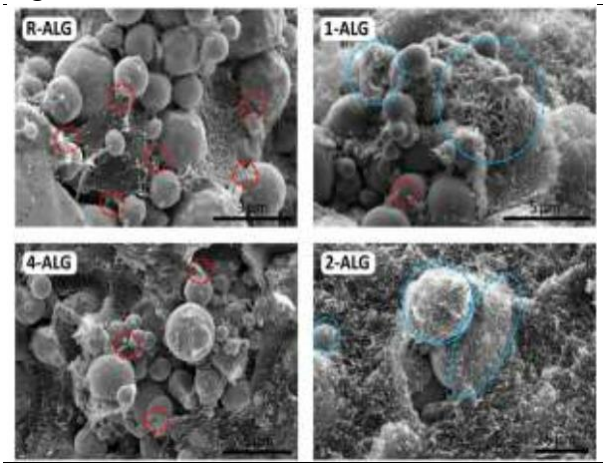


Figure 1: SEM microphotographs of the selected hydrogels (red circles show cobweb-like single point type joints, blue circles – multi point joints of the microparticles with alginate network) [13].

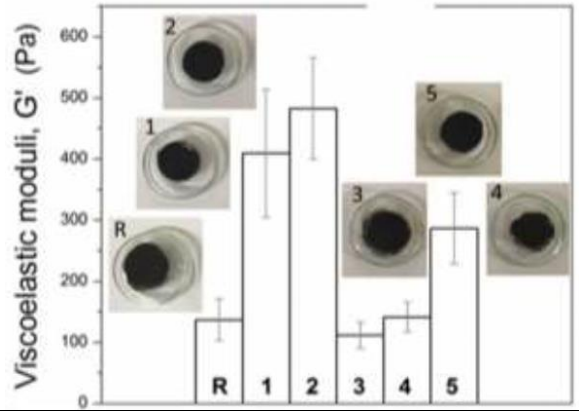


Figure 2: Comparison of the values of storage modulus (G') of the hydrogels studied without the presence of magnetic field [13].

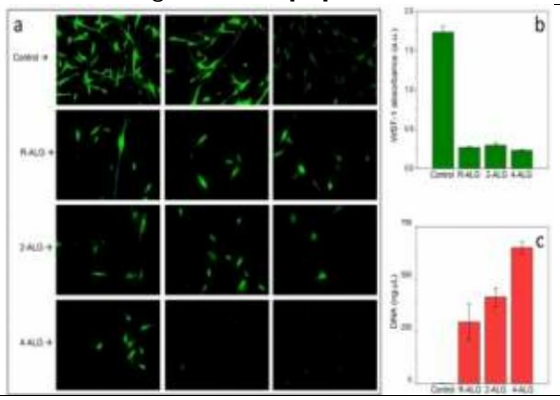


Figure 3: (a) Cytotoxicity of the selected hydrogels revealed by the fluorescence microscopy, (b) WST-1 absorbance test, (c) and DNA quantification in the cell medium [13].

Synthesis of water soluble fluorinated gold nanoparticles and *in vivo* 19F MRS.

Mónica Carril
Juan Manuel Arango, Jorge Blanco, Sonia López-Fernández, Daniel Padro, Pilar Castellnou, Abraham Martin

Instituto Biofisika UPV/EHU, CSIC, Barrio Sarriena s/n, E-48940, Leioa, Bizkaia, Spain.
Ikerbasque, Basque Foundation for Science, 48013, Bilbao, Spain

monica.carrilg@ehu.eus

Organic fluorine is not naturally occurring in human biological media for which it constitutes an interesting label or reporter. The absence of background signal allows for fluorinated species to be studied unequivocally and quantitatively by magnetic resonance (MR) related techniques [1,2], as long as sufficient local fluorine concentration is available. In this sense, ^{19}F Magnetic Resonance Imaging (^{19}F MRI) based on imaging exogenous fluorinated probes, is a versatile diagnosis technique complementary to conventional ^{1}H MRI. However, the applicability of ^{19}F MRI is currently limited by the detection sensitivity of the MRI technique and the need for high local concentration of fluorine, for which the design of highly fluorinated probes is an active field of research. Despite its interesting features, the prospects of fluorine in nanoparticle (NP) design for nanomedicine are somehow limited by several reasons, namely, (i) the high hydrophobicity of fluorinated molecules, (ii) the sometimes challenging synthesis of those, (iii) the need of high local concentration of fluorine for magnetic resonance (MR) applications and (iv) the usually poor relaxation times due to NP structural design. Thus, examples of fluorinated NPs composed of a metal core and fluorinated ligands that are water soluble are scarce in the literature. Herein, two methodologies are presented for their preparation: (i) a direct synthesis method using ad hoc prepared fluorinated ligands [1-3] and (ii) a fluorine labelling strategy based on the conjugation of custom made small fluorinated building blocks, obtained by simple synthetic transformations, with carboxylated gold NPs through a convenient phase transfer process. For the latter method, the synthesis of four fluorinated building blocks with different chemical shift in ^{19}F nuclear magnetic resonance and varied functionalities is presented, along with their conjugation onto NPs. Following these two synthetic methodologies, fluorinated NPs of small core size with very high (above the average) transverse relaxation times (T_2) ranging from 518 to 1030 ms and fluorine atoms per NP of up to 1260 atoms are obtained. Such T_2 and fluorine content values are challenging to achieve in fluorinated probes and make these NPs potential candidates for ^{19}F magnetic resonance related applications. Finally, non-targeted fluorinated NPs were probed *in vivo* by ^{19}F magnetic resonance spectroscopy (^{19}F MRS) in mice. NPs were clearly detected both at 1 hour and 2 hours after being injected and their fate was studied by analysing the gold content in tissues by ICP-MS.

References

[1] M. Carril, D. Padro, P. del Pino, C. Carrillo-Carrion, M. Gallego, W.J. Parak, Nat. Commun., (2017) 1542.
[2] D. Padro, P. Cienskowski, S. Loper-Fernandez, I. Chakraborty, C. Carrillo-Carrion, N. Feliu, W.J. Parak, M. Carril, Small (2020), in press.
[3] O. Michelena, D. Padro, C. Carrillo-Carrión, P. del Pino, J. Blanco, B. Arnaiz, W.J. Parak, M. Carril, Chem. Commun. (2017), 2447.

Figures

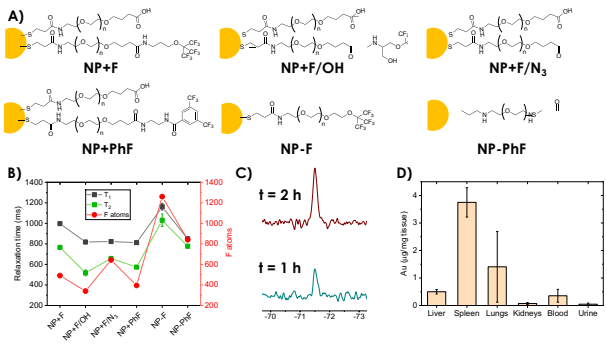


Figure 1: A) Fluorinated NPs prepared. B) Plot of relaxation times and number of fluorine atoms. C) *in vivo* ^{19}F MRS at 1 and 2 hours. D) ICP-MS analysis of extracted tissues and organs.

Nanotechnology at the Basque Research and Technology Alliance (BRTA)

Yolanda R. de Miguel

Tecnalia, Spain

yolanda.demiguel@tecnalia.com

BRTA has identified NANOTECHNOLOGY as a key enabling technology for the development of new products, mainly advanced materials, across a wide range of industrial sectors (e.g. Manufacturing, Health, Energy, Construction, Transport, etc.).

In this endeavor, the first stage is to generate the knowledge in nanoscience and nanotechnology, which can lead to high added value materials and products, ensuring economic impact and job creation coming from the resulting nanotechnology-based industrial applications; while taking into account issues like sustainability and circular economy as well as the environmental, health and safety (EHS) impacts of nanotechnology.

R&D activities at BRTA, from lab to pilot scale, span the industrial value chain from nanomaterials (e.g. graphene, nanocellulose, nanoparticles, nanofibers, etc.) all the way to the final nanotechnology-based products, which can either be nanostructured materials or nanomaterial-containing (3D bulk or 2D coating) materials or composites of different chemical nature, i.e. metallic, ceramic, polymeric, etc. State-of-the-art characterization for Nanotechnology is available as well as expertise in Modelling. The use of artificial intelligence in the design of the novel nanotechnology-enabled advanced materials is an emerging field which is also receiving special attention.

Unraveling the electronic properties of graphene with substitutional oxygen

Xabier D. de Cerio[1]
David M. A. Mackenzie*, Miriam Galbiati*, Ihor Y. Sahalianov*, Taras M. Radchenko*, Jianbo Sun*, Diego Peña*, Lene Gammelgaard*, Bjarke S. Jessen*, Joachim D. Thomsen*, Peter Bøggild*, Luca Camilli*, José M. Caridad*, Aran Garcia-Lekue[1,2]

[1]*Donostia International Physics Center (DIPC), Donostia-San Sebastian 20018, Spain*
[2]*Ikerbasque, Basque Foundation for Science, Bilbao 48013, Spain*
**Affiliation details in Ref. [3].*
xddecerio@dipc.org

Oxygen (O) is of undeniable importance in organic chemistry, being involved in a vast range of carbon (C)-based compounds. However, despite its wide variety of bonding configurations, scenarios involving O atoms with three C neighbors are rare in organic chemistry. In graphene, O plays an important role in the development of technological applications, but usually as part of out-of-plane functional groups [1]. For these reasons, the recent observation of substitutional O in the π-conjugated C honeycomb lattice [2] has generated great interest. Nevertheless, a detailed characterization of its electronic properties and an in-depth analysis of their potential novelty with respect to other type of impurities is still missing.

In this work, a combined theoretical and experimental exploration of in-plane substitutional O in monolayer graphene is presented [3]. The O implantation was realized via a controlled plasma-based process, allowing thorough atomic- to device-scale characterization. Using Density Functional Theory (DFT), we show that in-plane oxygen n-dopes graphene and we determine the distinctive character of the scattering potentials introduced in the most common impurity cases. Our simulations are combined with transport and scanning tunneling microscopy (STM) experiments, which serves to confirm the successful implantation of O, and to establish comparison with more conventional impurities like nitrogen (N)[4,5] or out-of-plane functional groups containing oxygen [1].

These achievements set up a cross-field understanding of a novel type of chemical doping in graphene and pave the way towards its implantation in other elaborate carbon nanostructures, such as graphene nanoribbons.

References

[1] D. A. Dikin et al., Nature, 448 (2007) 457
[2] C. Hofer et al., Nature Communications, 10 (2019) 4570
[3] D. M. A. Mackenzie et al. 2D Materials 8 (2021) 045035
[4] L. Zhao et al, Science, 333 (2011) 999
[5] Y. Tison et al., ACS Nano, 9 (2015) 670

Figures

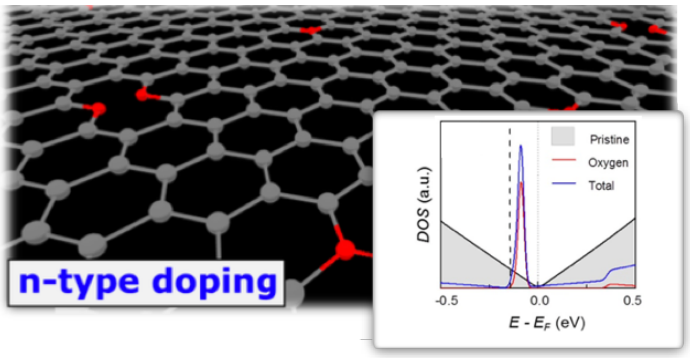


Figure 1: Illustration of different substitutional oxygen configurations, together with the effect of graphitic oxygen in the electronic structure of graphene.

Novel targeted devices based on Elastin-like polypeptides for diagnosis and gene therapy in breast cancer

Sara Escalera-Anzola[1]
Alessandra Girotti[2], Sofía Serrano[1], Raquel Muñoz[1], Purificación Cuadrado[1], F. Javier Arias[1]

[1]*Smart Biodevices for Nanomedicine Group, University of Valladolid, Edificio LUCIA, Paseo de Belén 19, 47011 Valladolid, Spain*
[2]*BIOFORGE (Group for Advanced Materials and Nanobiotechnology), CIBER-BBN, University of Valladolid, Valladolid, Spain*

sara.escalera@uva.es

Breast cancer is the principal malignancy diagnosed in women and the second most common cancer overall. Typical treatments for breast cancer are surgery, chemotherapy and radiotherapy; and although they improve the clinical outcome, they do not increase the cure rate [1]. The main problem of the current cancer treatments is the low specificity that translates into systemic toxicity and side-effects. In the last years, immunotherapy has emerged as an outstanding personalized treatment. Other approaches for cancer treatment such as the delivery of therapeutic genes via specifically targeted nanodevices stands out as an alternative therapy. Elastin-like polypeptides (ELPs), biomaterials derived from elastin-mimetic peptide sequences, are promising candidates as carriers for these gene therapies because of their excellent biocompatibility and low toxicity [2].

This work comprises the development of a selectively targeted nanodevice to eliminate tumor cells while keeping healthy ones safe. This devices are based on a polycationic Elastin-like backbone that complexes therapeutic DNA and interacts with the cell membrane allowing the DNA uptake. The device is also targeted to tumoral cell markers, and the expression of the therapeutic DNA is controlled by a tumoral promoter, which makes these nanoparticles doubly targeted to cancerous cells [3,4].

The genes codifying the different ELPs were created using genetic engineering techniques and the ELPs were bioproduced in a bacterial host. They were purified by affinity chromatography and characterized by MALDI-TOF, 1H-NMR, SDS-PAGE and DSC. Nanoparticles based on this ELPs and therapeutic plasmid DNA (pDNA) were formed by electrostatic interactions between the positively charged lysine-rich backbone of ELRs and negatively charged pDNA. The obtained nanoparticles were characterized by Dynamic Light Scattering (DLS). In addition, *in vitro* and *in vivo* experiments have been performed to prove the efficiency of the system.

Our nanoparticles presented a Zeta potential of about +40 mV and a size of about 140 nm. Their positive charge allows the interaction with the negatively charged cell membrane, facilitating the pDNA uptake. When loaded with a pDNA that encodes a fluorescent reporter protein, these nanoparticles can be used as imaging technique for diagnosis and when loaded with toxic pDNA, they can be used as selective gene therapy against cancerous cells. The developed in vitro studies showed transfection ability of the system facilitated mainly by micropinocytosis uptake and selective toxicity against cancer cells without harming the healthy cells. After the development of *in vivo* studies, an inhibition of tumor progression was observed with a decrease of the tumor growth of an 85% in comparison with the placebo group. In addition, a dose dependent reduction in tumor mass was observed, with a better result in the highest concentration of the therapeutic DNA tested which was 70 nM.

This versatile system can be tuned to target different tumoral targets making it a next-generation material with a promising scope.

References

[1] Gonzalez-Angulo AM, Morales-Vasquez F, Hortobagyi GN; Adv Exp Med Biol (2007) Ed 608:1-22.

[2] Rodriguez-Cabello JC, Arias FJ, Rodrigo MA, Girotti A; Adv Drug Deliv Rev (2016) Ed 97: 85−100

[3] Piña MJ, Girotti A, Santos M, Rodriguez-Cabello JC, Arias FJ; Mol Pharm (2016) Ed 13:795-808

[4] Piña MJ, Girotti A, Serrano S, Muñoz R, Rodriguez-Cabello JC, Arias FJ; Cancer Lett. (2020) Ed, 470:43-53

Figures

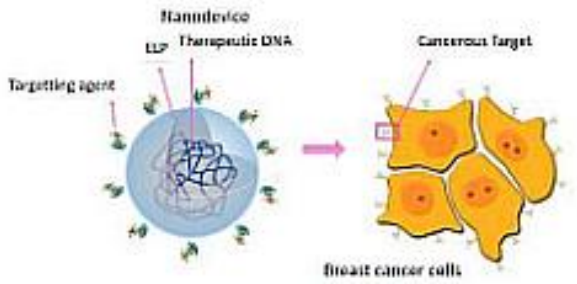


Figure 1: Scheme of the developed nanodevice

Lipid-gold clusters (Aurora™): improving gold nanoparticles for lipid membrane studies

Aritz B. García-Arribas
Jesús Sot, Sebastião A. Mendanha-Neto, Jon V. Busto, Shengrong Li, Stephen W. Burgess, Walt A. Shaw, David Gil-Carton, Félix M. Goñi, Alicia Alonso

Instituto Biofisika (UPV/EHU, CSIC), Barrio Sarriena s/n, 48940, Leioa, Spain.

aritzgarciaar@gmail.com

Lipid model membranes in lamellar phases (bilayers) of different phospholipid compositions have been prepared, in the form of vesicles, or of supported lipid bilayers, and doped with Aurora™ at 0.1 mol%. Aurora™ consists of an Au_{55} gold nanoparticle (about 1.4 nm in diameter) capped with triphenylphosphine ligands and a single diglyceride (distearoyl glycerol, DSG) ligand. Gold nanoparticles have been incorporated in the past inside liposomes, or grafted onto their surfaces, with diagnostic or therapeutic aims [1]. Including the gold nanoparticles in a stable form within the lipid bilayers has serious technical difficulties. We have tested the hypothesis that, because of the diglyceride ligand, Aurora™ would allow the easy incorporation of gold nanoclusters into cell membranes or lipid bilayers without significant effects in their biophysical properties. Our results show that Aurora™ readily incorporates into lipid bilayers, particularly when they are in the fluid phase, i.e. the state in which cell membranes exist. Calorimetric, fluorescence polarization or fluorescence confocal microscopy concur in showing that bilayer-embedded Aurora™ hardly changes the physical properties of the bilayers, nor does it perturb the phase equilibrium in lipid mixtures giving rise to lateral phase separation in the plane of the membrane. Atomic force microscopy shows, in fluid bilayers, well-resolved particles, 1.2 – 2.9 nm in height, that are interpreted as single Aurora™ conjugates (Figure 1). Cryo-transmission electron microscopy allows the clear observation of lipid bilayers with an enhanced contrast due to the Aurora™ gold nanoparticles; the single particles can be resolved at high magnification. Our studies support the applicability of Aurora™ as a membrane-friendly form of nano-gold particles for biological research or clinical applications [2].

References

[1] Miao Li, Theobald Lohmüller, Jochen Feldmann. Nano Lett, 15 (2015), 770-775.

[2] Jesús Sot, Sebastião A. Mendanha-Neto, Jon V. Busto, Aritz B. García-Arribas, Shengrong Li, Stephen W. Burgess, Walt A. Shaw, David Gil-Carton, Félix M. Goñi, Alicia Alonso. Chem Phys Lipids, 218 (2019), 40-46.

Figures

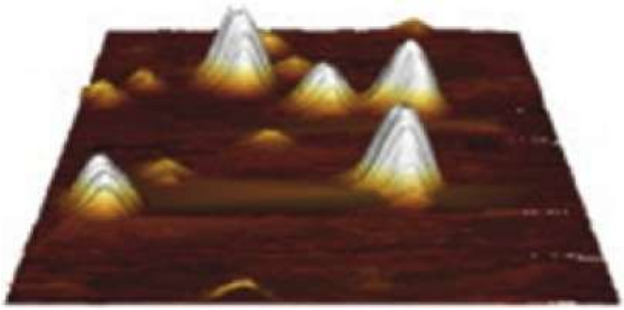


Figure 1: Contact mode AFM image of Aurora™ – DSG gold nanoparticles inserted into a lipid membrane (fluid phase).

Optomechanical detection of single bacterium mechanical modes

Eduardo Gil-Santos[1]
Jose Jaime Ruz[1], Oscar Malvar[1], Ivan Favero[2], Arestide Lemaître[3], Priscila Monteiro Kosaka[1], Sergio García-López[1], Montserrat Calleja1, Javier Tamayo[1]

[1]*Bionanomechanics Lab, Instituto de Micro y Nanotecnología, IMN-CNM (CSIC), Isaac Newton 8 (PTM), E-28760 Tres Cantos, Madrid, Spain.*
[2]*Matériaux et Phénomènes Quantiques, Université de Paris, CNRS, 10 rue Alice Domon et Léonie Duquet, 75013 Paris, France.*
[3]*Centre de Nanosciences et Nanotechnologies, CNRS, Université Paris-Saclay, 10 boulevard Thomas Gobert, 91120 Palaiseau, France.*

eduardo.gil@csic.es

Low-frequency phonon modes of biological particles such as proteins, viruses and bacteria involve coherent structural vibrations at frequencies in the THz and GHz domains (Figure 1). These modes carry information on its structure and mechanical properties that play a pivotal role in many relevant biological processes. Despite the rapid advances of optical spectroscopy techniques, detection of low-frequency phonons of single bioparticles has remained elusive. Here we harness a particular regime in the physics of mechanical resonator sensing that serves for detecting them. By depositing single bacterium on ultra-high frequency optomechanical disk resonators, we demonstrate that the vibration modes of the disk and bacterium hybridize when their associated frequencies are similar (Figure 2). A general theoretical framework is developed to describe the different regimes that can be found when an analyte adsorbs on a mechanical resonant sensor. Our model allows retrieving the mechanical frequencies and losses of the bacterium modes. This work opens the door for a new class of vibrational spectrometry based on high frequency mechanical resonators with the unique capability to obtain information on single biological entities [1].

References

[1] E. Gil-Santos, et. al. "Optomechanical detection of low-frequency phonon modes of single bacterium". Nature Nanotechnology, 15 (2020)469.

Figures

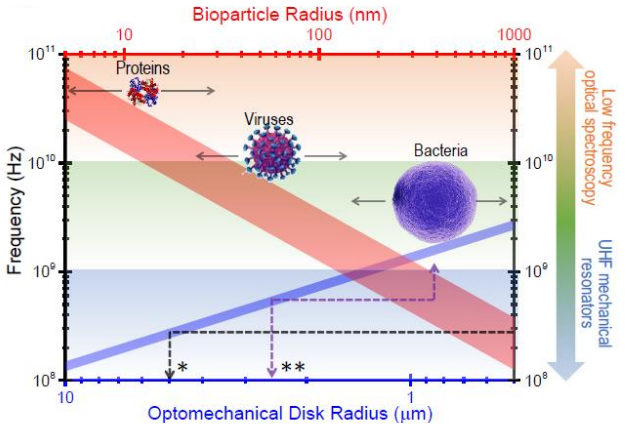


Figure 1: Frequency of the radial breathing mode of a 320 nm thick optomechanical disk (blue region) and of the fundamental mode of a quasi-spherical biological particle adsorbed on a rigid support (red region), as a function of the disk and bioparticle radii, respectively.

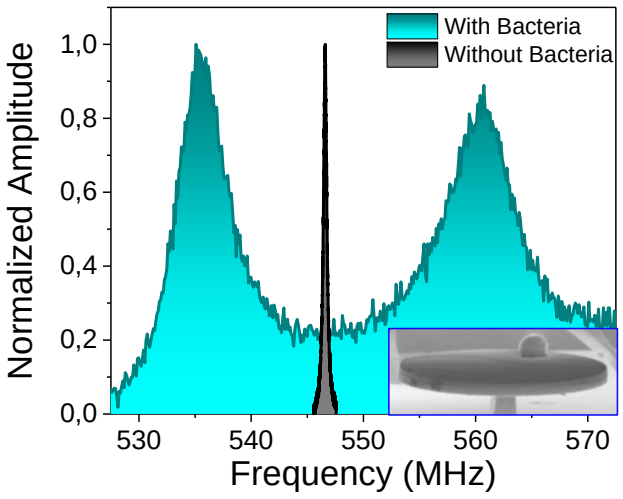


Figure 2: Effect of bacterium adsorption on the radial breathing mode of an optomechanical disk (2.5 μm in radius and 320 nm in thickness). The inset shows a scanning electron microscopy image of the optomechanical disk with an attached Staphylococcus epidermidis cell.

2D Layered MPX_3 Performance for Water Splitting Reactions

Rui Gusmão
Filipa M. Oliveira, Jan Paštika, Zdeněk Sofer

Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

rui.gusmao@vscht.cz

Two-dimensional (2D) layered materials are currently one of the most explored materials for developing efficient and stable electrocatalysts for energy conversion applications. Some of the 2D metal phosphorous trichalcogenides, $M_2P_2X_6$ or simply MPX_3, have been reported to be useful catalysts for water splitting,[1] although the results have been less promising for the sluggish oxygen evolution reaction (OER) due to insufficient activity or compromised stability.

We report on the water splitting performance of a series of MPX_3 (M^{2+} = Mn, Fe, Co, Zn, Cd; X = S, Se). For the series of MPX_3, $CoPS_3$ yields the best results with an overpotential within the range of values usually obtained for IrO_2 or RuO_2 catalysts. The liquid-phase exfoliation of $CoPS_3$ improves the OER activity due to the abundant active edges of the downsized sheets, accompanied by the presence of surface oxides. The influence of the OER medium and the underlying substrate electrode is studied, with the exfoliated $CoPS_3$ reaching the lowest overpotential also able to sustain high current densities, with excellent stability after multiple cycles or long-term operation.

The photoelectrochemical (PEC) responsivity of MPX_3 was also tested in the OER region, with excitation wavelengths from 385 to 700 nm, is reported. [3] The experimentally determined optical bandgaps of the MPX_3 materials range from 1.5 eV for $FePSe_3$ to 3.7 eV for $ZnPS_3$. At +1.23 V vs. RHE, the PEC activity in the OER region of $MnPSe_3$ exhibits superior performance, while the exfoliation of $CoPS_3$ improves its PEC activity up to double in contrast with its bulk counterpart. The influence of the substrate and applied potential is also optimized.

References

[1] R. Gusmão et al., Angew. Chemie Int. Ed. 58 (2019) 9326–9337.
[2] F.M. Oliveira et al. ACS Appl. Mater. Interfaces. 13 (2021) 23638–23646.
[3] F.M. Oliveira et al., Adv. Mater. Interfaces. (2021) 2100294.

Figures

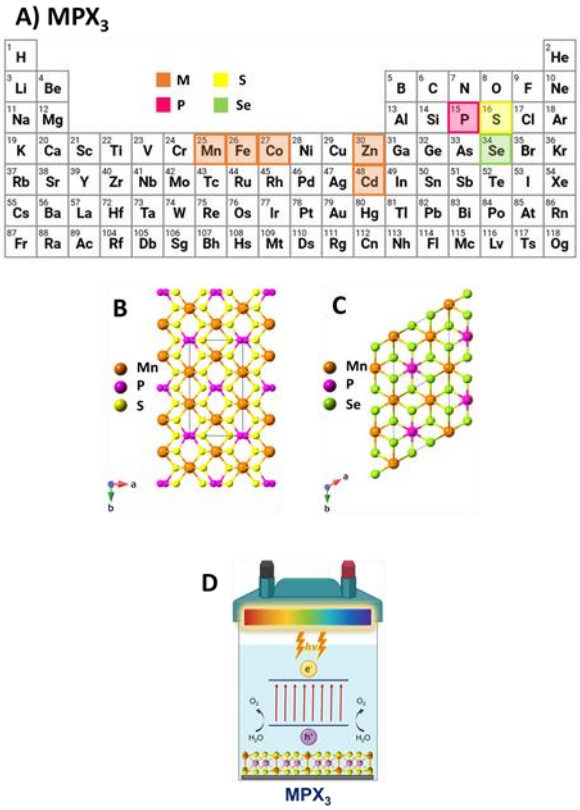


Figure 1: (A) Periodic table in which the filled blocks represent the elements selected for the synthesis of MPX3 materials. Top (c-axis) view of the crystal structures of (B) MnPS3 and (C) MPSe3. Color scheme: Mn – orange, P – pink, S – yellow, Se – green. D) Scheme of the photoelectrochemical response of MPX3 for OER.

SERS-active 3D printed scaffolds; combining hybrid materials to better understand the tumour environment

Malou Henriksen-Lacey[1,2]
Dorleta Jimenéz de Aberasturi[1,2,3]
Luis M. Liz-Marzán[1,2,3]

[1]*CIC biomaGUNE, Basque Research and Technology Alliance (BRTA), Paseo de Miramón 182, 20014 Donostia-San Sebastián, Spain*
[2]*Centro de Investigación Biomédica en Red de Bioingeniería Biomateriales, y Nanomedicina (CIBER-BBN), Paseo de Miramón 182, 20014 Donostia-San Sebastián, Spain*
[3]*Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain*

mhenriksen@cicbiomagune.es

Hybrid materials offer many advances in biomedicine thanks to their flexibility in physicochemical attributes such as geometry, scale, permeability, and responsive behaviour to externally applied stimuli. Specifically, the combination of inorganic nanoparticles and organic matrixes allows one to design biocompatible scaffolds in which mammalian cell growth (including aspects such as division, migration, differentiation) can be controlled and studied in real time.

With the aim of better understanding the tumour environment, we have designed a 3D printed scaffold which supports long term cell growth in 3D (Figure 1). The scaffolds are printed with a large (1cm^2) footprint yet retaining micro-scale resolution. Within the porous walls are embedded plasmonic gold nanoparticles (AuNPs), thereby simultaneously providing surface enhanced Raman spectroscopy (SERS) mapping and sensing components to allow high resolution imaging and detection of soluble components, respectively[1]. Additionally, we are investigating the ability to combine heterogenous 3D printed materials to produce complex 3D cell models to explore aspects such as drug delivery and metastatic cell migration from the tumour environment.

A key feature of our work involves SERS imaging and the technical aspects thereof. SERS offers important advantages over other commonly used microscopy techniques as it allows us to follow cell migration and division in a non-disruptive manner, avoiding the commonly encountered photobleaching and phototoxicity that otherwise occurs with fluorescence microscopy. Furthermore, imaging depths are increased thanks to the use of NIR excitation sources. Such bio-3D printed models provide an important stepping-stone or even alternative to in vivo studies. We foresee these models as systems in which factors such as local pH[2], temperature, degree of cellular migration, and metabolite production can all be studied in a controlled environment.

References

[1] García-Astrain, C., Lenzi, E., Jimenez de Aberasturi, D., Henriksen-Lacey, M., Binelli, MR., Liz-Marzán, LM. Advanced Functional Materials 30 (2020) 2005407
[2] Zhang, Y., Jimenez de Aberasturi, D., Henriksen-Lacey, M., Langer, J., Liz-Marzán, LM. ACS Sensors, 5 (2020) 3194-3206

Figures

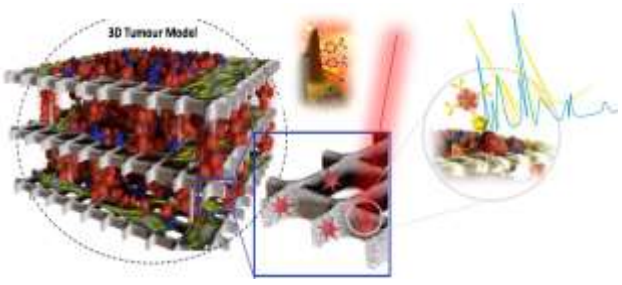


Figure 1: Model of a biocompatible 3D printed scaffold with SERS activity and supporting cell growth

MoS_2 Field-Effect Transistors for Ion Sensing: Ultrasensitive Hg^{2+} Detection

Fernando J. Urbanos
Sara Gullace, Paolo Samorì
Université de Strasbourg, CNR ISIS UMR 7006, 8 allée Gaspard Monge, Strasbourg, F-67000, France
jimenezurbanos@unistra.fr

Contamination of water with heavy metal ions represents a severe environmental problem resulting from the societal development. Among the various hazardous compounds, mercury (II) ions (Hg^{2+}) surely belong to the class of the most poisoning ones. Their accumulation in human bodies results in health deterioration, affecting all vital organs and eventually leading to chronic illnesses, overall lifespan shortening, and, in the worst-case scenario, premature death [1]. Because of this reason, the United States Environmental Protection Agency (EPA), the World Health Organization (WHO), and the European Union (EU) have established strict regulations on the quality of drinkable water. In particular, the maximum permitted concentration of Hg^{2+} has been set to 5-10 nM.

High performance can be achieved in chemical sensing by using suitable active materials capable to interact at the supramolecular level with the chosen species. Among those materials, 2D transition metal dichalcogenides (TMDCs) have attracted great attention as potential candidates because of their unique physical and chemical properties [2], which are highly susceptible to environmental changes. In this work, we have fabricated Hg^{2+} MoS_2-based sensors, relying on the affinity of heavy metal ions and point defects in TMDCs [3]. X-ray photoelectron spectroscopy characterization showed a significant reduction of the defectiveness of MoS_2 when exposed to Hg^{2+} solutions with increasing concentration. Low-temperature (77K) photoluminescence confirmed the defect healing, when observing a decrease of the defect-related bands after Hg^{2+} exposure. Transfer characteristics in the MoS_2 FETs provided unambiguous confirmation that Hg^{2+} acts as a p-dopant for MoS_2. Interestingly, we observed a strict correlation of this doping with the concentration of Hg^{2+}. Concentrations as low as 1 pM can be detected, being way below the restrictions imposed by health regulations. Moreover, the fabricated sensing devices displayed a high selectivity for Hg^{2+} against other metal ions. Electrical characterization also revealed that our sensing platform is reversible, since it can be washed and used multiple times without losing selectivity or sensitivity.

References:

[1] Holmes, P., James, K.A.F., Levy, L.S., Science of the Total Enviroment, 2009, 408 (2), 171-182
[2] Anichini, C.; Czepa, W.; Pakulski, D.; Aliprandi, A.; Ciesielski, A.; Samorì, P., Chemical sensing with 2D materials. Chemical Society Reviews 2018, 47 (13), 4860-4908
[3] Yi, H.; Zhang, X.; Jia, F.; Wei, Z.; Zhao, Y.; Song, S., Competition of Hg^{2+} adsorption and surface oxidation on MoS_2 surface as affected by sulfur vacancy defects. Applied Surface Science 2019, 483, 521-528

Figures:

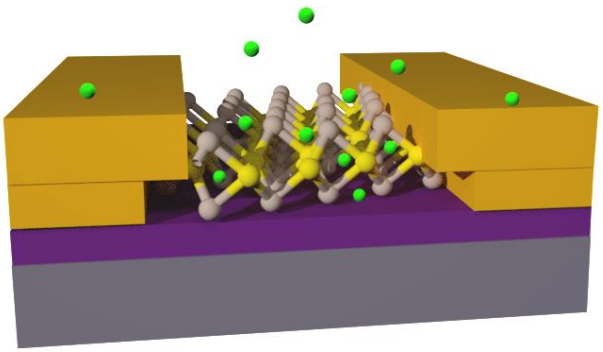


Figure 1: Schematic representation of Hg^{2+} ions (represented as green spheres) interacting with the MoS_2 flake, integrated in a back-gated FET geometry.

Gold nanoparticle-induced formation of reactive oxygen species in proton therapy is a surface effect

Jacob Johny[1]
Charlotte Erika Renate van Halteren[1], Carina Behrends[2,3,4], Christoph Rehbock[1], Christian Bäumer[2,3,4,5], Beate Timmermann[2,3,4,5], Stephan Barcikowski[1]

[1]*Technical Chemistry I and Center for Nanointegration Duisburg Essen (CENIDE), University of Duisburg-Essen, Germany*
[2]*West German Proton Therapy Centre Essen (WPE), Germany*
[3]*Department of Physics, TU Dortmund University, Germany*
[4]*Department of particle therapy, University Hospital Essen, West German Cancer Centre (WTZ), Germany*
[5]*German Cancer Consortium (DKTK), Germany*

jacob.johny@uni-due.de

Proton therapy is an emerging cancer treatment technique characterized by a well-targeted dose delivery to tumors located in or near sensitive organs and fewer adverse side effects in contrast to X-ray therapy [1, 2]. This makes proton therapy particularly useful in sensitive, growing tissues as present in pediatric oncology. Combining proton the apy with noble metallic nanoparticles is an effective strategy to further improve its efficacy [3]. So far, gold nanoparticles (AuNPs) have been at the center of attention as a radiosensitizer for proton therapy. However, nanoparticles of other metals such as platinum, iron, and gadolinium were also tested as sensitive agents to improve proton therapy [3-5]. Even though different mechanisms were proposed to explain the role of nanoparticles in proton beam therapy dose-enhancement, the primary mode of action is believed to be the generation of reactive oxygen species (ROS) leading to higher tumor cell death rates. Nevertheless, a clear idea of the correlation between a) the concentration of nanoparticles as well as b) the particle sizes and c) difference between the mass-driven vs. surface-driven effects on the dose enhancement, is to date not fully understood. In this work, we combined ligand-free noble metal and biocompatible AuNPs obtained via a modern laser ablation in liquids route [6] with proton irradiation. We first investigated the effects of laser-generated AuNPs size, concentration, and irradiation dose on the enhanced ROS production to explore the underlying mechanism by which the nanoparticles act as radiosensitizing agents for proton therapy. Different concentrations and sizes of AuNPs were therefore irradiated at different physical doses of proton fields and the generated ROS was quantified employing fluorescence spectroscopy using the oxidation of the dye coumarin into 7-OH-coumarin upon reacting with the .OH radicals [7]. Our results indicate that smaller particle sizes, higher irradiation doses, and nanoparticle concentration lead to more ROS generation as shown in Fig. 1 and Fig. 2. To further explore whether the observed particle size effects are solely related to the total particle surface area, additional irradiation tests at identical surface area concentrations were conducted for the three different particle sizes (5, 10, and 30 nm). We found that particle size-specific effects were greatly diminished when they are administered at identical surface area concentrations (Fig. 3), which seems to indicate a strong influence of the total available surface area on proton irradiation-induced ROS generation in the presence of gold nanoparticles. However, small but still significantly higher ROS generation was still found for the 5 and 10 nm particles in contrast to those administered at 30 nm, which still points at size effects, probably induced by higher curvature as well as a potentially higher extent of surface defects in the smaller nanoparticles. We further validated the formation of the ROS during proton irradiation of nanoparticles by mixing the AuNPs with sodium citrate, which is a radical scavenger. Here, we observed a significant reduction in the ROS formation (Fig. 4). As citrate is commonly used for the generation of AuNPs by chemical reduction methods, the efficiency of chemically-derived AuNPs in proton therapy is limited, due to the mandatory presence of citrate. The ligand-free AuNPs used in our approach, derived from the laser ablation in liquids

technique, proved to be superior ROS generators and highly suitable sensitizers in proton therapy. In the next steps, these analyses will be extended to *in vitro* and *in vivo* tumor models aiming at a transfer to the clinics.

References

[1] Mohan, R. and D. Grosshans, Proton therapy – Present and future. Advanced Drug Delivery Reviews, 2017. 109: p. 26-44.

[2] Wilson, R.R., Radiological Use of Fast Protons. Radiology, 1946. 47(5): p. 487-491.

[3] Schlathölter, T., et al., Improving proton therapy by metal-containing nanoparticles: nanoscale insights. International journal of nanomedicine, 2016. 11: p. 1549.

[4] Kim, J.-K., et al., Enhanced proton treatment in mouse tumors through proton irradiated nanoradiator effects on metallic nanoparticles. Physics in Medicine & Biology, 2012. 57(24): p. 8309.

[5] Polf, J.C., et al., Enhanced relative biological effectiveness of proton radiotherapy in tumor cells with internalized gold nanoparticles. Applied physics letters, 2011. 98(19): p. 193702.

[6] Zhang, D., B. Gökce, and S. Barcikowski, Laser Synthesis and Processing of Colloids: Fundamentals and Applications. Chemical Reviews, 2017. 117(5): p. 3990-4103

[7] Sicard-Roselli, C., et al., A New Mechanism for Hydroxyl Radical Production in Irradiated Nanoparticle Solutions. Small, 2014. 10(16): p. 3338-3346.

Figures

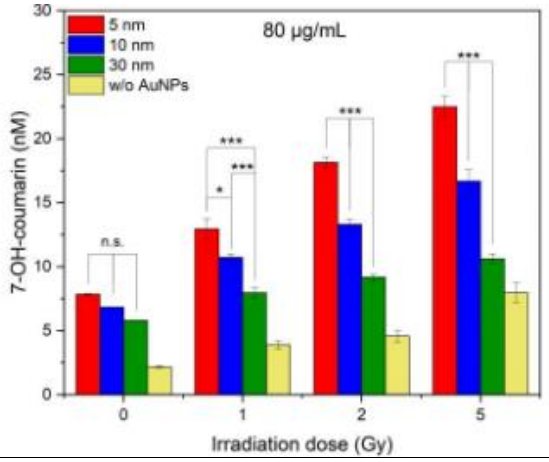


Figure 1: Amount of 7-OH-coumarin formed during the proton irradiation of water phantoms with different sized AuNPs at a constant mass concentration of 80 µg/mL at irradiation doses of 0, 1, 2, and 5 Gy (mean value ± SD of triplicate measurements).

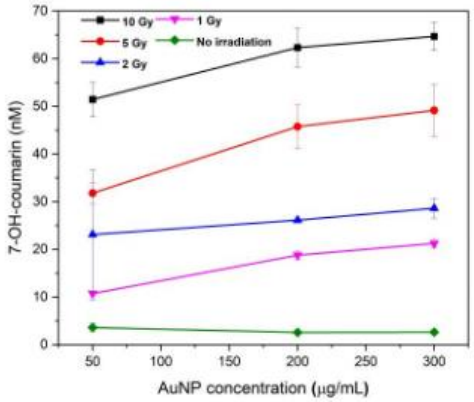


Figure 2: The effect of different AuNPs concentrations on the generation of 7-OH-coumarin (mean value ± SD of triplicate measurements) at different radiation doses. The solid lines connecting the data points are for guiding the eye.

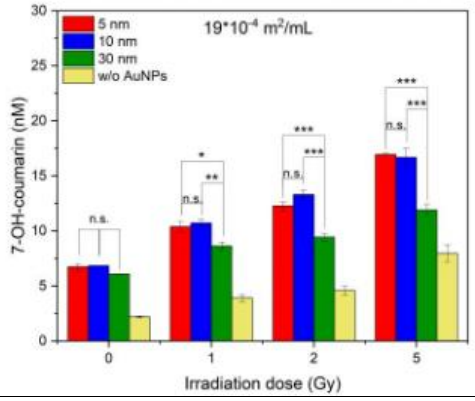


Figure 3: Amount of 7-OH-coumarin formed during the proton irradiation of water phantoms with different sized AuNPs at a constant total surface area of 19*10^{-4} m^2/mL at irradiation doses of 0, 1, 2, and 5 Gy for the evaluation of the size/mass effect (mean value ± SD of triplicate measurements).

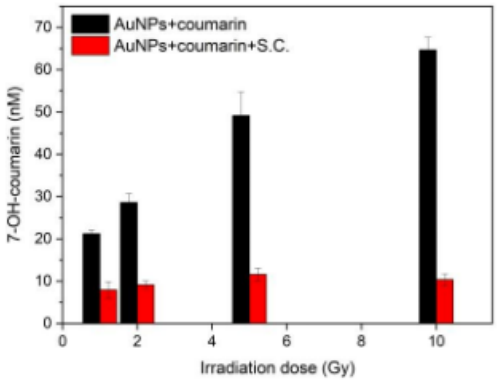


Figure 4: Amount of 7-OH-coumarin formed in the presence and absence of sodium citrate (S.C.) showing that the enhancement effect is due to the radical production which is significantly quenched in presence of the citrate molecules (AuNP+Coumarin+S.C.) (mean value ± SD of triplicate measurements).

2D-based nano/microrobots: Towards Biomedical and Environmental Applications

Bahareh Khezri
Seyyed Mohsen Beladi-Mousavi

University of chemistry and technology, Prague, Technická 5,166 28 Praha 6 – Dejvice, Prague, Czech Republic

Contact: bahareh.khezri@vscht.cz

Nano/microrobots with autonomous motion are the frontier of nanotechnology and nanomaterial research. These self-propelled nano/microrobots convert chemical energy obtained from their surroundings to propulsion. Particularly, the recent progress in targeted drug delivery[1] and efficient water purification systems[2] is very promising.
Graphene and the recently discovered layered materials -beyond graphene- have superior properties and have made a great impact on the new generation of energy, biomedical and environmental applications. Integration of single/few layers materials with extremely high surface area into nano/microrobots has been created a dynamic platform which could significantly enhance motor's functions in terms of adsorption capacity and mobility. We have employed 2D-based microrobots to demonstrate (i) organics[3, 4]/heavy metals[3]/ions[5] collection and DOX loading[1], (ii) a targeted transport system, (iii) the on-demand release mechanism, and (iv) the recovery of the robots for further usage.

References

[1] B. Khezri, S. M. B. Mousavi, L. Krejcova, Z. Heger, Z. Sofer, M. Pumera, Adv. Funct. Mater., 29 (2019) 10.
[2] L. Dekanovsky, B. Khezri, Z. Rottnerova, F. Novotny, J. Plutnar, M. Pumera, Nature Machine Intelligence 2 (2020) 711.
[3] S. M. Beladi-Mousavi, B. Khezri, L. Krejcova, Z. Heger, Z. Sofer, A. C. Fisher, M. Pumera, ACS Appl. Mater. Interfaces 11, (2019)13359.
[4] B. Khezri, K. Villa, F. Novotny, Z. Sofer, M. Pumera, Small 2020, 16, 8; B. Khezri, S. M. B. Mousavi, Z. Sofer, M. Pumera, Nanoscale 11 (2019) 8825.
[5] S. M. Beladi-Mousavi, B. Khezri, S. Matejkova, Z. Sofer, M. Pumera, Angew. Chem.-Int. Edit., 58 (2019)13340.

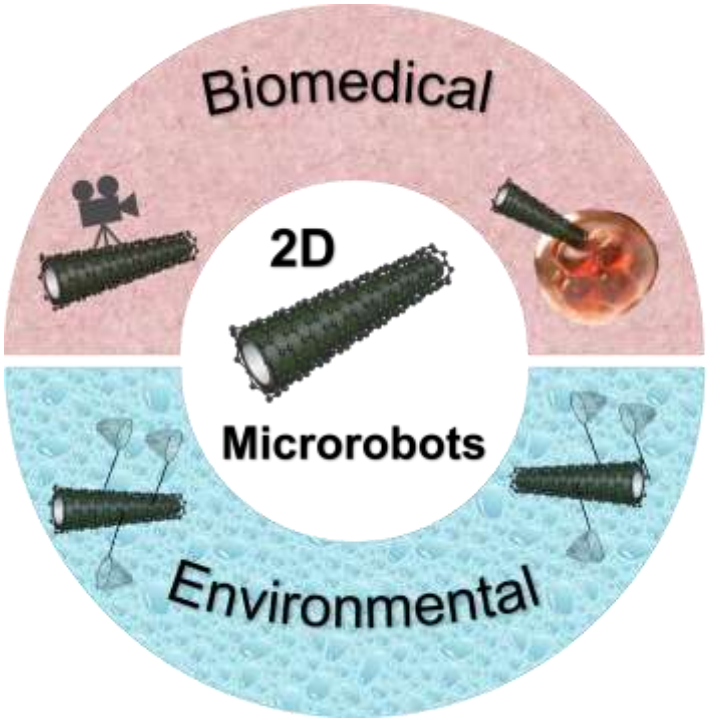


Figure 1: 2D-based nano/microrobots- Towards biomedical and environmental applications

Tkwant: a software package for time-dependent quantum transport

Thomas Kloss[1]
Joseph Weston[1,2], Benoit Gaury[1], Benoit Rossignol[1], Christoph Groth[1], and Xavier Waintal[1]

[1]*Université Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, 38000 Grenoble, France*
[2]*QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands*

thomas.kloss@cea.fr

Tkwant[1,2] is a Python package for simulating the dynamics of nanoelectronic devices which are driven out-of-equilibrium by external perturbations.
It is an extension of the Kwant[3] package and focusses on similar problems, involving semiconductors, graphene, topological materials, superconductors, metals and magnets, that can be described by tight-binding Hamiltonians. The simulated device typically consists of a scattering region of arbitrary dimension and shape, which is coupled to a number of semi-infinite electrodes in thermal equilibrium (Fig. 1).The problem is genuinely many-body even in the absence of interactions and is treated within the non-equilibrium Keldysh formalism. The code has been designed to be modular and easy to use (Fig. 2). Tkwant is free software distributed under a BSD license.

References

[1] T. Kloss, J. Weston, B. Gaury, B. Rossignol, C. Groth and X. Waintal, Tkwant: a software package for time-dependent quantum transport, *New J. Phys.* **23** 023025 (2021).
[2] https://tkwant.kwant-project.org/
[3] https://kwant-project.org/

Figures

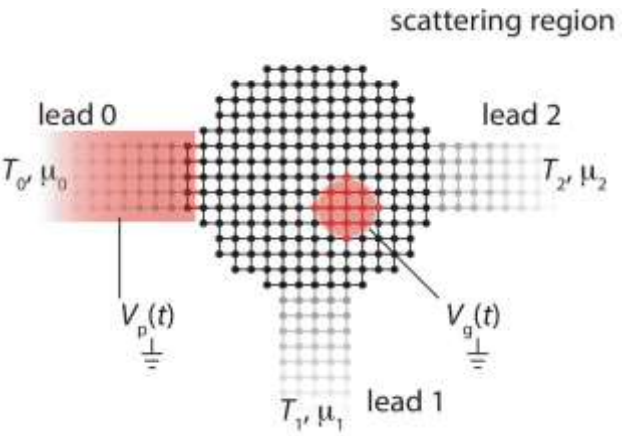


Figure 1: The system typically consists of a central scattering region which is connected to several leads.

```
import tkwant
import kwant

syst = make_system()

current_operator = kwant.operator.Current(syst)

state = tkwant.manybody.State(syst, tmax=1000)

for time in range(1000):
    state.evolve(time)
    current = state.evaluate(current_operator)
```

Figure 2: Using Tkwant is simple and consists in writing a small Python script that comes close to physical intuition.

Effects of energy metabolism on the mechanical properties of breast cancer cells

Marina L. Yubero[1].
Priscila M. Kosaka[1], Álvaro San Paulo[1], Marcos Malumbres[2], Montserrat Calleja[1] & Javier Tamayo[1].

[1]*Bionanomechanics Lab, Instituto de Micro y Nanotecnología, IMN-CNM (CSIC), Isaac Newton 8 (PTM), E-28760, Tres Cantos, Madrid, Spain.*
[2] *Cell Division and Cancer Group, Centro Nacional de Investigaciones Oncológicas (CNIO), C/ Melchor Fernández Almagro, 3, E-28029, Madrid, Spain.*

jtamayo@imm.cnm.csic.es

Tumorigenesis induces actin cortex remodelling, which makes cancerous cells softer [1]. Cell deformability is largely determined by myosin-driven cortical tension and actin fibre architecture at the cell cortex [2]. However, it is still unclear what the weight of each contribution is, and how these contributions change during cancer development, and little attention has been paid to the effect of energy metabolism on this phenomenon and its reprogramming in cancer.
Here, we perform precise two-dimensional mechanical phenotyping based on power-law rheology to unveil the contributions of myosin II, actin fiber architecture and energy metabolism to the deformability of healthy (MCF-10A), non-invasive cancerous (MCF-7), and metastatic (MDA-MB-231) human breast epithelial cells. The results show marked differences in the nature of the active processes that build up cell stiffness, namely that healthy cells use ATP-driven actin polymerization whereas metastatic cells use myosin II activity. Non-invasive cancerous cells exhibit an anomalous behaviour, as their stiffness is not as affected by the lack of nutrients and ATP, suggesting that energy metabolism reprogramming is used to sustain active processes at the actin cortex.

References

[1] Salbreux, G., Charras, G. & Paluch, E., *Trends Cell Biol.* Actin cortex mechanics and cellular morphogenesis. (2012) 22, 536-545.
[2] Calzado-Martín, A., Encinar, M., Tamayo, J., Calleja, M. & San Paulo, A. *ACS Nano.* Effect of actin organization on the stiffness of living breast cancer cells revealed by peak-force modulation atomic force microscopy. (2016) 10, 3365-3374.

Figures

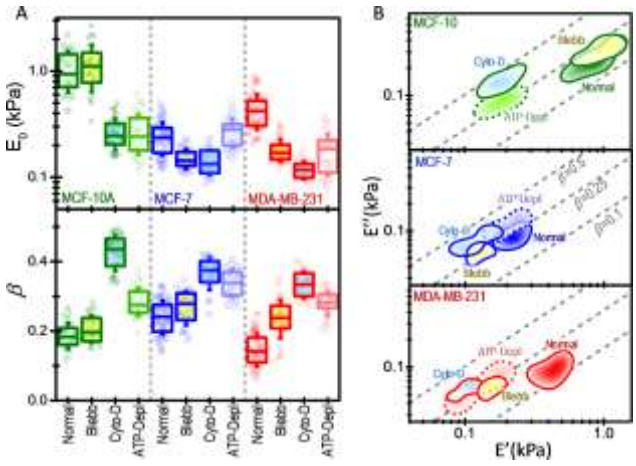


Figure 1: Power-law rheology parameters of the studied breast cell lines in normal conditions, treated with cytoskeletal drugs and in ATP-depletion conditions.

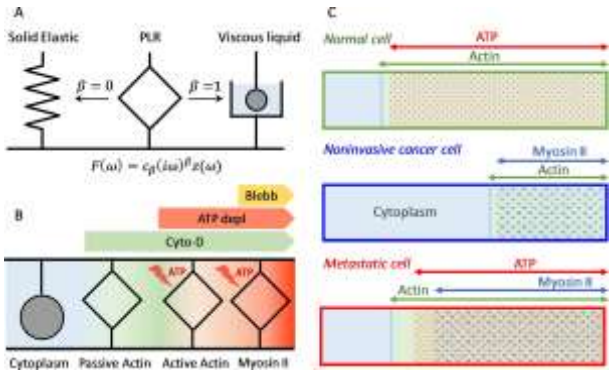


Figure 2: Sketch of uncoupling the effects of actin network, myosin II-driven contractility, and ATP hydrolysis on the cell stiffness.

Ultra-Sensitive High Dynamic Range Label Free Platform for Bioparticle Detection

Unai Ortiz-Orruño [1]
Jaime Ortega-Arroyo[1,2], Romain Quidant[1,2,3], Niek van Hulst[1,3], Matz Liebel[1]

[1]*ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain*
[2]*Nanophotonic Systems Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland*
[3]*ICREA-Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain*

unai.ortiz@icfo.eu

Scattering-based imaging has emerged as a suitable technique for detecting and tracking sub diffraction limited bioparticles with excellent resolution and sensitivity. Due to the intrinsically label-free nature of such scattering-sensors they have a large potential for imaging [1] and sizing bioparticles [2]. Albeit these advantages, this approach is intrinsically limited to quantifying nano-objects within a very narrow size-range which is due to the dramatic scattering-signal dependence on the particle size. This dependence drastically reduces its use due to the size heterogeneity of bioparticles.

Here, we present a microscope that is able to image heterogeneous size particles. Traditional microscopes are limited by their camera's single pixels dynamic range, as bright particles locally saturate the camera. Our platform, in contrast, employs all camera's pixels to acquire the signal of all the particles in the image all at once. Thus, the sum of the saturation limit of all pixels define our dynamic range, instead of individual pixels.

Our platform relies on off-axis interference of reciprocal-space representations of the images with a reference wave. Hence, we obtain interferograms that can be digitally processed for obtaining real-space intensity representations, which are equivalents of common images, albeit the dramatic increase in dynamic range. Additionally, we obtain the phase of the image, necessary for the use of digital holography tools. Therefore, we can computationally propagate and refocus the image, which allows single-shot 3D particle tracking and eliminates the need for mechanical focusing units thus dramatically reducing the sensors' cost.

I will show a pure scattering-signal quantification benchmark of 20 250 nm diameter gold nanoparticles as well as a size distribution chart showing the sizing and quantification of extracellular vesicles [3], probing its suitability for imaging heterogeneous biomolecules. Additionally, I will present some proof-of-concept experiments in which we characterize different nanoparticles by performing 3D nanoparticle tracking analysis (NTA), taking advantage of the phase retrieval and the digital holography tools.

References

[1] G. Young et al., "Quantitative mass imaging of single biological macromolecules," *Science (80-.).*, vol. 360, no. 6387, pp. 423–427, Apr. 2018.
[2] M. Liebel, J. T. Hugall, and N. F. Van Hulst, "Ultrasensitive Label-Free Nanosensing and High-Speed Tracking of Single Proteins," *Nano Lett.*, vol. 17, no. 2, pp. 1277–1281, 2017.
[3] U. Ortiz-Orruño, A. Jo, H. Lee, N. F. van Hulst, and M. Liebel, "Precise Nanosizing with High Dynamic Range Holography," *Nano Lett.*, vol. 21, no. 1, pp. 317–322, Jan. 2021.

Figures

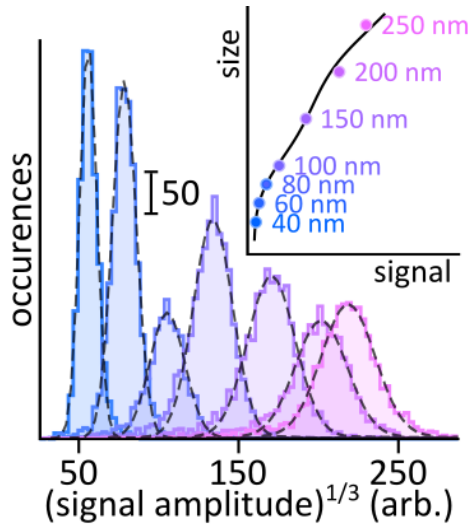


Figure 1: Dynamic range benchmark obtained by the quantification of different size gold nanoparticles scattering-signals

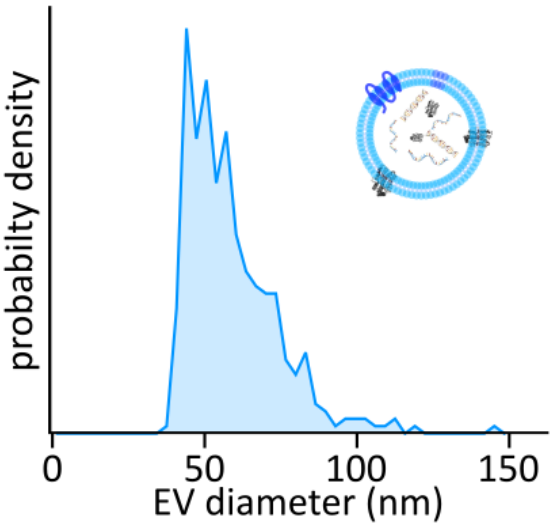


Figure 2: Obtained size distribution of different extracellular vesicles secreted by an ovarian cancer cell line

Gold-seeded lithium niobate nanoparticles as NanoZyme biosensors

Ana-María Pablo-Sainz-Ezquerra [1,3]
Rachael Taitt[1], Mathias Urbain[2], Florian Riporto[2], Sandrine Beauquis[2], Yannick Mugnier[2], Pyria Rose Divina Mariathomas[3], Rajes Ramanathan[3], Vipul Bansal[3], Yann Chevolot[4], Virginie Monnier[1]

[1]*Univ Lyon, Ecole Centrale de Lyon, CNRS, INSA Lyon, Université Claude Bernard Lyon 1, CPE Lyon, CNRS, INL, UMR5270, 69130 Ecully, France*
[2]*SYMME, Université Savoie Mont Blanc, 7 Chem. de Bellevue, 74940, Annecy, France*
[3]*RMIT, NanoBiotechnology Research Laboratory, Bowen Street, Melbourne, Victoria, 3000, Australia*
[4]*Univ Lyon, CNRS, INSA Lyon, Ecole Centrale de Lyon, Université Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69130 Ecully, France*
ana-maria.pablo-sainz-ezquerra@ec-lyon.fr

The need for a versatile, simple, fast and sensitive biosensor is crucial for environmental and health applications. Nowadays, enzyme-based assays in biosensing such as ELISA are one of the most used methods due to their high sensitivity and their selectivity. This sensing method basic principle relies on antigen-antibody interaction and the detection is carried out by an enzyme label, which generates a measurable colour product from a chromogenic substrate.[1] Initially, antibodies are fixed onto a solid surface support and they are incubated with the sample which contains the antigen. Subsequently, the antigen is bonded to an enzyme labelled antibody. The last step is the addition of the chromogenic substrate.[2] This method is simple as it is based on a colour change and presents high specificity. However, antibodies and enzymes are expensive and unstable in non-physiological conditions, and the experimental set up requires various steps.[3,4] To overcome these drawbacks, extensive research has been done to replace antibodies and enzymes for other recognition and detection elements.

Aptamers are molecular recognition elements based on single stranded DNA or RNA molecules which are generated by Systematic Evolution of Ligands by Exponential enrichment (SELEX).[5] Among the most remarkable advantages of aptamers over antibodies one can find, the cost reduction which is caused by the *in vitro* synthesis, the unlimited shelf-live, the ease of chemical modification and the relative stability in non-physiological conditions. Additionally, they present little or inexistent batch variation and reversible thermal denaturation.[6–10] SELEX method allows to diversify the targets of aptamer-based biosensors. Aptamers have successfully permitted the detection of a vast range of environmental and biological targets from metal ions to cells and bacteria and the development of various types of sensors.[8,10]

Nanoparticles which mimics enzyme activity are called NanoZymes. The high performance is achieved thanks to the high surface to volume ratio. Among them metal nanoparticles might be a solution. However unspecific aggregation remains a drawback. The immobilization of the metal nanoparticles on the oxide reduces the loss of performance related to this problem. This strategy allow one to to mimic the catalytic performance of enzymes.[11,12]

In addition, it produces a synergetic effect motivated by two complementary processes: a charge transfer between the materials and the creation of defects. This generates a hotspot for catalysis.[13,14] Since the pioneer work of Haruta et al.[15] gold nanoparticles deposited onto an oxide support has attracted lots of attention in catalysis in volatile organic compounds oxidation.

One can deposit directly metal nanoparticles onto the surface of the metal oxide, but the stability of the junction is not guaranteed. In addition, there is a lack of control on how the metal nanoparticles are distributed over the surface. Thus, to maximize the catalytic surface available, a link between the metal and the metal oxide can be introduced. Layer-by-layer method is a simple and rapid method to link the two types of nanoparticles.[16]

Exploiting this feature in peroxidase-mimics has already been investigated in hybrid nanoparticles composed of iron oxide-gold or cobalt oxide-gold.[17,18]

$LiNbO_3$ (LN) is one of the most versatile materials. Its non-centrosymmetric structure confers outstanding nonlinear optics, pyroelectric and piezoelectric properties which make it ideal for numerous applications in optics, batteries and optical communications.[19–21] At the nanoscale, LN NPs present low toxicity and lack of phase-matching conditions which makes it an excellent candidate for bio-imaging and photo-triggered drug delivery.[22,23]. Other features are the semiconducting properties and ferroelectricity which enhances catalysis

and photocatalysis, especially in redox reactions. These properties favour charge separation and polarization-induced facile adsorption of the species.[24]

We synthesized gold-coated lithium niobate nanoparticles with branched-polyethyleneimine as an intermediate linker between these two components.[25] We showed that the intrinsic peroxidase-mimic NanoZyme activity of gold nanoparticles is upgraded when they are deposited onto lithium niobate nanoparticles. We also probed that the presence of a link between the two nanomaterials was necessary to ensure maximum efficiency. In addition, we optimized the conditions to maximize the colorimetric response (pH, temperature, quantity and surface coverage). The subsequent addition of aptamers, which bind to the gold nanoparticles, quenches the enzyme-mimics which is restored in the presence of the target. We managed to successfully attach the aptamer and the optimization of the biosensing of antibiotics is being carried out.

References

[1] Y. Gao, Y. Zhou, R. Chandrawati, ACS Appl. Nano Mater. 3 (2020) 1–21.
[2] L. Zhan, W.B. Wu, X.X. Yang, C.Z. Huang, New J. Chem. 38 (2014) 2935–2940.
[3] D. Jiang, D. Ni, Z.T. Rosenkrans, P. Huang, X. Yan, W. Cai, Chem. Soc. Rev. 48 (2019) 3683–3704.
[4] A. Mohamad, H. Teo, N.A. Keasberry, M.U. Ahmed, Crit. Rev. Biotechnol. 39 (2019) 50–66.
[5] T. Kumar Sharma, R. Ramanathan, P. Weerathunge, M. Mohammadtaheri, H. Kumar Daima, R. Shukla, V. Bansal, Chem. Commun. 50 (2014) 15856–15859.
[6] G. Paniagua, A. Villalonga, M. Eguílaz, B. Vegas, C. Parrado, G. Rivas, P. Díez, R. Villalonga, Anal. Chim. Acta 1061 (2019) 84–91.
[7] P. Weerathunge, R. Ramanathan, V.A. Torok, K. Hodgson, Y. Xu, R. Goodacre, B.K. Behera, V. Bansal, Anal. Chem. 91 (2019) 3270–3276.
[8] J. Zhou, M.R. Battig, Y. Wang, Anal. Bioanal. Chem. 398 (2010) 2471–2480.
[9] J.O. Lee, H.M. So, E.K. Jeon, H. Chang, K. Won, Y.H. Kim, Anal. Bioanal. Chem. 390 (2008) 1023–1032.
[10] S. Song, L. Wang, J. Li, C. Fan, J. Zhao, TrAC - Trends Anal. Chem. 27 (2008) 108–117.
[11] Q. Gao, Y. Xing, M. Peng, Y. Liu, Z. Luo, Y. Jin, H. Fan, K. Li, C. Chen, Y. Cui, Chinese J. Chem. 35 (2017) 1431–1436.
[12] S. Zhang, H. Li, Z. Wang, J. Liu, H. Zhang, B. Wang, Z. Yang, Nanoscale 7 (2015) 8495–8502.
[13] N. Guijarro, M.S. Prévot, K. Sivula, Phys. Chem. Chem. Phys. 17 (2015) 15655–15674.
[14] S.M. Kim, H. Lee, J.Y. Park, Catal. Letters 145 (2015) 299–308.
[15] M. Haruta, N. Yamada, T. Kobayashi, S. Iijima, J. Catal. 115 (1989) 301–309.
[16] Y. Liu, Q. Kou, D. Wang, L. Chen, Y. Sun, Z. Lu, Y. Zhang, Y. Wang, J. Yang, S.G. Xing, J. Mater. Sci. 52 (2017) 10163–10174.
[17] Y. Lee, M.A. Garcia, N.A. Frey Huls, S. Sun, Angew. Chemie Int. Ed. 49 (2010) 1271–1274.
[18] J. Lu, H. Zhang, S. Li, S. Guo, L. Shen, T. Zhou, H. Zhong, L. Wu, Q. Meng, Y. Zhang, Inorg. Chem. 59 (2020) 3152–3159.
[19] D. Mohanty, G.S. Chaubey, A. Yourdkhani, S. Adireddy, G. Caruntu, J.B. Wiley, RSC Adv. 2 (2012) 1913–1916.
[20] R.S. Weis, T.K. Gaylord, Appl. Phys. A Solids Surfaces 37 (1985) 191–203.
[21] M. Niederberger, N. Pinna, J. Polleux, M. Antonietti, Angew. Chemie - Int. Ed. 43 (2004) 2270–2273.
[22] J. Vuilleumier, G. Gaulier, R. De Matos, Y. Mugnier, G. Campargue, J.P. Wolf, L. Bonacina, S. Gerber-Lemaire, Helv. Chim. Acta 103 (2020).
[23] D. Staedler, T. Magouroux, R. Hadji, C. Joulaud, J. Extermann, S. Schwung, S. Passemard, C. Kasparian, G. Clarke, M. Gerrmann, R. Le Dantec, Y. Mugnier, D. Rytz, D. Ciepielewski, C. Galez, S. Gerber-Lemaire, L. Juillerat-Jeanneret, L. Bonacina, J.P. Wolf, ACS Nano 6 (2012) 2542–2549.
[24] M.A. Khan, M.A. Nadeem, H. Idriss, Surf. Sci. Rep. 71 (2016) 1–31.
[25] R. Taitt, M. Urbain, Z. Behel, A.M. Pablo-Sainz-ezquerra, I. Kandybka, E. Millet, N. Martinez-Rodriguez, C. Yeromonahos, S. Beauquis, R. Le Dantec, Y. Mugnier, P.F. Brevet, Y. Chevolot, V. Monnier, Nanomaterials 11 (2021).

Acknowledgement

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 801512.

Figures

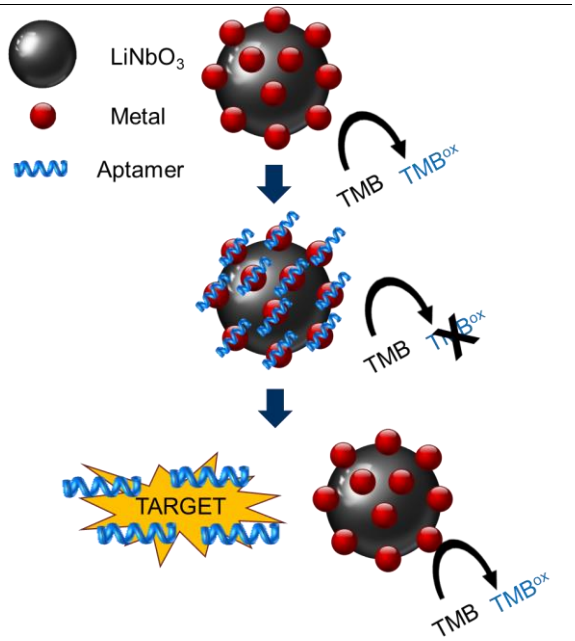


Figure 1: Gold-seeded lithium niobate based aptasensor. Mechanism of action.

Breath-level detection of hydrogen sulphide in humid air by arrays of gold nanoparticle-functionalized carbon nanotubes

Luis Antonio Panes Ruiz [1]
Leif Riemenschneider[1], Viktor Bezugly[2], Bergoi Ibarlucea[1], Gianaurelio Cuniberti[1]

[1]*Institute for Materials Science, Max Bergmann Center of Biomaterials, Technische Universität Dresden, Dresden 01062, Germany.*
[2]*Life Science Incubator Sachsen GmbH & Co. KG, Dresden 01307, Germany*
[3]*Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Dresden 01062, Germany*
luis_antonio.panes_ruiz@tu-dresden.de

During the past decade, the analysis of exhaled breath has been intensively considered as a non-invasive and cost-effective method for the precise identification of certain diseases [1]. For example, it has been previously demonstrated that increased concentrations of NH_3 can be correlated to kidney failure and *Helicobacter Pylori* infections [2]. Similarly, H_2S has been recently proposed as a marker for the precise identification of gastrointestinal diseases like irritable bowel syndrome (IBS) and small intestinal bacterial overgrowth (SIBO) [3]. Nevertheless, the high complexity of exhaled breath, containing over 3500 components, keeps representing a great challenge for emerging gas sensing technologies in terms of response time, sensitivity and selectivity.

In this context, we present the selective detection of low concentrations of H_2S gas in humid air and room temperature using a multichannel sensing platform based on semiconducting single-walled carbon nanotubes (sc-SWCNTs) functionalized with gold nanoparticles (AuNP). The platform consisted of 64 sensors individually addressed by a dedicated multiplexing system (Figure 1a). The electrodes we fabricated by standard UV-lithography and metal deposition techniques followed by the deposition of sc-SWCNTs using a controlled dielectrphoretic process (DEP). The nanotubes were then functionalized with gold nanoparticles (AuNP) using a potentiostatic electrodeposition technique achieving an average particle diameter of 60 nm and separation lengths of around 100 nm along the nanotube lattice (Figure 1b). AuNP-functionalized sensors demonstrated an increased and reproducible sensing performance to all tested H2S gas concentrations compared to non-functionalized sensors of 0.122 %/ppb and a calculated limit of detection of 3 ppb, similar to the odor threshold (Figure 1c and 1d). Furthermore, the sensors showed low cross-sensitivity to NH_3 and NO gases, also expected to be present in exhaled breath, as well as higher sensitivity and stability compared to commercial electrochemical-based gas sensors (AlphaSense, UK) [4]. These results suggest the potential application of our platform in the field of exhaled breath analysis.

References

[1] Zhou, X., et al. J. Mater. Chem. B, 8 (2020), 3231-3248.
[2] Panes-Ruiz, L.A., et al. ACS Sensors, 3 (2018), 79-86.
[3] Banik, G. D., et al. J. breath Res., 10 (2016), 026010.
[4] Panes-Ruiz, L.A., et al. Nano Res, (2021).

Figures

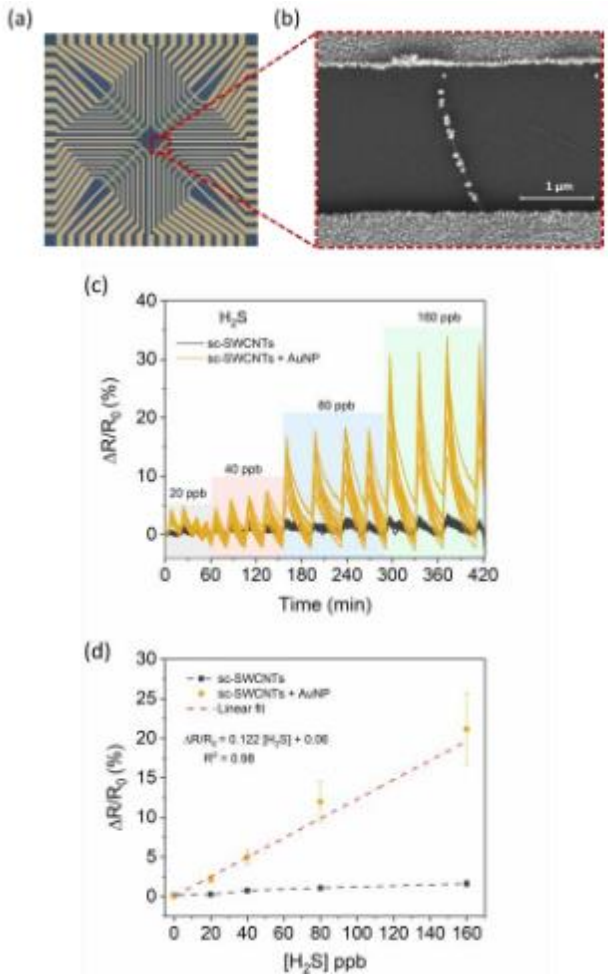


Figure 1: Multichannel gas sensing device. (a) Photographic image of microelectrodes on Si/SiO_2 wafer. (b) Scanning electron micrograph of aligned sc-SWCNT functionalized with AuNP. (c) Dynamic sensing response ($\Delta R/R_0$) of AuNP-functionalized and non-functionalized sensors to 20, 40, 80 and 160 ppb of H_2S gas in humid air (25% Rel. Humidity). (d) Average sensing response of AuNP- and non-functionalized sensors. [4]

A potential catalytic therapy in oncology: Cu-Fe Nanoparticles responsive to tumor microenvironment

Jesús Santamaría
Javier Bonet-ALeta, María Sancho-Albero, Javier Calzada, Silvia Irusta, M.Pilar Martín-Duque, Jose L. Hueso,

1) Department of Chemical and Environmental Engineering, Institute of Nanoscience and Materials of Aragon (INMA), University of Zaragoza; 2) Networking Research Center in Biomaterials, Bioengineering and Nanomedicine, CIBER-BBN; 3) Instituto Aragonés de Ciencias de la Salud

jesus.santamaria@unizar.es

Heterogeneous catalysis has emerged as a promising alternative for the development of new cancer therapies. Also, regarding the tumor microenvironment as a reactor with very specific chemical features has provided a new perspective in the search for catalytic nanoarchitectures with specific action against chemical species playing a key role in tumor metabolism. One of these species is glutathione (GSH), whose depletion is the cornerstone of emerging strategies in oncology, since this metabolite plays a pivotal regulatory role as antioxidant agent, dampening the harmful effects of intracellular reactive oxidative species (ROS). Herein, we present copper-iron oxide spinel nanoparticles that exhibit a versatile and selective catalytic response to reduce GSH levels while generating ROS in a cascade reaction. We demonstrate a clear correlation between GSH depletion and apoptotic death in tumor cells in the presence of the copper-iron nanocatalyst. Furthermore, we also provide a novel analytical protocol, alternative to state-of-the-art commercial kits, to accurately monitoring the concentration of GSH intracellular levels in both tumor and healthy cells. We observe a selective action of the nanoparticles, with lower toxicity in healthy cell lines, whose intrinsic GSH levels are lower, and intense apoptosis in tumor cells accompanied by a fast reduction of GSH levels.

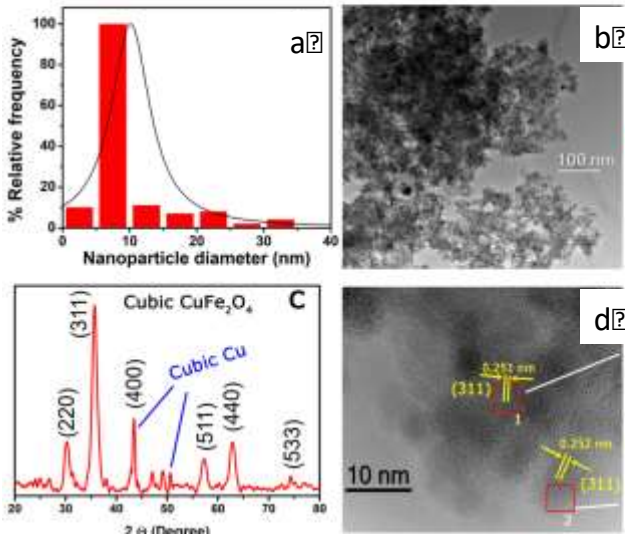


Figure 1: Characterization of Cu-Fe nanoparticles. a) Particle size distribution. b)Low magnification TEM image. c) XRD pattern showing a predominant cubic apinel phase of CuFe2O4 and a secondary phase of Cu. d) HRTEM images of CuFe nanoparticles

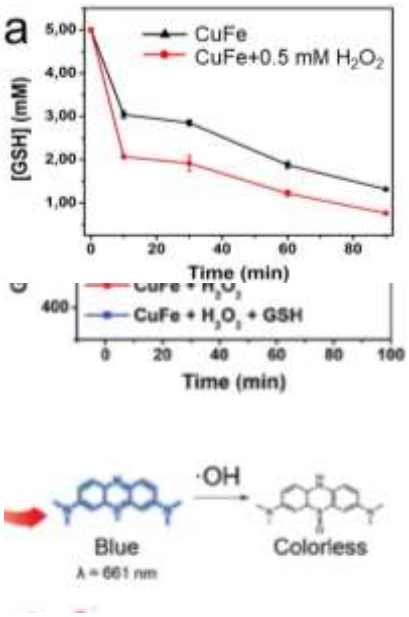


Figure 2: Starvation therapy: glutathione and glucose conversion under different reaction scenarios

nano-FTIR and correlation nanoscopy for organic and inorganic material analysis

Philip Schäfer,
Andreas J. Huber, Adrian Cernescu

Attocube (Germany)

philip.schaefer@neaspec.com

Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) is a scanning probe approach to optical microscopy and spectroscopy that achieves a spatial resolution below 20nm. s-SNOM exploits the strong confinement of light at the apex of a sharp metallic AFM tip to create a nanoscale optical hot-spot. Analysing the scattered light from the tip enables the extraction of the optical properties (dielectric function) of the sample directly below the tip, yielding nanoscale resolved optical images simultaneous to topography or local spectroscopic information about a specimens reflectivity and absorption in the infrared regime [1,2]. This allows direct material identification on the 10nm length scale.

In latest s-SNOM applications, the combined analysis of complex nanoscale material systems by correlating near-field IR spectra with information obtained in a wider spectral range (VIS to THz frequencies) has gained significant interest. For example, the material-characteristic nano-FTIR spectra measured for nanoscale Acetaminophen (Paracetamol) particles can be directly compared with nanoscale resolved tip-enhanced Raman spectra (TERS) obtained on the very same sample location [3]. Further, correlative measurements of the near-field optical response of semiconducting samples like Graphene (2D) or functional SRAM devices (3D) and Kelvin Probe Force Microscopy (KPFM) measurements reveal complementary quantitative information about the local conductivity in engineered nanostructures.

Consequently, s-SNOM systems have the potential to characterize complex material systems by different near-field and AFM-based methods at the nanoscale for a wide field of different applications, ranging from doped semiconductors, plasmonic wave-guides, 2D materials, metamaterials and polymeric and biological samples.

Recently, s-SNOM imaging and spectros-copy have been realized also at cryogenic temperatures [4].

References

[1] F. Keilmann, R. Hillenbrand, Phil. Trans. R. Soc. Lond. A (2004) 362, 787
[2] F. Huth, *et al.*, Nano Lett. (2012)12, 3973
[3] P. Kusch *et al*., J. Phys. Chem. C (2018) 122, 28, 16274
[4] W. Luo, *et al*. Nature Comm. (2019) 10, 2774

Figure

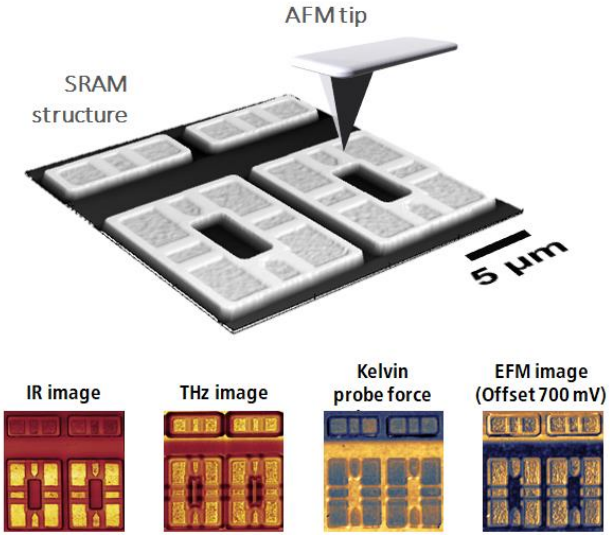


Figure: Correlation nanoscopy on SRAM sample, with optical IR and THz response as well as KPFM and EFM image.

Tumor-penetrating polymersomes encapsulating a novel anthracycline for cancer treatment

Lorena Simón-Gracia & Valeria Sidorenko
Ain Uustare, Ivan Ogibalov, Andrus Tasa, Olga Tshubrik, Tambet Teesalu.

Laboratory of Precision and Nanomedicine, Institute of Biomedicine and Translational Medicine, University of Tartu, Ravila 14b, 50411 Tartu, Estonia
Lorena.Simon.Gracia@ut.ee

Novel anticancer compounds and their precision delivery systems are actively developed to create potent and well-tolerated anticancer therapeutics. Tumour-penetrating peptides (TPPs) can be used to increase the accumulation and penetration of nanocarriers in the tumour [1]. We encapsulated a novel anthracycline, Utorubicin (UTO), which is more toxic to cultured tumour cell lines than doxorubicin, in biocompatible polymeric nanovesicles (polymersomes, PS) functionalized with TPPs [2]. Nanoformulated UTO reduced the viability of cultured malignant cells and this effect was potentiated by functionalization with the TPP. Systemic peptide-guided PS showed preferential accumulation in triple-negative breast tumour xenografts implanted in mice (Fig. 2A), and enhanced the UTO accumulation in tumour. Moreover, in an experimental treatment of mice with peritoneal carcinomatosis, UTO-loaded PS decreased the tumour growth after systemic administration (Fig. 2B). Our studies show the potential application of our novel UTO-loaded polymersomes in precision cancer therapy.

References

[1] Teesalu et al. Frontiers in Oncology, 216 (2013),1
[2] Simón-Gracia and Sidorenko et al. Angew. Chem. Int. Ed., 31 (2021), 17018

Figures

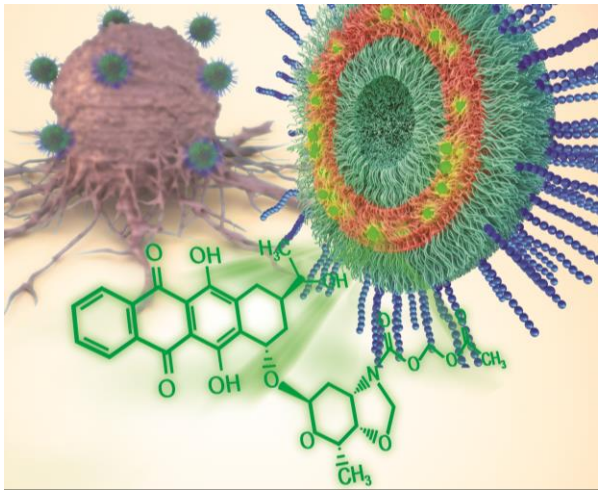


Figure 1: New anthracycline Utorubicin loaded in peptide-functionalized polymersomes for targeting solid tumours

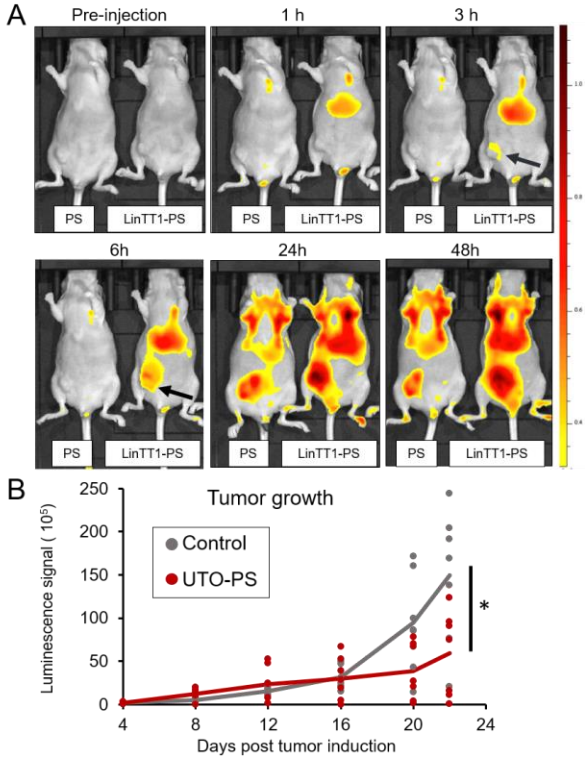


Figure 2: A) Peptide-guided polymersomes (LinTT1-PS) accumulated in triple-negative breast tumour xenografts. PS=untargeted polymersomes. **B)** UTO-loaded PS decreased the tumour growth in experimental treatment of peritoneal carcinomatosis

Striking Influence of Nickel Surface Changes on the Growth of Cobalt Nanostructures

Srdjan Stavrić[1,3]
Valeria Chesnyak[1,2], Mirco Panighel[2], Giovanni Comelli[1,2], Maria Peressi[1], Cristina Africh[2]

[1]*Physics Department, University of Trieste, via A. Valerio 2, Trieste 34127, Italy*
[2]*CNR-IOM, Laboratorio TASC, Trieste 34149, Italy*
[3]*Vinča Institute of Nuclear Sciences, University of Belgrade, M. Petrovića Alasa 12-14, Belgrade, Serbia*

sstavric@units.it

The influence of the carbide (Ni_2C) layer, formed on Ni(100) surface, on the growth of Cobalt (Co) nanostructures, is revealed via complementary scanning-tunneling microscopy (STM) measurements and the first-principles calculations [1]. On clean Ni(100) below 200°C, Co forms randomly distributed two-dimensional (2D) islands, while on Ni_2C three-dimensional (3D) two-atomic-layers thick islands are observed in STM images. We present a simple yet powerful model that elucidates the substantial differences in the Co growth mode on the two surfaces. On stepped surfaces, the observed formation of jagged step decoration of Ni_2C, not visible on Ni(100), is explained by the sharp differences in the mobility of Co atoms in the two cases. With the increase of temperature, the dissolution process starts and finally STM scanning of Ni(100) surface at 250°C revealed almost no remaining Co, whereas some Co islands are still being visible on Ni_2C surface up to 300°C. Computational results corroborated the ability of Co to persist on the Ni_2C surface up to higher temperatures and suggested a vacancy-assisted model for its dissolution in Ni(100). The methodology presented here systematically combines the STM measurements with the first-principles calculations and computational modeling, thus opening the new route towards the selective modification of metallic surfaces through the deposition of metal atoms of another species and the control of temperature.

References

[1] V. Chesnyak, S. Stavrić, M. Panighel, G. Comelli, M. Peressi, C. Africh, to be submitted

Figures

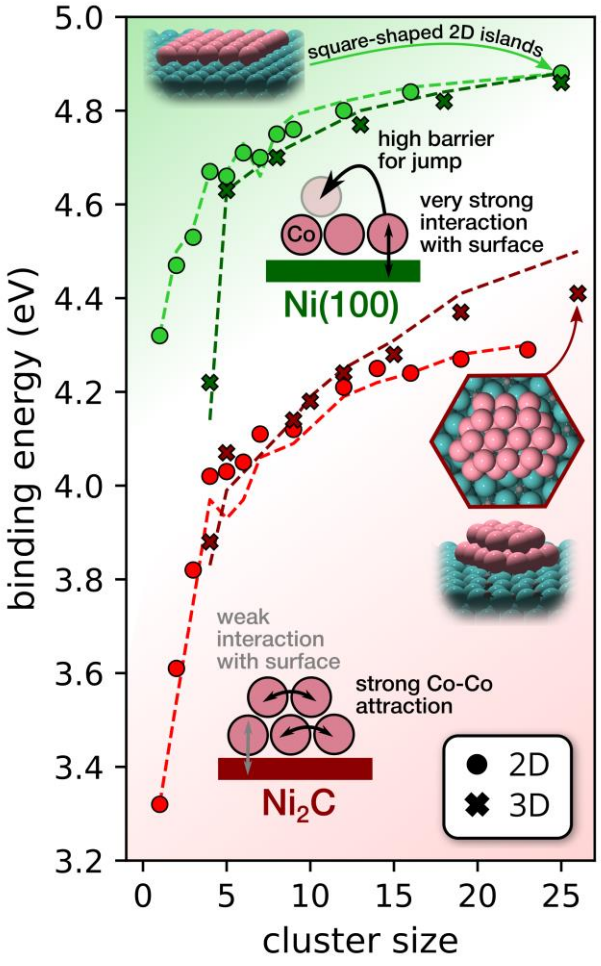


Figure 1: Binding energy of Co clusters up to ~25 atoms in size calculated directly by DFT (circles and crosses) fitted to the estimate from the model (dashed lines). In the inset the schematic representation of the important players that determine the shape of Co nanostructures on each surface together with the most stable structures with ~25 atoms are depicted.

Reduction of the Thermal Conductivity by the Nanostructuration of Electrodeposited CuNi Alloys

Cristina V. Manzano[1,2*], Olga Caballero-Calero[1], Maxime Tranchant[2], Enrico Bertero[2], Pablo Cervino-Solana[1], Marisol Martín-González[1], Laetitia Philippe[2]

[1] Instituto de Micro y Nanotecnología, IMN-CNM, CSIC (CEI UAM+CSIC) Isaac Newton, 8, E-28760, Tres Cantos, Madrid, Spain

[2] Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Feuerwerkerstrasse 39, CH-3602 Thun, Switzerland

cristina.vicente@csic.es

The application of inexpensive and scalable materials in the industry for thermoelectric applications has received great interest, such as CuNi alloys in the last ears. Nanocrystalline CuNi alloys with different compositions were grown by pulsed electrodeposition reducing the crystallite size of the CuNi down to 30-40 nm by the incorporation of saccharine in the electrolyte [1]. The thermoelectric properties, such as electrical conductivity, Seebeck coefficient, and thermal conductivity of these nanocrystalline alloys, were studied. The maximum figure of merit at room temperature obtained was (6.4 ± 1.5) $\cdot 10^{-2}$ for nanocrystalline $Cu_{0.65}Ni_{0.35}$. The thermal conductivity of CuNi alloys was reduced by the nanostructuration to a value of 9.0 ± 0.9 W/m·K, making these nanocrystalline CuNi alloys more competitive than other more classical thermoelectric materials [2]. This work opens a new field to be investigated, that can be described as the use of commercial alloys such as CuNi for thermoelectric applications, and shows the use of a new approach to enhance the thermoelectric properties of inexpensive and/or fewer pollutant materials.

References

[1] Cristina V. Manzano, Patrik Schürch, Laszlo Pethö, Gerhard Bürki, Johann Michler, and Laetitia Philippe, *Journal of The Electrochemical Society*, 166 (10), (2019) E1-E7 (2019).

[2] Cristina V. Manzano, Olga Caballero-Calero, Maxime Tranchant, Enrico Bertero,Pablo Cervino-Solana, Marisol Martin-Gonzalez and Laetitia PhilippeJ. Mater. Chem. C, 9 (2021) 3447.

Figures

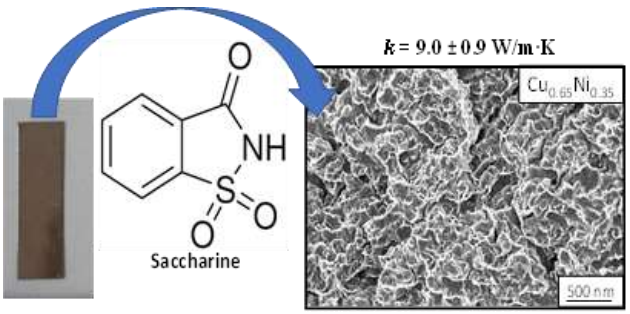


Figure 1: The thermal conductivity of CuNi alloys is reduced by the nanostructuration.

Fe_3O_4 Nanoparticles Embedded in Phase Change Materials

A. Baron[1], A. M. Goitandia[2], C. Monteserín[2], K. Vidal[2], M. Blanco[2], I. Castellanos-Rubio[1], M. Insausti[1].

[1]*Dept. Organic and Inorganic Chemistry, Faculty of Science and Thecnology,UPV/EHU, Leioa 48940, Spain.*
[2]*Surface Chemistry and Nanotechnologies, BRTA, Tekniker, Eibar 20600, Spain.*

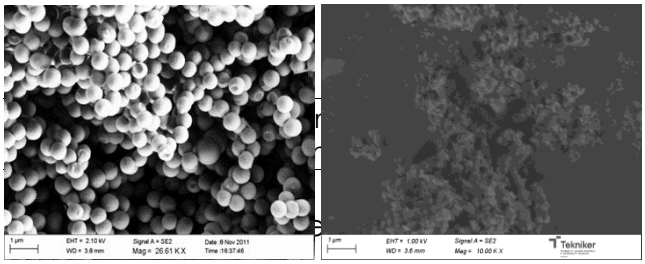
ander.baron@ehu.eus

Phase change materials (PCMs) have the ability to release and absorb large amounts of thermal energy during their isothermal phase change. Because of this, they are able to store and release energy as heat and maintain stable temperatures, so they find their application in electronics, clothing and construction sector [1]. According to the material which releases the heat, PCMs can be categorized in organic compounds, hydrated salts and eutectic compounds, being paraffin waxes (n-alkanes) the most suitable ones, due to their high heat storage capacity, little overcooling, little volume change, good chemical and thermal stability, low vapor pressure, little corrosion of the storage vessel and low toxicity. However, they can suffer from liquid leakage, which limits their application. Proper encapsulation of PCMs using organic or inorganic supporting materials could be an effective way to overcome these kind of problem [2].

In different electronic devices, electromagnetic radiation and heat are released. Magnetic PCMs could alleviate these drawbacks due to their latent heat and electromagnetic shielding, as well as being able to be controlled by a magnetic field [3]. The aim of the present work would be to achieve a system of encapsulated organic PCMs containing magnetic nanoparticles (MNPs).

For this purpose, we have prepared NPs of magnetite, Fe_3O_4, as they have become the formulations preferred by the industry, due to their low toxicity and modulable magnetic response by two different routes. From precipitation in basic medium superparamagnetic ones (SPM-NPs) with sizes less than 20 nm and with no remanent magnetization have been obtained and ferromagnetic nanoparticles (FM-NPs), greater than 20 nm, with non-fluctuating magnetic moment and remanence, have been prepared by thermal decomposition of a metallo-organic precursor of iron(III) oleate. Both kinds of MNPs have been characterized by X-ray diffraction and transmission electron microscopy and their magnetic behavior has also been analyzed.

Both kind of MNP have been employed for the preparation of magnetic encapsulated PCMs, using a sol-gel method, in which hexadecane with a 0.5 – 5 % (in weight) Fe_3O_4 dispersion of NPs has been successfully encapsulated in silica spheres (Fig. 1).



The contents of PCM vary in the 55 – 76 % range and the size of the microcapsules obtained are around 50 μm. Magnetic measurements of the PCMs with embedded MNPs leads to the estimation of the amount of NPs loaded in the PCMs.

References

[1] Zhu, Y. et al, Energy Conversion and Management, 119 (2016) 151-162.
[2] Bourne, S., Novoselac, A., Building and Environment, 98 (2016) 133-144.
[3] Sangphil, P., Colloids and Surfaces A: Physicochem. Eng. Aspects, 450 (2014) 46-51.

Analysis and production of dsRNA-layered double hydroxides nanocomposites for plant protection

J. Delgado Martín[1]
L.J. Alemany[2], C. Herrera[2], S. Molina-Ramírez[2], L. Ruiz[3], D. Janssen[3] & L. Velasco[1]

[1]*IFAPA Centro de Málaga, 29140 Málaga, Spain*
[2]*Departamento de Ingeniería Química, Universidad de Málaga, 29071 Málaga, Spain*
[3]*IFAPA Centro La Mojonera, 04745 Almería, Spain*
leonardo.velasco@juntadeandalucia.es

Layered double hydroxide (LDH) nanoparticles are an increasingly popular tool in biomedical applications as carriers of drugs, chemicals or nucleic acids [1], and have recently been proposed for the control of plant pathogens by RNAi [2]. We are considering LDHs as carriers of viral-derived dsRNAs for the control of virus diseases in vegetable crops, as alternative to traditional breeding or transgenic development. For that, we have developed tools and protocols for *in vitro* and *in vivo* synthesis of specific dsRNAs in addition to the standardized synthesis of LDH nanoparticles. Binding conditions were optimized and the loading capacity of LDHs for dsRNAs was determined. In addition, physical-chemical characterization and microscopy of the particles and nanocomposites was performed by using RAMAN, EDX, IR, Z-potential, PDi, PI, and TEM spectroscopy, among other tools.
dsRNAs (about 500 bp) derived from two genes of each of the cucurbit-infecting viruses *Cucumber green mild mottle virus* (CGMMV) and *Tomato leaf curl New-Delhi virus* (ToLCNDV) have been obtained. LDH nanoparticles were produced by Al-Mg coprecipitation (1: 3). TEM allowed the determination of the particle size, averaging 100 nm, and their structure was found to be laminar hexagonal shapes, characteristic of these nanoparticles. Binding of the dsRNAs to the LDH was performed and the LDH binding ratio of LDH with respect to dsRNA resulted 15: 1 (w/w). dsRNAs seem to attach electrostatically to the laminar LDHs and does not intercalate between sheets.

References

[1] Arrabito G., Bonasera A., Prestopino G. et al., Crystals, 9 (2019).
[2] Fletcher S.J., Reeves P.T., Hoang B.T., Mitter N., Frontiers in Plant Science, 11 (2020).

Figures

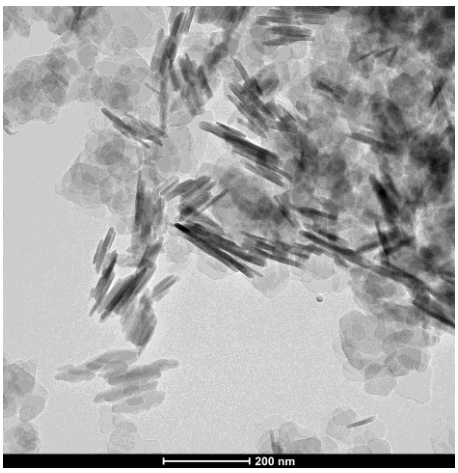


Figure 1: TEM of Mg-Al layered double-hydroxides.

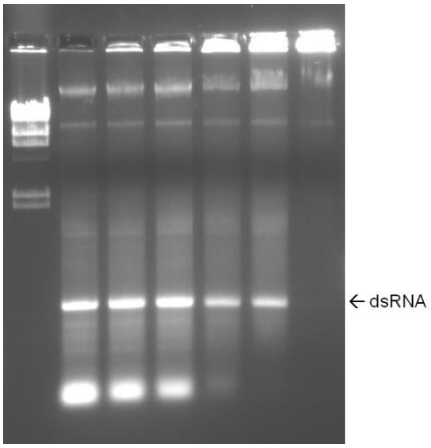


Figure 2: Loading of dsRNA-enriched nucleic acid samples with increasing amounts of LDH in 1% agarose gels stained with RedSafe. LDH-dsRNA nanocomposites do not migrate in electrophoresis.

Breathable Nano-coated Waterproof Functional Textile Surfaces for Wound Dressing Applications

Yüce Denizli
Mustafa Karaman
Serdar Murat Cam

KORTEKS, OSB Sari Cd. No.3, Bursa, Turkey
Konya Technical University

yuce.denizli@zorlu.com

In recent years, studies on the functionalization of conventional textile surfaces have become widespread. Particularly in medical applications, there are considerable studies on wound dressings. In this study, plasma enhanced chemical vapor deposition (PECVD) was used for hydrophobic surface-functionalization of raw textile surfaces. PECVD is a one-step and all-dry polymer coating technique, in which energetic particles generated during the plasma discharge start the polymer coating reactions. For the top layer of a wound dressing surface, it should be waterproof to protect the wound from contaminated fluids and risk of infection. In addition, the structure should have air permeability and water vapor transmission, as well as good mechanical and thermal performance for comfortable wearing. Within this scope, PECVD nanoscale functional coating technique is used for antibacterial and waterproof effect and biocompatible multi channeled poly lactic acid (PLA) yarns for enhanced air and vapor permeability. In the experiments, hydrophobic monomer vapors were delivered to system until the desired pressure is reached. Next, plasma source was turned on to generate a plasma discharge of monomer. The effects of plasma power and the pressure on the morphology and structure of the coated filaments were studied. Figure 1 summarizes the functional monomers deposited on PLA surfaces in this study. The behavior of the liquids with different properties on the waterproof surface obtained after the study is as in Figure 2.

References

Figures

Monomer	Polymer	Function
Perfluoro decyl acrylate	Poly(Perfluoro decyl acrylate)	Hydrophobic
Hexa florobutyl acrylate	Poly(Hexafloro butyl acrylate)	Hydrophobic
Dimethyl aminoethyl methacrylate	Poly(Dimethylamino) ethylmethacrylate)	Antibacterial

Figure 1: Functional monomers used in this study

Figure 2: The behavior of the liquids with different properties on the standard and waterproof surface

Ferroelectric Oxide/Halide Perovskite heterojunctions: application as solar cells and solar transistors

Saptam Ganguly[1]
Haibing Xie[1], Amador Perez-Tomas[1], Maria Lourdes Calzada[2], Anders Hagfeldt[3], Mónica Lira-Cantu[1]*.
1 Catalan Institute of Nanoscience and Nanotechnology and The Barcelona Institute of Science and Technology (BIST), Edifici ICN2, Campus of the UAB, Barcelona, Spain -08193
2 Instituto de Ciencia de Materiales de Madrid, ICMM-CSIC. C / Sor Juana Inés de la Cruz 3, 28049, Cantoblanco, Madrid, Spain
3 Laboratory of Photonics and Interfaces, Institute of Chemical Sciences and Engineering, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

monica.lira@icn2.cat

Metal halide perovskite materials exhibit exceptional performance characteristics for low-cost optoelectronic applications[1] . State-of-the-art halide perovskite solar cells (PSCs) employ semiconductor oxides as electron transport layers (ETL) for example, TiO_2[2][3][4]. This oxide, under UV irradiation and Oxygen, directly affects the stability of the solar cells, owing to the defects such as Oxygen vacancies (O_{vac}). In this work, we demonstrate the application of Ferroelectric oxides such as $PbZrTiO_3$ (PZT) and $BiFeO_3$ (BFO), as the electron extraction material in halide perovskite solar cells. The application of a bias voltage (poling) up to 2 V, under UV light, is a critical step to induce charge transport in these materials[5]. For PZT, champion cells result in power conversion efficiencies of ~13% after poling. Stability analysis, carried out at 1-sun AM 1.5 G, including UV light in air for unencapsulated devices, shows negligible degradation for hours[6]. For BFO, the solar cells reach a maximum efficiency of around 4 % which is the highest efficiency reported up to date for this type of devices. For BFO, the stability analyses carried out inside a nitrogen chamber under continuous light irradiation at 1 sun show reversible switching properties with a typical T_{80} (time at which it reached the 80 % of the initial efficiency) of around 180 mins. Our results were supported by characterization analysis with XRD, XPS, AFM, IPCE, UV-vis spectroscopy, photoconductivity techniques apart from J-V curves. In conclusion, we introduced ferroelectric oxides as ETL and successfully incorporated into solar cells, giving better UV and moisture stability for PZT based solar cells compared to BFO based solar cells. The switching property of our devices permits also their application as solar transistors, which is a step forward applications in self-power electronics for the future IoT [7].

References

[1] J. S. Manser, J. A. Christians, P. V. Kamat, *Chem. Rev.* **2016**, *116*, 12956–13008.
[2] A. Mingorance, et al., *Adv. Mater. Interfaces* **2018**, *5*, 1.
[3] M. Coll, et al.,. *Appl. Surf. Sci.* **2019**, *482*, 1.
[4] A. Pérez-Tomás, et al, In *The Future of Semiconductor Oxides in Next-Generation Solar Cells*; Elsevier, **2018**; pp. 267–356.
[5] A. Pérez-Tomas,et al, *Sustain. Energy Fuels* **2019**.
[6] M. Lira-Cantú, *Nat. Energy* **2017**, *2*, 1.
[7] A. Pérez-Tomás, et al., *Adv. Funct. Mater.* **2018**, *28*, 1707099.

Figures

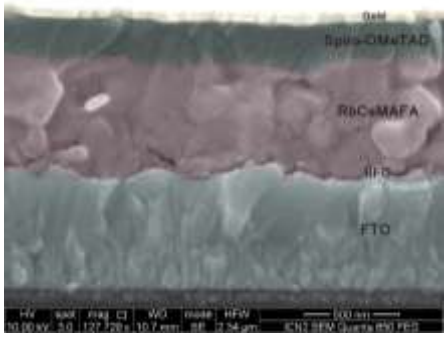


Figure 1: Cross-sectional SEM view of a typical Perovskite solar cell applying the BFO as the electron transport layer.

Fabrication and characterization of ThMn12-type compounds for applications as permanent magnets

Andrés García-Franco
James J. Rosero, Bosco Rodríguez-Crespo, Paula G. Saiz, Jorge Lago, Daniel Salazar

BCMaterials, Bld. Martina Casiano, 3rd. Floor, UPV/EHU Science Park, Barrio Sarriena s/n, 48940 Leioa, Spain

andres.garcia@bcmaterials.net

The growing interest in searching novel magnetic materials for permanent magnet applications is related to the key role they play in the energy efficiency of electrical motors, wind turbines or hard disk drives.

Among others, NdFeB, SmCo5 and similar alloys are the most commonly employed for permanent magnet applications. However, their high content of critical raw materials (CRM), as rare earth elements or Co, motivates the scientific community to explore and find novel eco-friendly materials for that applications. In this context, one of the preferred are the magnetic materials based on the ThMn12-type structure which present a lower amount of CRM and are considered a suitable material to replace the commercial ones due to its high performance.

In this work, three ThMn12-based samples with compositions: $Sm_{1.2}Fe_{11}Si_{0.5}Mo_{0.5}$, $Sm_{1.2}Fe_{11.3}B_{0.2}Mo_{0.5}$ and $Sm_{1.2}Fe_{11.1}B_{0.4}Mo_{0.5}$ were synthesized by arc-melting in order to investigate the effect of the Si and B additives on their properties. Moreover, ribbons of these alloys were fabricated by melt-spinning in order to investigate the extrinsic properties. Magnetic properties of all the samples were evaluated in terms of anisotropy field, Curie temperature, coercive field, remanence and saturation magnetization via VSM, while the crystalline structure was determined by XRD patterns. Elemental mapping and surface topography were also investigated by SEM/EDX and AFM, respectively. This study demonstrates that hard magnetic alloys with the 1:12 structure and Si and B additives are good candidates for permanent magnet applications.

References

[1] L.E.Z. Alfonso, J.S.T. Hernandez, D.Salazar, G.A.P. Alcázar, Effect of Nitrogenation on the Intrinsic Magnetic Properties of the Compounds (Nd1 −x Cex)1.1Fe10CoTi, 56 (2020).

[2] A. Martin-Cid, D. Salazar, A.M. Schönhöbel, J.S. Garitaonandia, J.M. Barandiaran, G.C. Hadjipanayis, Magnetic properties and phase stability of tetragonal Ce1- SmxFe9Co2Ti 1:12 phase for permanent magnets, J. Alloys Compd. 749 (2018) 640–644. doi:10.1016/j.jallcom.2018.03.325.

[3] D. Salazar, A. Martín-Cid, J.S. Garitaonandia, T.C. Hansen, J.M. Barandiaran, G.C. Hadjipanayis, Role of Ce substitution in the magneto-crystalline anisotropy of tetragonal ZrFe10Si2, J. Alloys Compd. 766 (2018) 291–296. doi:10.1016/j.jallcom.2018.06.225.

Imaging microviscosity in mesenchymal stem cells and their differentiated counterparts using a viscosity-sensitive molecular nanorotor and FLIM

Džiugas Jurgutis[1,2]
Greta Jarockytė[1], Aurimas Vyšniauskas[2], Vitalijus Karabanovas[1,2,3], Ričardas Rotomskis[1,4]

[1]*Biomedical Physics Laboratory, National Cancer Institute, P. Baublio str. 3b, Vilnius, Lithuania*
[2]*State research institute Center for Physical Sciences and Technology, Saulėtekio av. 3, Vilnius, Lithuania*
[3]*Department of Chemistry and Bioengineering, Vilnius Gediminas Technical University, Saulėtekio av. 9-III, Vilnius, Lithuania*
[4]*Biophotonics group of Laser Research Centre, Vilnius University, Saulėtekio av. 9, Vilnius, Lithuania*

dziugas.jurgutis@nvi.lt

Changes in microscopic viscosity (microviscosity) signal about the ongoing intracellular alterations or the onset of various diseases, e.g. diabetes or atherosclerosis [1]. Imaging microviscosity before and after differentiation would enable a greater understanding of the differentiation mechanism and a more accurate characterization of stem cells, e.g. mesenchymal stem cells (MSC), which are able to differentiate into fat, bone or other connective tissue. Microviscosity bioimaging can be achieved by utilising molecular nanorotors with fluorescence lifetime imaging microscopy (FLIM) [1,3]. In this work, we utilise BDP-H molecular nanorotor (Figure 1). In low-viscosity environments, intramolecular rotation of BDP-H meso-phenyl ring is unhindered, and the relaxation from the excited state primarily occurs through a non-radiative energy transition leading to a shorter fluorescence (FL) lifetime. In more viscous environments, the rotation is restricted and energy is released through a radiative decay, thus resulting in longer FL lifetime [1,2]. The aim of our study was to determine intracellular localization of BDP-H and to apply the molecular nanorotor for microviscosity determination in live human skin MSC and their differentiated cultures – adipocytes and osteoblasts. Live cells were imaged with a confocal laser scanning microscope. FL lifetimes of BDP-H in live MSC were determined using time-correlated single photon counting based FLIM. Localisation experiments showed that BDP-H accumulates in lipid droplets (LD) and cytosol of live MSC (Figure 1A). In addition, BDP-H intensely accumulates in enlarged LD of adipocytes, while in osteoblasts, cytosolic staining is more pronounced. Finally, by using a calibration curve obtained in toluene-castor oil mixtures of known bulk viscosities, and the τ_1 of BDP-H decays obtained with FLIM (Figure 1B), we were able to assign microviscosities values of ca. 120 cP and 104 cP to LD of undifferentiated MSC and mature adipocytes, respectively.

References

[1] Kuimova, M.K., Physical Chemistry Chemical Physics, 14 (2012) 12671-12686.
[2] Toliautas, S. et al., Chemistry – A European Journal, 25 (2019) 10342-10349.
[3] Vyšniauskas, A. & Kuimova, M.K., International Reviews in Physical Chemistry, 37 (2018) 259-285.

Figures

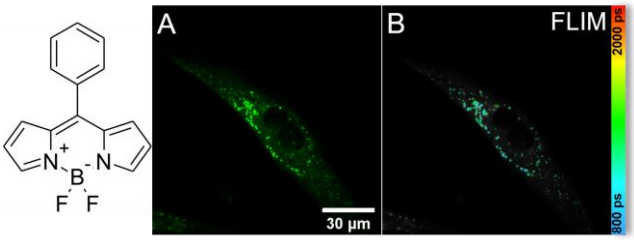


Figure 1: Structure of the BDP-H molecular nanorotor and its accumulation in lipid droplets of MSC (A). B – FLIM image obtained by applying a biexponential fit (τ_1 = 871±3 ps, mean lifetime – 1215±4 ps) (λ_{ex} = 490±5 nm).

Acknowledgements: supported by the Research Council of Lithuania, Grant No. S-MIP-19-6.

Modelling the interaction between graphene surfaces and metallic nanoclusters

Isabel Lado-Touriño
Arisbel Cerpa Naranjo
Mariana P. Arce

School of Architecture, Engineering and Design, Universidad Europea de Madrid, c) Tajo s/n, 28670 VIllaviciosa de Odón (Spain

misabel.lado@universidadeuropea.es

Abstract

The overuse of antibiotics has led to the flourishment of antibiotic-resistant bacteria [1] and consequently to the need to develop new, more efficient pharmacological compounds. Several advanced materials are being studied, among which are metallic nanoparticles and certain graphene oxides (GO) modified with polyethylene glycol (PEG) [2-4]. In this work, molecular dynamics (MD) simulations of the adsorption of small Ag and Cu clusters on pristine graphene and PEGylated graphene oxide (GO_PEG) surfaces were carried out. The results are presented as a function of nanoparticles concentration, adsorption energies, mean equilibrium distances between nanoparticles and graphene surfaces (figure 1), radial distribution functions and diffusion coefficients of the metallic nanoclusters. These preliminary results show that PEGylation of the surface is critical to strengthen the interaction between the surfaces and the metallic clusters, which, in turn, is a key factor for improving the efficacy of these compounds.

References

[1] P. Spigaglia, Therapeutic Advances in Infectious diseases, vol. 3 (2015) 23-42
[2] B.K Kim, Y.L. Jo Hu, J.J Shim, Supercrit. Fluids 72 (2012) 28-35
[3] J. Li, G. Wang, H. Zhu, M. Zhang, X. Zheng, Z. Di, X. Liu, X. Wang, Sci. Rep. 4 (2014) 4359
[4] J. Chen, H. Peng, X. Wang, F. Shao, Z. Yuan, H. Han, Nanoscale 4 (2014) 1879–1889

Figures

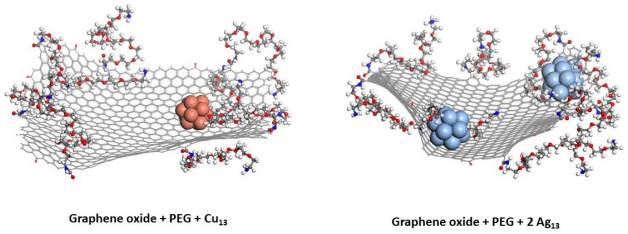


Figure 1: Final position of one Cu_{13} cluster and two Ag_{13} clusters on a PEGylated graphene oxide surface after 3 ns of simulation time.

Polymer-based nanocomposite materials, catalytic and photocatalytic applications

Angel Leiva[1]
Oscar Ramirez[1], Alexander Córdoba[1], Cesar Saldias[1], Marcela Urzúa[2].

[1]*Pontificia Universidad Católica de Chile, Vicuña Mackenna 4860 Macul, Santiago, Chile.*
[2]*Departamento de Química, Facultad de Ciencias, Universidad de Chile, Santiago, Chile*

aleivac@uc.cl

Abstract
Hybrid nanocomposites based on polymers containing catalytic and photocatalytic nanoparticles in different formats have been obtained. Herein, three examples corresponding to, powder, thin films and nanofibers, are included.
Chitosan-based nanocomposite materials containing different amounts of gold nanoparticles were prepared as powder and thin films. The powder was obtained in solid phase by a thermal process, while the thin films were obtained by a wet chemistry method (Fig.1). In both cases, the materials were tested as catalysts in the reaction the reduction of 4-nitrophenol (4NP) to 4-aminophenol (4AP) as model reaction.
Additionally, nanofibers of chitosan and polycaprolactone mixtures (C-PCL), containing photocatalytic TiO_2 nanoparticles (Fig. 2), were obtained and tested in the photochemical decomposition of rhodamine B in water. The hybrid materials were designed and produced taking advantage of the special characteristics of chitosan biopolymer and the biodegradable poly ester PCL.

Acknowledgements: The authors thank to projects FONDECYT N°1211124 and FONDAP N°15110019.

References

[1] O. Ramirez, S. Bonardd, C. Saldías, D. Radic, A. Leiva, ACS Appl. Mater. Interfaces, 9, (2017) 16561-16570.

[2] S. Bonardd, C. Saldías, O. Ramírez, D. Radić, F. J. Recio, M. Urzúa, A. Leiva, Carbohydrate Polymers 207 (2019) 533–541534

Figures

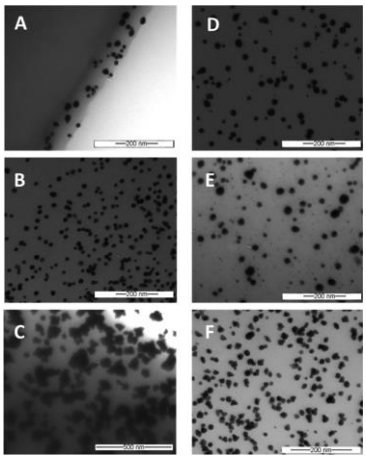


Figure 1: A- TEM images of gold-chitosan nanocomposite films obtained from immersion into different KAuCl4 solutions. (a, d) 5%, (b, e) 10%, and (c, f) 20% of $KAuCl_4$ and reduced with hydrazine (left side) and L-ascorbic acid (right side).

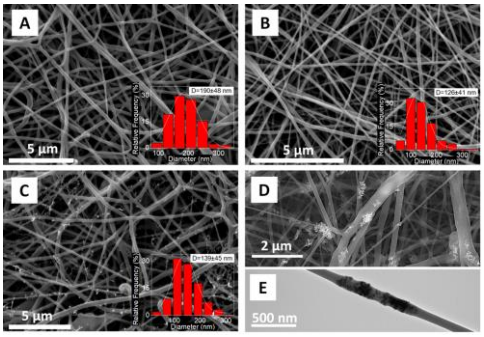


Figure 2: SEM micrographs of electrospun mats. A) PCL, B) PCL-CS, C) PCL-CS-TiO_2TX. Insets show the corresponding fiber diameter distribution. (D) SEM Imagen of PCL-CS-TiO_2TX mat without being coated in gold. (E) Imagen TEM of a single fiber of PCL-CS-TiO2TX.

Bioinspired nanoparticles as trastuzumab and paclitaxel targeted carrier for HER2-positive breast cancer treatment

Eva M. Martín del Valle
Celia Nieto, Milena A. Vega

University of Salamanca, Plaza de los Caídos s/n, Salamanca, Spain

emvalle@usal.es

Abstract

HER2-overexpression has long been associated with a worse prognosis for patients suffering from breast cancer. However, this overexpression has also allowed the development of targeted anti-HER2 agents that have remarkably improved patient outcomes, like trastuzumab, whose administration, along with taxanes, has notably increased the overall survival rate of this disease. Nevertheless, both trastuzumab and the taxanes, have significant side toxicity, and the apparition of resistances to them is frequent [1,2]. In this way, in other to overcome these drawbacks, a drug targeted nanovehicle made up of polydopamine nanoparticles (PDA NPs) (180 nm) was developed in the current work to transport both paclitaxel (PTX) and trastuzumab (Tmab). Since PDA has strong ability to load drugs [3,4], the mentioned taxane and antibody could be directly incorporated to the NPs synthesized. Besides, Tmab was also covalently bound to PDA NPs by means of the carbodiimide chemistry to compare the results obtained following both loading strategies. The effectiveness and selectivity of the NPs obtained were validated *in vitro* with different human HER2-overexpressing tumour and normal cells. They proved to have more noticeable antitumour activity than a nanosystem previously developed for the transport of PTX and Tmab and, in addition, to be more selective than the parent drug. Moreover, loaded PDA NPs, which were capable of highly increasing the number of apoptotic HER2-positive breast cancer cells upon administration, maintained their therapeutic activity when validated in HER2-overexpressing breast tumour spheroids. Thus, this novel Tmab and PTX nanocarrier may represent a great approach to reduce the severe side effects of the HER2-positive breast cancer therapies that already exist, while reducing the probability of the apparition of treatment resistances.

References

[1] C. Nieto, M.A. Vega, E.M. Martín del Valle, Nanomaterials, 10, (2020), 1674

[2] C. Nieto, A. Centa, J.A. Rodríguez-Rodríguez, A. Pandiella, E.M. Martín del Valle, Nanomaterials, 9, (2019), 948

[3] C. Nieto, M.A. Vega, G. Marcelo, E.M. Martín del Valle, RSC Adv., 8, (2018), 36201

[4] C. Nieto, M.A. Vega, J. Enrique, G. Marcelo, E.M. Martín del Valle, Cancers, 11 (2019), 1679

Multifunctional coatings and innovative fabrication process for low voltage electrowetting on dielectric applications

Ana L. Martínez Díez
Maria Fe Menéndez Suárez
Pascal Sanchez
Fundación Idonial, C/Calafates 11, Avilés

Ana.martinez@idonial.com

Electrowetting on dielectric (EWOD) based digital microfluidics is explored as a promising device to manipulate droplets by controlling the wetting behavior of liquids on the dielectric surfaces applying a voltage [1, 2].

In this work a study of EWOD actuations on coplanar electrodes under parallel configuration, fabricated with not expensive processes for low actuation voltage, is carried out.

To accomplish this aim the innovation on processes and the use of multifunctional coatings has been developed:

(i)Starting from a conductive layer of 100nm of ITO deposited by sputtering, the electrodes have been designed and fabricated by using laser ablation instead of photolithography, with the advantage of the speed of this process. The electrodes have been designed with a gap of 50nm between them.

(ii)A unique low cost layer, developed by sol-gel technology, based on silica precursors (TEOS/MTES) under acid catalysis, which meets both properties dielectric and hydrophobic, has been developed. This reduces the manufacturing time (from a bilayer, usually PMMA and Teflon to only one) besides lowering the price of the device.

The device has been tested with a nonaqueous droplet (Ethylene glycol as solvent and sodium dodecyl sulfate as surfactant 0.1%) [3] and its movement takes place at low voltage as it can be seen in Figure 1.

References

[1] Junghoon Ledd, Hyejun Moon, Jesse fowler, Thomas Schoellhammer, Chang- Jin Kim. Sensors and Actuators A95 (2002) 259-268
[2] Xu. Xiaowei, Zhang Yuliang, Sun Lining, Chinese Journal of Physics, 56 (2018) 2887-2896
[3] Debalina Chatterjee, Boonta Hetayothin et al. Lab chip, 6(2006)199-206

Figures

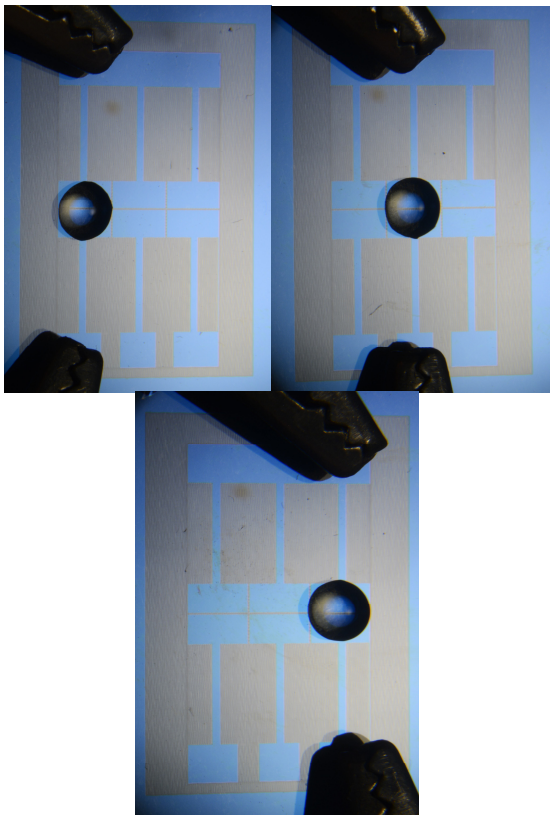


Figure 1: EWOD droplet movement after applying a voltage

Next-Generation of Tribological Lubricants Modified with Magnetic Nano-Microwires

Mª Fe Menéndez Suárez [1]
Ana L. Martínez Díez [1]
Pascal Sánchez [1]
Juan Carlos Sánchez López [2]

[1] *Fundación IDONIAL, C/ Calafates 11, 33490, Avilés, Spain*
[2] *ICMS (CSIC-US), C/Américo Vespucio 49, 41092, Sevilla, Spain*

marife.menendez@idonial.com

Nowadays, there is a high interest in developing new advanced lubricants that improve the performance and life-service of the materials, by reducing friction coefficients and wear rates [1].

It has been shown that one of the strategies that pays off for improving the tribological properties of lubricants is the addition of nanoparticles, which act as nano-bearings, thanks to the formation of a protective film that decreases the contact between surfaces [2].

In this work a commercial lubricant (Shell Donax TD 10W-30) has been modified by selectively incorporating of differents magnetic metallic nano and microwires (Ni-NWs, Fe-Nws, Co-MWs, Figures 1-3) synthesized by Fundación IDONIAl. The experimental results obtained on AISI 430 stainless steel substrate are highly promising, showing that the novel nanolubricant significantly improved anti-wear tribological properties in relation to unmodified oil. Tribological tests have been performed on a tribometer in *pin-on-disc* configuration.

Additionally, these advanced lubricants are environmentally friendly, due to the fact that metallic additives can be separated by an external magnetic field and subsequently they can be reused.

References

[1] Holmberg K., Kivikytö-Reponen P., Härkisaari P., Valtonen K., Erdemir A. Global energy consumption due to friction and wear in the industry. Tribol. Int. 2017, 115, 116–139.
[2] Gulzar, M.; Masjuki, H.H.; Kalam, M.A.; Varman, M.; Zulkifli, N.W.M.; Mufti, R.A. Tribological performance of nanoparticles as lubricating oil additives. J. Nanoparticle Res. 2016, 18, 223.

Figures

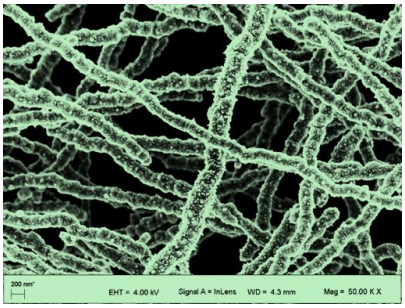


Figure 1: FEG-SEM Images of Niquel Nanowires

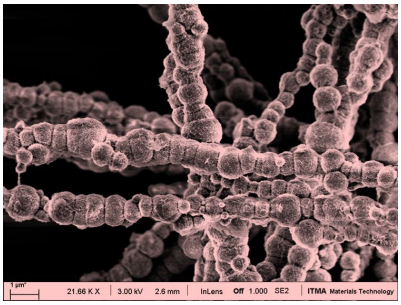


Figure 2: FEG-SEM Images of Cobalt Microwires

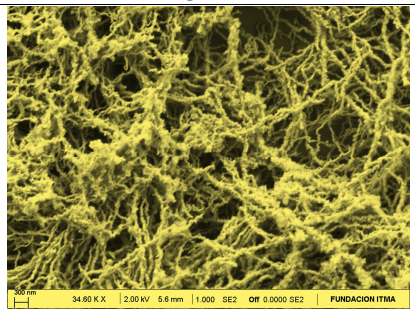


Figure 3: FEG-SEM Images of Iron Nanowires

BIONANOPOLYS Open Innovation Test Bed (OITB)

Natalia Ortuño

ITENE, Albert Einstein, 1, Paterna, Spain

natalia.ortuno@itene.com

Abstract

The Horizon 2020 project Bionanopolys unites 27 European partners to create an Open Innovation Test-Bed (OITB) for an improved performance for packaging, textile, agriculture, cosmetics, pharma or food. In order to create a more sustainable future for all of us, the project team is eager to develop biomaterials with high quality and, therefore, to provide potential alternatives to fossil-based materials. These novel biomaterials must offer functional properties for high-volume applications and need to perform even better in order to drive their adoption by industry and end users. Besides, fossil-based materials are still cheaper – a barrier for a successful market entry of biomaterials.

Bionanopolys opens up a platform for driving "open innovation" in this field. In order to provide materials with the requested properties, the Bionanopolys community makes use of sustainably sourced renewable feedstocks in Europe for manufacturing innovative bionanocomposites and producing bio-based nano-products for different industry sectors. To speed up the introduction of bio-based nano-enabled materials into the market, a single entry point (SEP) for stakeholders, who are willing to contribute or to make use of the OITB services is a central objective of the project.

For the start, Bionanopolys created a network of 14 pilot plants and their complementary services: Five pilot plants will focus on the development of bionanomaterials from biomass, three pilot plants are dedicated to bionanocomposites and six pilot plants aim at manufacturing bio-based nanoproducts in order to reach a wide range of applications in different sectors. Pilot lines are going to be upgraded and fine-tuned across the entire Bionanopolys value chain.

Therefore, Bionanopolys offers to create an integrated platform of technologies and scientific expertise as well as technicians devoted to the nanotechnology based on bio-based raw materials for the first time. A comprehensive portfolio of services for the development and integration of new bio-based nano-enabled products complements the outputs of the project. The services of the OITB comprise scientific consultancy for the production on the one hand, and complementary considerations in terms of ethics, security, life cycle assessment, economic analyses etc. on the other.

References

[1] www.bionanopolys.eu

Figures

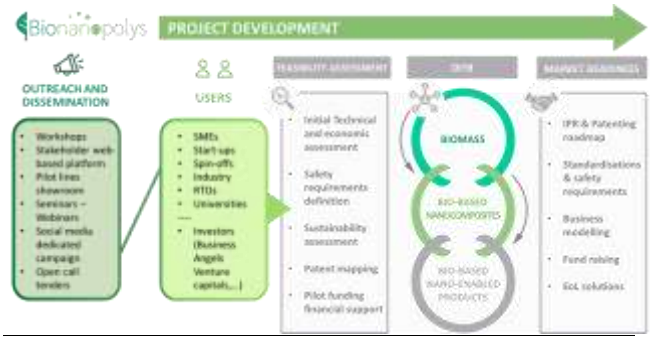


Figure 1: Overall concept of BIONANOPOLYS Test Bed

Oxaliplatin-loaded magnetoliposomes associated to LGR5 for targeted therapy of colorectal cancer

J. Prados[1,2,3], A. Cepero[1,2,3], B. García-Pinel[1,2,3], L. Gago[1,2], Y. Jabalera[4], G. Iglesias[4], L. Cabeza[1,3], C. Mesas[1,2], F.J. Quiñonero[1,2,3], G. Perazzoli[1,2], R. Ortiz[1,2,3], C. Jiménez-López[4], Melguizo[1,2,3]

[1]*Institute of Biopathology and Regenerative Medicine (IBIMER), Center of Biomedical Research (CIBM), University of Granada, 18100 Granada, Spain.*
[2]*Department of Anatomy and Embryology, Faculty of Medicine, University of Granada, 18071 Granada, Spain*
[3]*Instituto de Investigación Biosanitaria ibs. Granada, 18012 Granada, Spain*
[4]*Department of Microbiology, Sciences School, University of Granada, Campus de Fuentenueva, 18002 Granada, Spain.*

jcprados@ugr.es

Abstract

Introduction: Oxaliplatin (OXA) is one of the of the main chemotherapeutic drugs for colorectal cancer (CRC) treatment, the third most frequent cancer worldwide. In advanced stages, CRC has a five-year survival rate of 14%, with the appearance of multiple resistances being one of the main problems in treatment failure. In this context, colorectal cancer stem cells (CSCs), which are derived from intestinal stem cells positive for LGR5 marker, appear to be responsible for resistance to chemotherapy, radiotherapy and the development of metastases [1]. Thus, the development of new nanoformulations that selectively target colorectal CSCs appears as a promising strategy to improve the prognosis of these patients. In this context, magnetoliposomes (MLPs) are a type of nanocarriers with multiple properties, such as the controlled release of anti-tumor agents, active targeting through binding monoclonal antibodies and high bioavailability [2,3].
Materials and Methods: Protein expression of the LGR5 marker was analyzed by western blot in colorectal cancer cell lines MC38 and T84, in normal colon cell line CCD18, and in the hepatocellular carcinoma control line HepG2. MLPs loaded with OXA (MLP-OXA) (Fig.1) were synthesized, functionalized with anti-LGR5 (MLP-OXA-LGR5) and tested in the above cell lines. Cell proliferation percentages were analyzed using the Sulforhodamine B assay.
Results: LGR5 is expressed in MC38, T84, CCD18 and HepG2 cell lines. In MC38 and T84, treatment with MLPs-OXA-LGR5 showed greater cytotoxic effect than free drug and non-targeted nanoformulations. However, in CCD18 and the HepG2 control line, treatment with MLP-OXA-LGR5 produced the same antitumor effect as MLP-OXA.
Conclusions: MLP-OXA-LGR5 may be a promising strategy to selectively eliminate colon CSCs. Further in vitro and in vivo studies are needed to validate the antitumor effect of these nanocarriers.

References

[1] Ortíz R, Quiñonero F, García-Pinel B, Fuel M, Mesas C, Cabeza L, Melguizo C, Prados J. Cancers (Basel). 2021, 13(2021):2058.

[2]Garcia-Pinel B, Jabalera Y, Ortiz R, Cabeza L, Jimenez-Lopez C, Melguizo C, Prados J. Pharmaceutics. 2020 12(2020):589.

[3]Jabalera Y, Garcia-Pinel B, Ortiz R, Iglesias G, Cabeza L, Prados J, Jimenez-Lopez C, Melguizo C. Pharmaceutics. 11(2019):395.

Figures

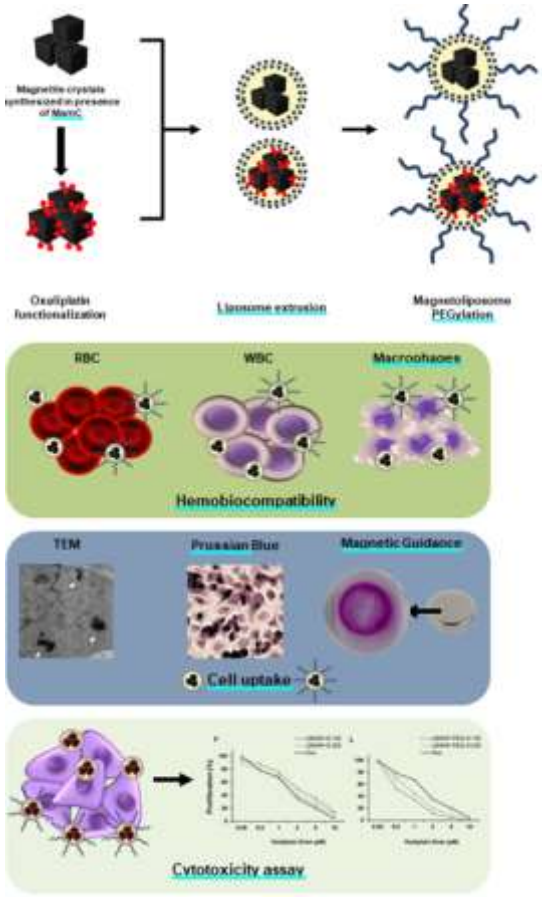


Figure 1: Representative image: magnetoliposome-OXA synthesis and in vitro analysis.

GOLD NANOPARTICLES TO MODULATE THE TUMOUR MICROENVIRONMENT

Comas, L.
Uranga-Murillo, I.; Artiga, A.; Serrano, I.; Ramírez-Labrada A.; Arias, M.; Martinez de la Fuente, J.; Pardo, J.; Gálvez, E.

Instituto de Carboquímica, ICB-CSIC, Zaragoza, Spain

lcomasc@hotmail.com

The number of patients benefiting from Immune Checkpoint Inhibitors (ICIs) is still relatively low, restricted to specific tumour types [1]; those presenting specific inflammatory immune cell populations at tumour microenvironment: the so-called hot tumours. Development of protocols to selectively modulate inflammation and increase tumour sensitivity to ICIs is required. Some nanoparticles (NPs) are able to modulate the immune response [2]. Yet, their effect on tumour microenvironment and inflammation has not been explored.

M1/M2 macrophages and dendritic cells (DCs) were differentiated from mouse bone marrow. Gold nanoparticles (GNPs) were synthetized and characterised (Figure1). Production of inflammatory cytokines in myeloid cells and the mechanism involved were analysed in vitro. Immunomodulation in vivo was analysed in the B16 melanoma model.

As a result, GNPs are not cytotoxic in vitro at any tested concentration. Nevertheless, GNPs were able to induce the release of TNFa and IL6 in macrophages in vitro, and, in combination with LPS, they also induced IL1β. The latter depended on the canonical caspase-1-inflammasome. NPs also induced DC maturation in vitro. GNPs increased in vivo LPS immunomodulation in tumours, modifying the tumour growth and the microenvironment, including cell populations and the profile of inflammatory cytokines.

In conclusion, GNPs are able to modulate the inflammatory response in tumour microenvironment in vitro and in vivo. Further studies will required to analyse if they modulate the sensitivity of tumour to ICIs.

References

[1] P. Bonaventura *et al.*, *Frontiers in Immunology* (2019).
[2] B. S. Zolnik, Á. González-Fernández, N. Sadrieh, and M. A. Dobrovolskaia, *Endocrinology* 151, 458–465 (2010).

Figures

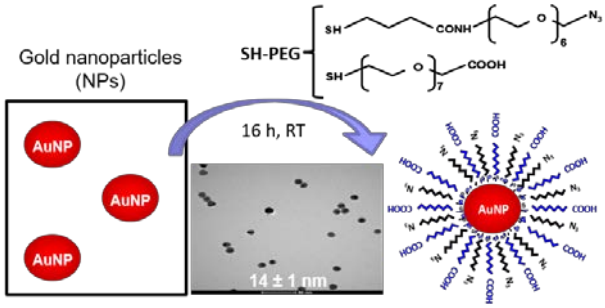


Figure 1: Synthesis of gold nanoparticles

Role of Defects in Optical Properties of 2D h-BN

Junkai Ren
Luigi Stagi, Luca Malfatti, and Plinio Innocenzi

Laboratory of Materials Science and Nanotechnology, Department of Chemistry and Pharmacy, CR-INSTM, University of Sassari, Via Vienna 2, 07100, Sassari, Italy

E-mail: j.ren@studenti.uniss.it

Abstract

Two-dimensional hexagonal boron nitride (2D h-BN) is representing one of the most popular layered materials whose excellent properties are expected to have great potentials in optics and electronics.[1-2] The introduction of tailored defects can endow 2D h-BN with many new properties, such as fluorescence and photocatalytic activity.[3-4] Therefore, managing defects in h-BN is a key process to exploit its advanced functions. However, a clear correspondence between defects and properties still has not been well established in terms of h-BN basic research.

In this report, h-BN nanosheets (h-BNNSs) have been prepared by sonication-assisted liquid-phase exfoliation of the bulk powders. In one hand, the exfoliation in water can make cavitation and allow producing hydroxyl-defective h-BNNSs which show a visible photoluminescence (**Figure 1a**).[5] In another hand, the exfoliation in N-methyl-2-pyrrolidone (NMP) only produces relatively defect-free h-BNNSs, consequently, without that visible fluorescence. It highlights the critical role of hydroxylation and oxidation in the fluorescent emission as well as the rising optical absorbance of the 2D h-BN structure. Subsequently, the nanosheets have been successfully incorporated into titania (TiO_2) mesoporous films to form heterostructures via a template-assisted self-assembly (**Figure 1b**).[6] Both bare and defective BN sheets do not show photocatalytic properties but can contribute to the anatase TiO_2 crystallization by heterogeneous nucleation. Importantly, the defects of h-BNNSs can further increase the UVA absorbance and thereby enhance the photocatalytic response of the film.

In a summary, defective h-BNNSs can be prepared via sonication-assisted exfoliation of their bulk counterpart in water-phase. The tailored defects not only can induce visible emission from h-BN layer but also enhance the photocatalytic property of BN-TiO_2 heterojunction. Prospectively, only through a better understanding of multiple defects, it is possible to create new properties of h-BN materials and develop their advanced functions.

References

[1] **J. Ren**, L. Stagi, P. Innocenzi *J. Mater. Sci.*, 56 (2021) 4053.
[2] L. Stagi, **J. Ren**, P. Innocenzi. *Materials*, 12 (2019) 3905.
[3] **J. Ren**, P. Innocenzi. *Small Struct.*, 2 (2021) 2100068.
[4] **J. Ren**, L. Stagi, L. Malfatti, C. M. Carbonaro, G. Granozzi, L. Calvillo, S. Garroni, S. Enzo, P. Innocenzi. *Appl. Surf. Sci.*, 567 (2021) 150727.
[5] **J. Ren**, Luigi Stagi, C. M. Carbonaro, L. Malfatti, M. F. Casula, P. C. Ricci, A. D. Rio, F. Bonaccorso, L. Calvillo, G. Granozzi, P. Innocenzi. *2D Mater.*, 7 (2020) 045023.
[6] **J. Ren**, L. Stagi, L. Malfatti, S. Garroni, S. Enzo, P. Innocenzi. *Langmuir*, 37 (2021) 5348.

Figures

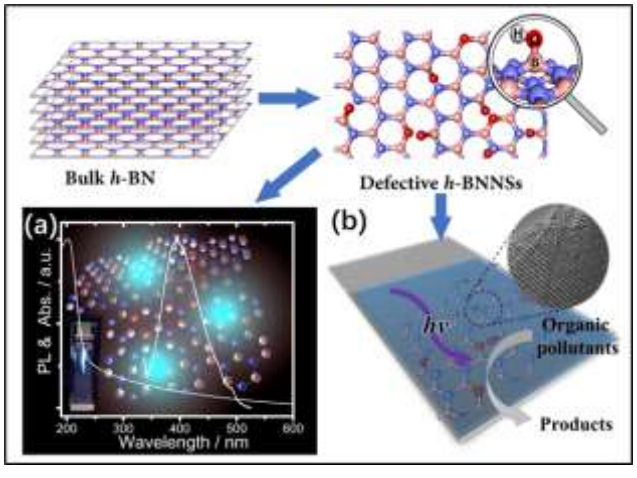


Figure 1: Defect-assisted (a) luminescence from h-BNNSs and (b) enhanced photocatalysis in BN-TiO_2 film heterostructure.

Chitosan-based nanosystem as pneumococcal vaccine delivery platform

Robla Álvarez, Sandra[1]
Prasanna, Maruthi[1,2]; Varela Calviño, Rubén[3]; Grandjean, Cyrille[2]; Csaba, Noemi[1].

1. Center for Research in Molecular Medicine and Chronic Diseases- CIMUS, University of Santiago de Compostela.
2. Unit Function & Protein Engineering, UMR CNRS 6286, University of Nantes, France.
3. Department of Biochemistry and Molecular Biology, University of Santiago de Compostela, Spain.

Sandra.robla@outlook.es

Abstract

Chitosan-based nanosystems have been described as interesting tools for antigen delivery, enhancing the immunogenicity of nasally administered vaccines [1]. The design of chitosan nanocapsules with the *Streptococcus pneumoniae* cell membrane protein PsaA (pneumococcal surface adhesin A), involved in adhesion and nasopharyngeal colonization processes [2] are proposed as an antigen-loaded vaccine delivery system candidate. This nanocarriers should reach to nasal subepithelial lymphoid follicles for their uptake by dendritic cells (DCs), for activation of specific T cells, producing an adaptive immune response against pneumonia [3].

Chitosan nanoparticles with thiol-maleimide conjugation between the polymer (chitosan) and the antigen (PsaA) were designed to enable surface presentation of PsaA for immune cell recognition. Spherical shaped particles, with size of 266±32 nn, positive charge of +30±1 mV and good stability profiles in simulated nasal fluids (up to 24 hours) were achieved. PsaA association rates were three times higher compared to nanocapsules without covalent polymer-protein conjugation.

The maturation of pre-incubated inmature DCs in the presence of antigen-conjugated nanocapsules, and subsequent studies of lymphocyte activation after this antigen presenting cells (APCs) presentation showed a higher capacity of nanocapsules to activate CD4 (CD4+/CD25+, 19% activation) and lower to CD8 T lymphocytes (CD8+/CD28+, 17% activation) compared to immature DCs (CD4+/CD25+ 16% and CD8+/CD28+, 18% activation). The evaluation of antigen-specific responses and cytokine profiles are currently underway to further evaluate the potential of these nanocapsules as vaccine delivery systems.

References

[1] C. Prego, D. Torres, M. J. Alonso. *J. Drug Deliv. Sci. Technol.* 2006, 16, 5.

[2] M. Prasanna *et al. Eur. J. Pharm. Sci* .2018, 129.

[3] N. Csaba, M. Garcia-Fuentes, M. J. Alonso. *Adv. Drug Deliv. Rev.* 2009, 61, 2.

Figures

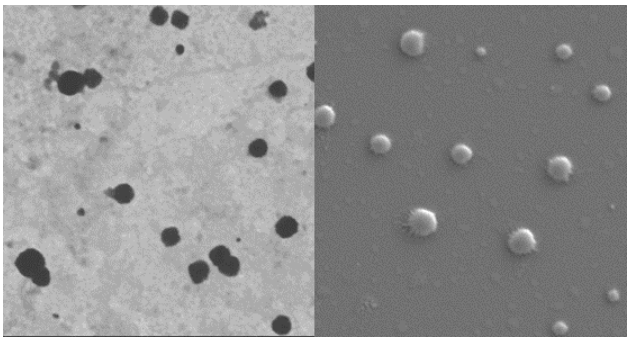


Figure 1: TEM and SEM images of Chitosan-maleimide PsaA-SATA nanocapsules.

Aluminium matrix composites reinforced with ceramic nanoparticles for additive manufacturing

James J. Rosero
Paula G. Saiz, Daniel Salazar, Rafael Morales

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

james.rosero@bcmaterials.net

Abstract

Aluminium alloys have been widely employed in different fields such as defense, aerospace or automotive technologies as a result of its high corrosion resistance, low density, high strength and specially because of their low cost. Nevertheless, some disadvantages such as poor wear resistance are also found in classic aluminium alloys, which limit their range of application. In this context, Aluminium Matrix Composites (AMCs) are gaining attention as their improved physical and mechanical properties allow for excellent stiffness and ductility as well as enhanced wear resistance.

In this work, AMCs have been prepared using TiC and TiB2 ceramic nanoparticles as additives (50 nm) and Al particles (45 µm) as the metallic matrix. Powders were mixed by ball milling using different weight ratios (from 0.5 to 8 %wt.) and subsequently prepared in the form of pellets by cold isostatic pressing. Finally, samples underwent a thermal treatment for deoxygenation and subsequent sintering. Obtained samples before and after thermal treatments were characterized by different techniques. X-ray diffraction and SEM-EDX were employed to analyse the crystalline structure and the morphology and distribution of the resulting AMCs. Mechanical properties of these materials were also investigated by DMA. Samples show a well distribution of the filler along the matrix as well as the formation of secondary intermetallic phases above certain temperatures. Further analysis of their potential for additive manufacturing applications is being performed.

References

[1] G. Langelandsvik, M. Grandcolas, K. G. Skorpen, T. Furu, O. M. Akselsen, and H. J. Roven, Metals (Basel)., vol. 10, no. 11, pp. 1–17, 2020, doi: 10.3390/met10111485.

[2] S. B. Boppana, J. Mater. Sci. Chem. Eng., vol. 08, no. 01, pp. 1–10, 2020, doi: 10.4236/msce.2020.81001.

[3] C. Selcuk and A. R. Kennedy, Mater. Lett., vol. 60, no. 28, pp. 3364–3366, 2006,doi:10.1016/j.matlet.2006.03.021

[4] P. Li, E. G. Kandalova, and V. I. Nikitin, *Mater. Lett.*, vol. 59, no. 19–20, pp. 2545–2548, 2005, doi:10.1016/j.matlet.2005.03.043

Figures

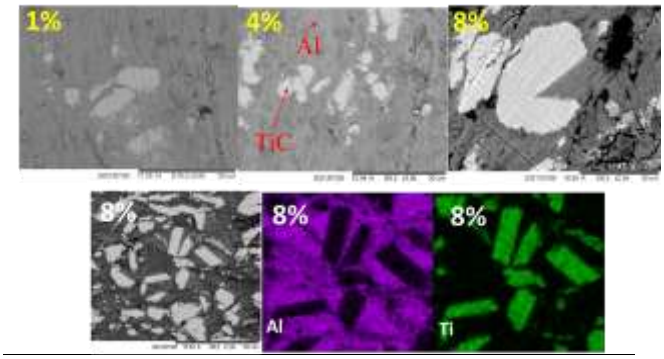


Figure 1: $TiAl_3$ intermetallic phases for AMCs reinforced with TiC nanoparticles.

ICARUS-INAS: Integrated Nanostructures Assessment Service

Juan Antonio Tamayo Ramos
Sonia Martel Martín
Rocío Barros García
David Blanco Alcántara
Julieta Díez Hernández
Jesús Ibáñez Porras

University of Burgos – ICCRAM
Plaza Misael Bañuelos s/n

jatramos@ubu.es
smartel@ubu.es
rbarros@ubu.es
dblanco@ubu.es
jdhernandez@ubu.es
jesusibanez@ubu.es

Abstract

The innovation idea of ICARUS-INAS comes from the integration of nanosafety and Life Cycle Assessment (LCA) by the calculation of high-quality Characterisation Factors (CF) for novel nanostructured materials (NMs). Some limitations have been identified by the European Commission in the use of valid CF. Therefore, in this EU funded project, a complete exploitation plan to commercialise these services has been developed, assessing the economic viability of the nanosafety and LCA integration, identifying potential stakeholders, barriers and opportunities in the related markets. The growing tendency on the identification of environmental impacts of novel NMs provide a large market niche to commercialise nanosafety-LCA integrated analyses, together with additional services, such as physico-chemical characterisation of NMs, as well as the determination of potential economic and social impacts, which will allow to create a complete sustainability assessment. The methods used for the nanotoxicological assessment will be competed with the calculation of the CF, in order to integrate the obtained results in a single model for the implementation of Sustainability by Design strategies in the development of new nanomaterials.

References

Saouter, E., Biganzoli, F., Ceriani, L., Versteeg, D., Crenna, E., Zampori, L., Sala, S, Pant, R. (2018). Environmental Footprint: Update of Life Cycle Impact Assessment Methods – Ecotoxicity freshwater, human toxicity cancer, and non-cancer. EUR 29495 EN, Publications Office of the European Union, Luxembourg, ISBN 978-92-79-98183-8, doi:10.2760/611799, JRC114227.

Figures

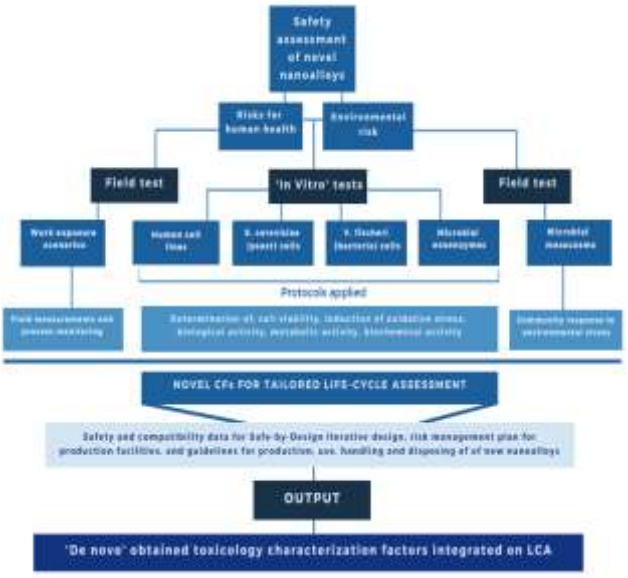


Figure 1: Overview of nanosafety approach for the determination of CF in LCA

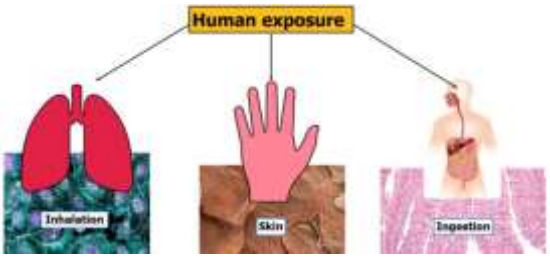


Figure 2: Human cell lines to be used in the determination of human hazard

Polymer thin film for immobilization of Laccase enzyme

N. González[a], A. González[a], Catalina Sosa[a], V. Villalobos[b], J. Blamey[c,d], L. Tamayo [a], **M. Urzúa** [a]

[a]*Dpto. de Química, Facultad de Ciencias, Universidad de Chile. Las Palmeras 3425, Santiago, Chile*
[b]*Instituto de Ciencias Químicas Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, El Llano Subercaseaux 2801, San Miguel, Santiago, Chile.*
[c]*Fundación Biociencia, José Domingo Cañas 2280, Santiago, Chile.*
[d]*Facultad de Química y Biología. Universidad de Santiago. Santiago, Chile*
Contact@E-mail: maurzua@uchile.cl

Immobilization of enzyme has become an important element of bioprocess development in recent years due to its high specificity and high activity under industrial conditions, where the biocatalysis is considered an efficient method of biotransformation[1,2]. This work reports the study of the immobilization of the Laccase enzyme on thin films of poly (maleic anhydride-alt-styrene), poly (maleic anhydride-alt-ethylene) and poly (maleic anhydride-alt-styrene) modified with L-glutamic acid (Figure 1). The thin films of polymers were prepared by spin-coating on previously treated Si-wafer. The surface modified with the different polymers studied was characterized by ATR-FTIR spectroscopy, AFM microscopy and contact angle measurements to obtain molecular characterization, morphology and wettability, respectively. The thickness of the surface was measured by Ex-Situ ellipsometry and ATR-FTIR. The Laccase enzyme was immobilized on the different polymeric films at pH 7. Studies of the activity of the Laccase enzyme were carried out by means of UV-Vis spectroscopy against a solution with persistent organic pollutants by means of.
The results show that the wettability (Figure 2) and morphology of the polymeric films are dependent on the comonomeric unit and on the presence of L-glutamic acid from the side chain of poly (maleic anhydride-alt-styrene). The thicknesses of the different polymeric films determined by ellipsometry are in agreement with those determined by ATR-FTIR. The activity of the Laccase enzyme immobilized on the surface of polymeric films depends on the hydrophobicity / hydrophilicity of the surface of the polymeric film.

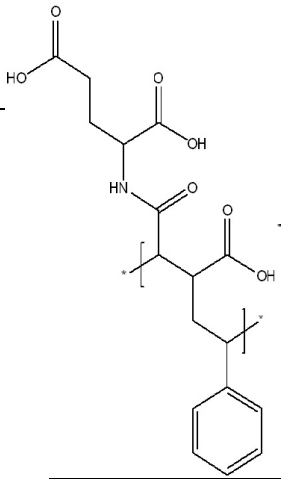


Figure 1: Poly(maleic anhydride-*alt*-styrene) modified with L-Glutamic Acid.

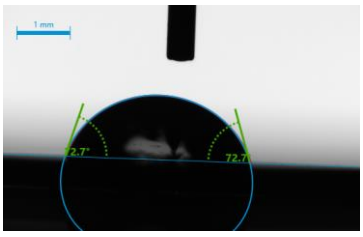


Figure 2: The contact angle for a drop of water on the modified polymer surface adsorbed in the previously treated surface (Silicon wafer)

References

[1] Nerea Ormategui, Antonio Veloso, Gracia Patricia Leal, Susana Rodriguez-Couto and Radmila Tomovska, ACS Appl. Mater. Interfaces 7 (2015) 14104−14112
[2] Mohd Syahlan Mohd Syukri, Zurina Mohamad, Roshanida A. Rahman, Rosli Md Illias and Hideaki Tokuyama J Chem Technol Biotechnol 2021,12 September 2021 DOI 0.1002/jctb.6919

Acknowledge

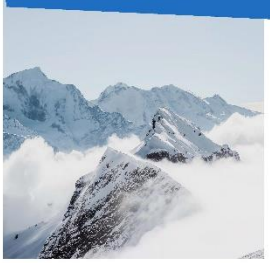
Project: FONDECYT N°1191467

IKUR STRATEGY AT A GLANCE

ikur estrategia

+ Info: ikur@euskampus.eu

1 What it is



IKUR 2030 is the Strategy to position the Basque Country as a scientific pole of international reference...

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

2 Its objectives

- Development of Advanced Capabilities
- "Tractor effect" of Research in the Basque Country
- Reference in Europe
- Economic and Social Impact

3 Flagship Areas

- Neurobiosciences
- Quantum Technologies (QT)
- NeutriOnics

High Performance Computing & Artificial Intelligence (HPC-AI)

4 Expected impact

- **Research personnel**: +400
- **Publications**: +4.000
- **EPO Patents**: +30
- **Spin offs**: +20
- **Turnover**: +350 M€
- **Employment**: +3.200

5 Governance

- ikerbasque Basque Foundation for Science — Recruitment and attraction of research personnel
- Management of IKUR funds
- EUSKO JAURLARITZA GOBIERNO VASCO — HEZKUNTZA SAILA / DEPARTAMENTO DE EDUCACIÓN
- Fundación Biofísica Bizkaia / Biofisika Bizkaia Fundazioa — Neurobiosciences
- DIPC — QT + HPC-AI
- MPC Materials Physics Center — NeutrIOnics
- euskampus FUNDAZIOA — Monitoring and evaluation the impact of the IKUR Strategy

Scientific Direction of IKUR's Flagship Areas