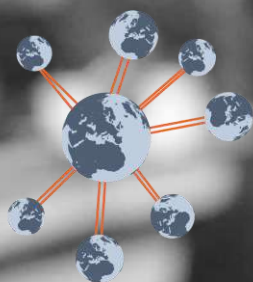


October 03-07, 2022 • Tirana, Albania



2022 TNT nanoBałkan



Abstracts Book

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2022 TNT nanoBalkan

October 03-07, 2022 • Tirana (Albania)

TNT2022 Foreword

On behalf of the International and Technical Committees, we take great pleasure in welcoming you to Tirana (Albania) for the "Trends in NanoTechnology" International Conference (TNT2022).

The 22nd edition of the Trends in Nanotechnology International Conference (TNT2022) is being launched following the overwhelming success of earlier Nanotechnology Conferences. TNT2022 will take place in Tirana (Albania) for the 2nd year in a row in particular to launch a new conference series denominated nanoBalkan.

This high-level scientific meeting TNT series aims to present a broad range of current research in Nanoscience and Nanotechnology as well as related policies or other kind of initiatives such as nanoAlb. TNT events have demonstrated that they are particularly effective in transmitting information and establishing contacts among workers in this field.

The TNT2022 structure will keep the fundamental features of the previous editions, providing a unique opportunity for broad interaction.

On the occasion of TNT2022 several specific sessions on hot topics will be organised: "Graphene and 2DM" one-day Symposium, Meet Editors of Biosensors and Bioelectronics journal, Future projects/Networking, etc.

We are indebted to the following Government Agencies for their financial support: Academy of Sciences of Albania and MAEC/Embajada de España en Albania.

In addition, thanks must be given to the staff of all the organizing institutions whose hard work has helped planning this conference.

TNT2022

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The Institut Català de Nanociència i Nanotecnologia with its official English translation Catalan Institute of Nanoscience and Nanotechnology and acronym ICN2, is a non-profit international research institute located close to Barcelona (Catalonia, Spain). It is devoted to the generation of knowledge, materials and devices in the broad fields of ICT, health and medicine, energy and the environment. ICN2 Quantum gathers seven research laboratories covering a broad range of quantum science & technologies, including the growth of high-quality topological quantum matter for next generation devices & quantum technologies, the control of phononic and photonic degrees of freedom for innovative ultralow power actuators, sensors and information processing protocols, ultrafast dynamics of energy/heat/information in quantum materials, fabrication of atomically precise 2D nanoarchitectures as quantum platforms and ultimate atomic scale characterization and 3D atomic modelling of nanoscale materials for quantum technologies.



www.iit.it/cmi-sssa

The Center for Materials Interfaces – CMI@SSSA is an interdisciplinary R&D center dedicated to the investigation, development, characterization, and exploitation of materials at the nanoscale, with particular attention to the biomedical and technological sectors, and with a special focus on interface effects. The Center is highly multidisciplinary, and materials science, physics, chemistry, life science and engineering merge to find how innovative materials and interfacial processes can be developed and exploited for specific applications.



<https://emerge-infrastructure.eu/>

EMERGE – Emerging Printed Electronics Research Infrastructure

EMERGE is a pioneering research infrastructure, comprised of top-ranked European partners, supporting free-of-charge access to applicants to develop short-term projects related to sustainable flexible large-area printed electronics and photonics (FLAPEP) at partners' laboratories. EMERGE tackles the challenges concerning all the FLAPEP value chain, offering a true open-access facility that connects scientific expertise and technological competencies to a vast network in the ecosystem. Apply not to create sustainable solutions, synergies, save time and minimize risks when introducing FLAPEP technologies in new products.



www.tntconf.org/2022/Files/hidrofarm.pdf



HidroFarm was founded in order to return the attention in the national and regional market to quality and healthy production through the use of professional skills and technology while preserving regional cultivars without harming the environment.

The mission of the Innovation Center (Hub) in the Ministry of Defense is to bring some out-of-the-box solutions to problems that this sector encounters, including problems that might arise at NATO level. In addition, the Center is focused on the development of new ideas and startups by encouraging innovation and entrepreneurship, stimulating demand in the fields of national security, civil defense, and cyber security, and building connections between important ecosystem actors, such as academia, industry, think-tanks, NGOs, and non-governmental organizations.



<https://everestie.com/>

ETNA POLIMER was founded in 2008, and is operating in collection, recycling, producing, printing and converting plastic materials made from Polyethylene. The company has about 50 people employed directly and around 500 more indirectly in the collection network. With the latest, state of the art technology and equipment, ETNA POLIMER capabilities and production are comparable to the best practices in the EU countries



DNS Medikal.shpk was founded on March 23, 2009 as a private company with limited liability and carries out its activity in the field of medical equipment. It is licensed by the National Registration Center with the object of activity: wholesale and retail trade, import export of medical devices, accessories, spare parts, service, testing and maintenance of medical devices. DNS Medikal aims to offer high quality medical equipment on the medical market in Albania at reasonable prices, as well as service and maintenance for medical equipment at the highest contemporary levels.



The Ministry of Agriculture and Rural Development is the institution in charge not only of policies regarding agriculture, but also aims to develop and update new technology that will help farmer's production. Through its Centers for the Transfer of Agricultural Technology, we work to present the farmers with new technology that will help them lower the cost of their product, raise the production but most importantly to slowly turn the farms towards environmentally sustainable agriculture.

<https://bujqesia.gov.al/>



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2D Nanostructures at Atomic Scale: From Energy and Environmental Applications to Quantum Devices

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Abstract

Technology at the nanoscale has become one of the main challenges in science as new physical effects appear and can be modulated at will. As developments in materials science are pushing to the size limits of physics and chemistry, there is a critical need for understanding the origin of these unique properties and relate them to the changes originated at the atomic scale, e.g.: linked to structural changes of the material, many times related to the presence of crystal defects or crystal surface terminations. Especially on 2D materials designed for electrocatalysis in energy and environmental applications, crystallography and distribution of the atomic species are of outmost importance in order to determine the active sites that will improve the reaction performance, including efficiency and selectivity towards certain reactions. In 2D nanomaterials the distribution and coordination of metal species at the surface are determining their final electrocatalytic behavior as the reactions of interest mainly occur at the surface. The presentation will show how pristine and perfect crystalline surfaces may tend to be inert versus particular reactions, while creation of certain types of defects or even a predetermined surface amorphization may highly improve the catalytic activity of these 2D nanomaterials [1-4].

In the present work, a combination of advanced electron microscopy imaging with electron spectroscopy, in an aberration corrected STEM will allow us to probe the elemental composition and structure in a high spatial detail, while determining the growth mechanisms and correlating the structural properties to their physical and chemical properties [5].

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Figures

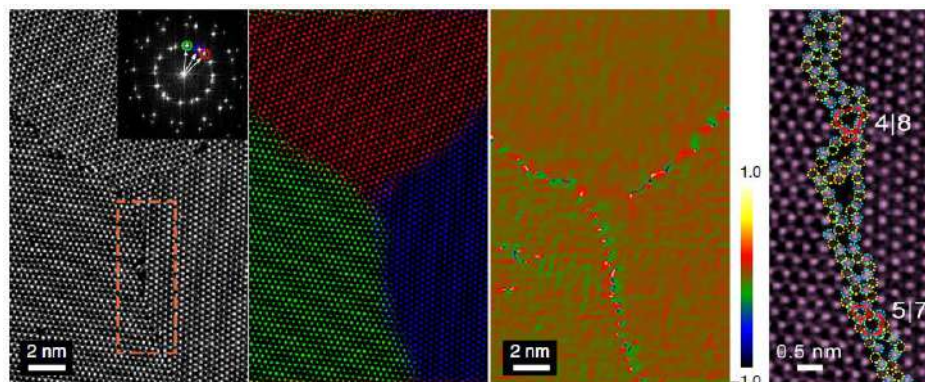


Figure 1: AC HAADF STEM magnified example of a triple grain boundary and a detail of the complex bonding coordination [1].

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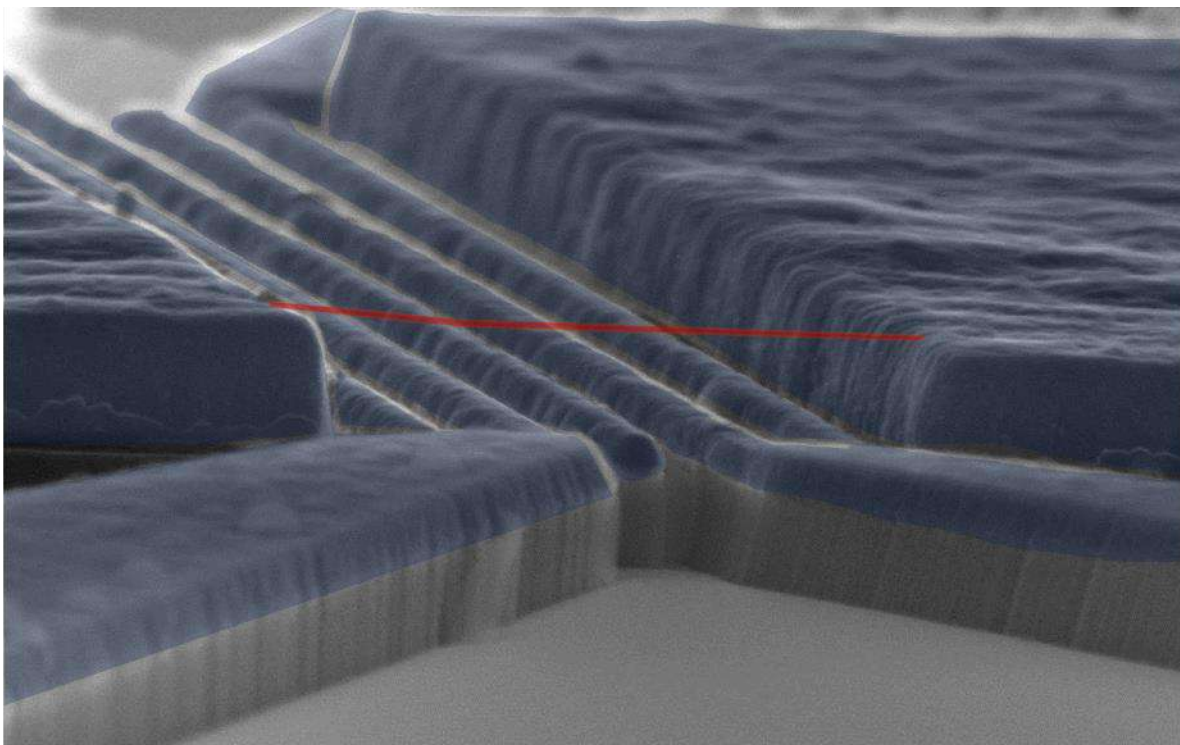
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Abstract

Mechanics has historically played a pivotal role in science by providing the basis for classical physics. Today, with the advent of nanoscale mechanical devices combined with quantum electronic devices, we are witnessing a renaissance in the field of mechanics. Here, I will discuss our recent advances on resonators based on carbon nanotubes. In particular, single-electron tunneling enables coupling mechanical vibrations to electrons by a large amount in these systems. I will show how to use this coupling to create a nonlinear mechanical oscillator approaching the quantum regime, where the resulting quantum energy levels of the mechanical oscillator are no longer evenly spaced. Using mechanical nanotubes hosting multiple quantum dots, we expect that our approach may enable the realization of a mechanical qubit [1] and a quantum simulator of quantum matters featuring strong electron-phonon correlations [2].

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One dimensional nanostructures serving as backbone of the sensor device, have attracted attention as highly efficient elements due to their high surface-to-volume ratio, which simplifies the detection of biochemical species. Use of nanowires enable to ultimately decrease the dimensions of the sensing area of the device and thus increase the resulting sensitivity of the assay (1-3). Finally, nanoscale sensors integrated into lab-on-a-chip system offer attractive opportunity of the multifunctional and multiplexed bio- and chemical analysis that can be performed in real time, directly in-flow.

Focusing on two different subsystems based on (a) silicon nanowire based field effect transistors and (b) gold nanowire based nanocapacitors, we explore their applications in the field of immunology. Namely, first subsystem is used for evaluation of the binding affinities of the peptides, relevant for the immunotherapy of the cancer using modified CAR-T cells. Second subsystem is used to realize an ultra-compact nanosize flow cytometer for real-time impedimetric detection and classification of subpopulations of immune cells. Both investigations demonstrate ability of the nanoscopic sensors to deliver new information about biological species.

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Detection, characterization, and toxicological assessment of nano- and other advanced materials in consumer products: Progress, challenges, needs and opportunities

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Abstract

Many engineered nano/materials (ENMs) eventually reach large scale production and routine use in consumer goods, foods, and personal care products. Millions of workers and consumers are being exposed on a regular basis to these ENMs across the life cycle of nano-enabled products, from synthesis to end-of-life. Assessing toxicological properties of these ENMs in complex matrixes, under realistic exposure scenarios to humans, present serious technical and methodological challenges related to nanoparticle detection in products and biological tissues, their quantitation, documentation of physio-chemical and morphological transformations that happen as part of the process, and biomonitoring, to name a few. Significant progress has been made in the past two decades in our collective understanding of the fundamental relationships between nanoparticle physio-chemical properties and nanoparticle biokinetics with mechanistic toxicology using raw or pristine materials. Progress in untangling these dose-effect relationships in humans for ENMs in complex product matrixes under mixed exposure scenarios in the real world has been notably slower. Major unmet challenges include determination of the more relevant dose metric for health effects studies, the contribution of ENMs relative to matrix components and incidental nanoparticles on adverse health effects, interactive/catalytic effects of ENMs with the matrix components, and lack of ENM-specific biomarkers of exposure (especially for carbonaceous ENMs) or effects.

The presentation will start with a brief historical perspective of major developments in the field of nanotoxicology over the last two decades and use select case studies to illustrate the challenges and the lessons learned. One such case study involves ENMs incorporated in toner-based laser printing and photocopying and human health. Through a comprehensive case series of 40 studies that were developed over a decade of interdisciplinary and multi-PI research efforts, we offers insights into some of the unique ENM-mediated phenomena on chemical composition of laser printer emissions, dose metrics and their toxicology on the respiratory and cardiovascular systems, inflammation and oxidative stress, immune system, and airway microbiome remodeling, across multiple testing platforms - cell co-cultures, animal inhalation studies, and human molecular epidemiology investigations. A second case study involves ingested ENMs (specifically titanium dioxide E171) in foods and gastrointestinal health (such as barrier integrity and inflammation). The presentation will conclude with (i) how such research experiences can inform and guide our collective scientific approaches and responses to the studying of applications and implications of the new generation of emerging advanced materials and technologies for solving challenging societal and security challenges; and (ii) how the nano scientists can work closer with nanotoxicologists to develop new technology to meet unique sensing and metrology needs for the nanotoxicology community.

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Abstract

The development of industrial-scale, reliable, inexpensive production processes of graphene and related two-dimensional materials (GRMs)[1,2] is a key requirement for their widespread use in several application areas,[1-6] providing a balance between ease of fabrication and final product quality. In particular, the production of GRMs in liquid phase [2,6] represents a simple and cost-effective pathway towards the development of GRMs-based next-generation devices, presenting huge integration flexibility compared to other production methods. Here, I will first present our strategy to produce GRMs on large scale by wet-jet milling [7] of their bulk counterpart and then an overview of their applications in the energy sector. [3,8-14]

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The current advances in nanotechnology allows for a wide spectrum of possible applications in different fields, in particular in medicine. Nanoparticles can be exploited as efficient drug delivery systems thanks to their capacity to encapsulate high payloads of drugs that are otherwise poorly soluble in the biological milieu, increasing their bioavailability and biocompatibility. In other cases, nanoparticles can act themselves as a therapeutic or diagnostic agent (e.g., superparamagnetic iron oxide nanoparticles, -SPIONs-). Nanostructured lipid carriers (NLCs) offer several advantages as compared to other systems, such as a relatively easy, green, low-cost, and scalable preparation protocol, biocompatibility / biodegradability ensured by the lipid constituents, a high drug payload, and physicochemical stability in bodily fluids. We demonstrated that NLCs loaded with SPIONs and a chemotherapeutic agent are able to selectively induce apoptosis in glioblastoma multiforme cells.^[1,2] In the aim of reaching full targeting potential and provide a patient-personalized treatment, we are now working on developing new nanocarriers based on NLCs and coated with extract of glioblastoma cell membranes derived from patients' samples. Cancer cell membrane coating confers extraordinary targeting abilities to the nanovectors, increasing the accumulation of therapeutics in diseased tissues and significantly reducing side effects.^[3] These nanovectors co-deliver both SPIONs, for hyperthermia treatment, and chemotherapeutic drugs. The targeting efficiency, the ability of crossing the blood-brain barrier, and the selective anticancer activity of the nanovectors are studied by means of state-of-the-art fluidic systems to closely mimic the complex tumor microenvironment *in vitro*. This work will be of great importance in the development of new technologies for precision medicine and for theranostic applications, thanks to abilities of SPIONs to act both as a therapeutic tool and as a magnetic resonance imaging -MRI- contrast agent, depending on the magnetic field used. Moreover, thanks to the versatility of the formulation and testing tools, this new approach could be easily remodeled to be applied for the treatment of other oncological pathologies.

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Solid lipid nanoparticles (SLNs) have been explored as alternative to colloidal drug delivery systems, such as lipid emulsions, liposomes and polymeric nanoparticles. They have many advantages over traditional drug delivery systems such as: low toxicity, high stability and loading capacity for both hydrophilic and hydrophobic drugs, other therapeutic molecules for instance peptides and nucleic acids and even small nanoparticles (SPIONs and QDs). Despite their great potential, translation from the preclinical formulation to the industrial scale-up production might have limitations. In recent years, microfluidic nanoparticle production strategies have been developed with the goal of providing a successful approach to scale-up the nanoparticle synthesis process in a reliable and reproducible manner [1].

Recently, we developed the first set-up to produce SLNs by microfluidics (Figure 1)[2].

SLNs have been produced using the glass-capillary microfluidic device, through a systematic optimisation process, opening a new avenue for future standardisation and scale-up of the production of such nanocarriers.

The achievement of a continuous and reproducible method producing SLNs has encouraged us to explore devices of different material and geometry to offer a versatile platform for engineering SLNs and encapsulating bioactive molecules.

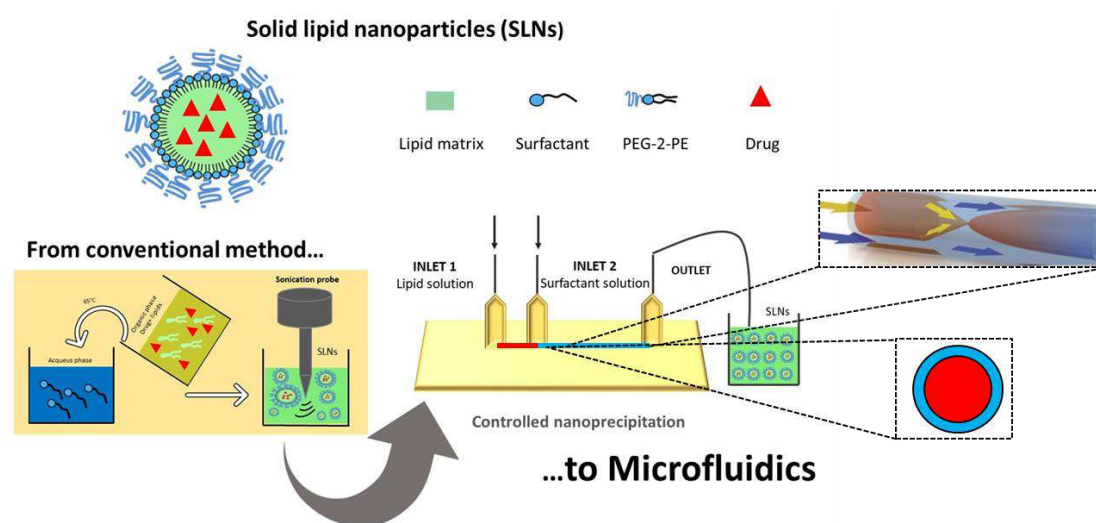


Figure 1: 3D glass capillary co-flow microfluidic nanoprecipitation platform for the production of SLNs

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Nanomaterials Modified Electrochemical Nucleic Acid Biosensors

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Abstract

The electroactivity of nucleic acids was discovered by Prof. Emil Palecek [1]. Many electrochemical techniques have been then developed for the analysis of nucleic acids as well as DNA interactions [2-6].

Nanomaterials like nanofibers, nanotubes, nanoparticles, graphenes etc. have received a great attention to design nanomaterials enriched electrochemical biosensors that could be implemented into the areas of biomedical engineering and drug discovery.

Electrochemical nucleic acid biosensors based on nanomaterials have become the one of the imperative topics due to the advantages of various nanomaterials as they have unique electronic, optical, and catalytic properties [5,6]. Electrochemical nucleic acid biosensors based on nanomaterials are overviewed herein and discussed with their applications on monitoring the detection of sequence-selective nucleic acid hybridization, and the biointeraction of nucleic acids with drugs, proteins, etc.

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Diagnosis of neonatal sepsis is very challenging especially in very low birth weight infants, having so small blood volume and given their increased vulnerability to infection due to the immature immune system. That is why ICU care for these patients is more expensive to save the incipient life [1].

Micromotors (MM) represent one of the most exciting horizons in micro and nanotechnologies. The utilization of self-propelled micromotors in (bio)-chemical assays has led to a fundamentally new approach where their continuous movement around the sample and the mixing associated effect, greatly enhances the target-receptor contacts and hence the binding efficiency and sensitivity of the assay. Catalytic tubular micromotors are constituted by few microscale layers that confer them sensing/(bio)-functionalization capabilities (outer external layer, i.e., graphene oxide, GO), magnetic properties (internal layer, i.e., Ni), and self-propulsion (catalytic layer, i.e., Pt) (**Figure 1**). These catalytic MM have demonstrated to be a powerful tool for (bio)sensing [2].

While catalytic MM covalently functionalized with antibodies have previously been used in the diagnosis of neonatal sepsis [3-5], here we also explore the possibilities of aptamers on board on MM technology for this type of diagnosis, due to their high stability. They can also be produced by chemical synthesis and are therefore less expensive to manufacture, have less variability between batches and very controlled post-production modification all without losing its selectivity and sensitivity.

In this Keynote, novel GO/Ni/Pt MM-based aptassays will be presented and their neonatal sepsis diagnosis capabilities will be discussed.

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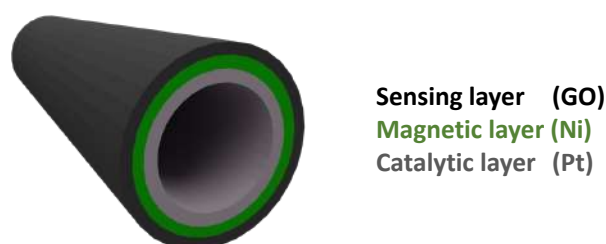


Figure 1: Schematics for layered catalytic tubular GO/Ni/Pt micromotors

Optically active self-organised quantum dots in marginally twisted MoSe₂/WSe₂ and MoS₂/WS₂ bilayers

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Moiré superlattices in twistrionic heterostructures are a powerful tool for materials engineering. In marginally twisted (small misalignment angle, ϑ) bilayers of nearly lattice-matched two-dimensional (2D) crystals moiré patterns take the form of domains of commensurate stacking, separated by a network of domain walls (NoDW) with strain hot spots at the NoDW nodes. Here, we show¹ that, for type-II transition metal dichalcogenide bilayers MoX₂/WX₂ (X=S, Se), the hydrostatic strain component in these hot spots creates quantum dots for electrons and holes. We investigate the electron/hole states bound by such objects, discussing their manifestations via the intralayer intraband infrared transitions. The electron/hole confinement, which is the strongest for $\vartheta < 0.5^\circ$, leads to a red-shift of their recombination line producing single photon emitters (SPE) broadly tunable around 1.2 eV by misalignment angle. These self-organised dots can form in bilayers with both aligned and inverted MoX₂ and WX₂ unit cells, emitting photons with different polarizations. We also find that the hot spots of strain reduce the intralayer MoX₂ A-exciton energy, enabling selective population of the quantum dot states.

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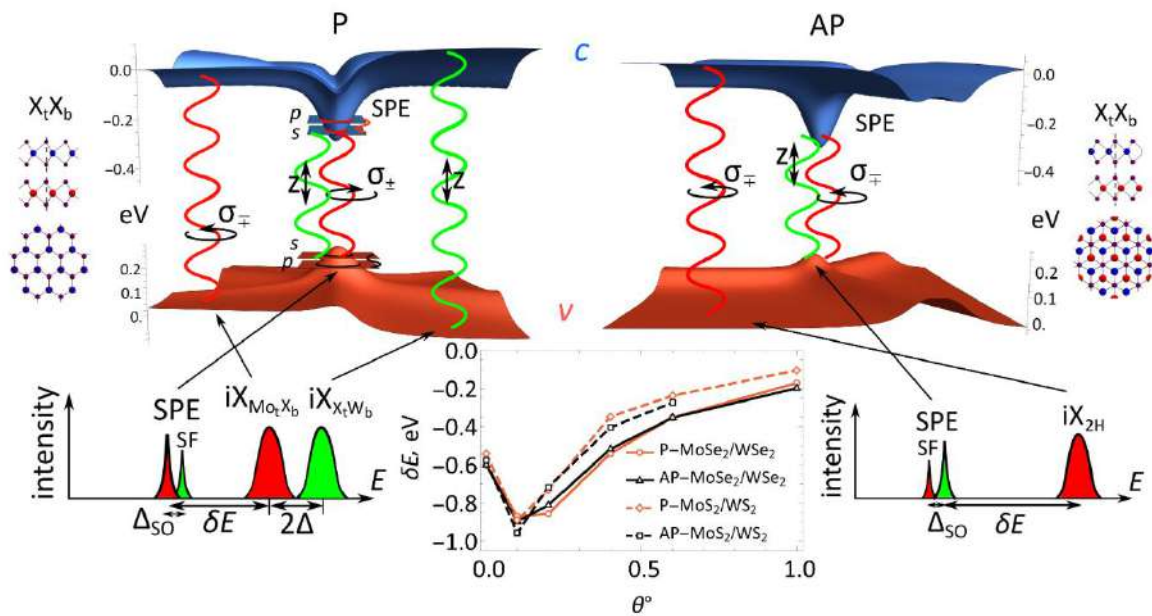


Figure 1: Self-organised quantum dots and spectral features of SPE and the interlayer excitons, iX. (Top) Conduction (c) and valence (v) band edge profiles in vicinity of X_tX_b nodes of the network of domain walls in a reconstructed P- and AP-MoX₂/WX₂ bilayers with $\theta = 0^\circ$. Colors of wavy lines encode polarisations of emitted light in $\pm K$ -valleys: red for circular and green for z-polarisation. Upper/lower subscript of circular polarisation (σ^\pm or σ^\mp) indicates helicity of light emitted in $+K/-K$ -valleys. Left and right bottom panels show sketches of predicted optical spectra in marginally twisted P- and AP-MoX₂/WX₂ bilayers, respectively. Middle bottom panel shows the calculated shift of the SPE energy (3) with respect to energy of iX inside of Mo_tX_b/2H domains for P- and AP- bilayers.

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The topological structure associated with the branchpoint singularity around an exceptional point (EP) can provide tools for controlling the propagation of light. Using graphene-based devices, we demonstrate the emergence of EPs in the electrically controlled interaction of light with a collection of organic molecules in the terahertz regime at room temperature. We show that the intensity and phase of terahertz pulses can be controlled by a gate voltage which drives the device across the EP. Our electrically tuneable system allows reconstructing the Riemann surface associated with the complex energy landscape and provides a topological control of light by tuning the loss-imbalance and frequency detuning of interacting modes. Our approach provides a platform for developing topological optoelectronics and studying the manifestations of EP physics in light-matter interactions.

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Figures

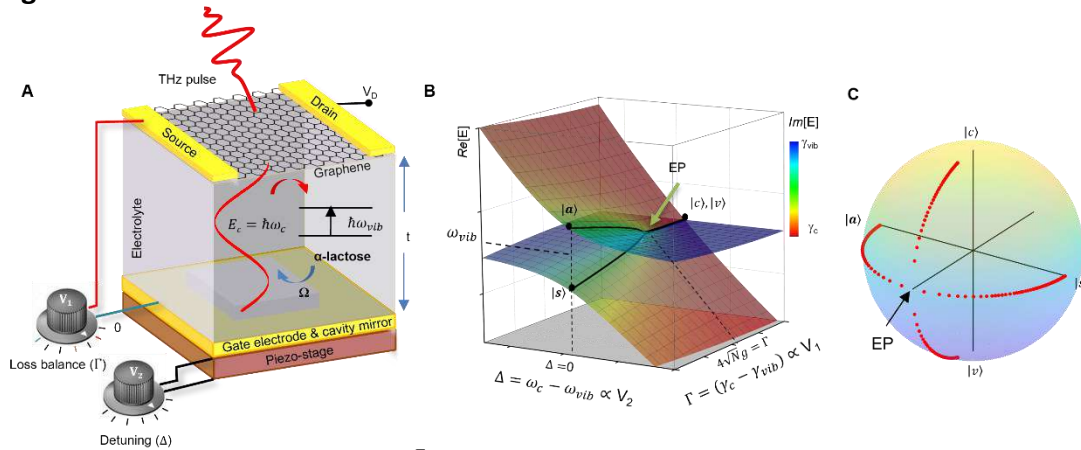


Figure 1: Electrically tuneable EP device. A, Schematic of the electrolyte-gated graphene transistor embedded with lactose microcrystals. B, Riemann surface obtained using numerical simulations shows the complex energy eigenvalues of the device plotted on the two-parameter voltage space defined by V_1 and V_2 . C, Visualization of the evolution of the supermodes of the coupled system on a Bloch sphere as the gate voltage V_1 is varied (loss imbalance Γ is tuned).

Mixed-Halide Perovskites meet 2D materials: An ideal materials platform for efficient energy harvesting and neuromorphic computation

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An aggressive technological deployment will soon affect the planet's energy landscape, demanding a swift transformation from the predominant use of fossil fuels to that of renewable energy installations. With its concurrent arrival the Internet-of-Things (IoT) promises to create a largely distributed global network of wireless sensors and wearables connected to the "cloud": Humankind is exploiting new technological platforms able to impact sustainable development and prosperity toward Industry 4.0 revolution. These platforms will create a robust demand of energy for their supply with power, making a battery-free operation mandatory together with low manufacturing cost and reduced environmental impact. GRM-enabled "harvesters" span across a wide range of scales. The demonstrated prototypes include self-powered miniaturized IoT devices, to large scale renewable energy installations.¹

The heterogeneity of peculiar ions and carriers observed in hybrid organic/inorganic materials is the source of their emergent cross-coupled light and electric field tuneable functions with potential utility in novel opto-electronic applications. Mixed halide perovskites (HPs) have been used as active layers in high performing perovskite solar cells (PSCs) that led to efficient solar energy harvesting. The power conversion efficiency (PCE) of PSCs has rapidly increased and is now approaching the state-of-the-art PCE of 26.1% obtained by crystalline-silicon PVs. However, this impressive PCE obtained on small-area cells and in laboratory conditions should be also valid to large-area PV panels in real outdoor conditions. Through interface engineering, the incorporation of the 2D materials improves the charge dynamics of the interfaces and most importantly protects the perovskite layer against degradation². Graphene Flagship partners demonstrated the validity of this technology through the entire value chain, from materials development, perovskite modules and panels fabrication and their integration in an autonomous solar farm (of 5m² perovskite PV panels), to outdoor field tests, and assessment of the real energy production output.³ The energy production of the solar farm was monitored for 12 months, demonstrating a remarkable 20% reduction (T_{80}) of the PV performance over 8 months of operation². The data analysis demonstrated that the perovskite panels enabled by 2D materials are promising for outdoor operation at elevated temperatures, such as in high-irradiance global locations.

Targeting beyond PV applications, HPs' rich dynamics enabled by inherently coupled ionic and electronic degrees of freedom have also led to the demonstration of optoelectronic memristors that emulate synaptic- and neural-like dynamics⁴. A single printable material stack fabricated with low manufacturing cost at low temperature, combining both efficient solar energy harvesting and memristive functionalities would constitute a transformational breakthrough. We have demonstrated that an inverted PSC with an average PCE of >17% with appropriate electric biasing procedure exhibits stable resistance switching characteristics at low voltages without losing its PCE performance even after thousands of switching cycles. Moreover, a high resistance state (HRS) to low resistance state (LRS) ratio of up to 10⁵ and light-tunable switching cycles in the millisecond regime with an endurance of 3 x 10³ cycles with no detectable HRS/LRS ratio drop.

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Figure 1: A) A photograph of the solar farm. B) Demonstration of a PSC operating simultaneously as an efficient, stable memristor and solar energy harvester.

MXenes as Transport Layer Materials for Halide perovskite Solar Cells

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Halide perovskite solar cells (PSCs) have already demonstrated power conversion efficiencies above 25%, which makes them one of the most attractive photovoltaic technologies. However, several challenges must be defeated for the technology to be competitive and commercially available. One of these is their long-term stability and several are the strategies currently employed to stabilize PSCs, for example, the use of complex metal oxides as transport layers, the passivation of defects in the halide perovskite layer through additive engineering, or the replacement of metal electrodes by carbon-based electrodes. In our laboratory, we have explored the use of 2D materials, such as MXenes, as transport layers in halide perovskite solar cells. In this work we present our most novel results on the application of MXenes, $\text{Ti}_3\text{C}_2\text{T}_x$, as transport layers and the effect of the intercalation of organic additives. We prepared complete halide perovskite solar cells and analysed device lifetime. Special emphasis is given to their effect on the stability of PSCs under environmental conditions such as humidity, atmosphere, light irradiation (UV, visible) or heat, considering the recently reported ISOS protocols, especially outdoor testing.

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Abstract

Epithelial tissues contain three-dimensional (3D) microstructures that guide cell self-organization at the tissue level. In the small intestine, crypts and finger-like villi microstructures improve its absorbance function, provides specific microenvironments and compartmentalizes cell types [1–3]. Despite its physiological relevance, tissue architecture and multicellular population are neglected in the standard in vitro models, thus compromising their predictive capabilities [4]. Our efforts in addressing these shortcomings by including key elements to mimic the native tissue in vitro will be discussed in this talk. First, this will include strategies to promote cell's self-organization capabilities giving rise to crypt-villus domains on 2D monolayers [5], and strategies to engineer cell spatial positioning through micropatterning. Then, our approach to include the 3D architecture of the tissue will be addressed. In here, light-based biofabrication techniques to produce 3D villus-like structures [6,7] will be discussed. Finally, I will introduce our biofabrication proposal to produce tissue engineered models that include the epithelial and the stromal compartments [8]. Improving the prediction capabilities of cell-based assays is a growing strategy to lead to more efficient drug development processes. As 2D-based systems are showing their limits, new 3D strategies are gaining acceptance among the scientific community [9]. Our approaches aim to further accelerate this trend by providing feasible strategies to routinely incorporate 3D multicellular structures at the tissue level in cell culture systems.

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Soft electronics is a new emerging exciting field of study, targeting seamless integration of electronics components and devices into non-rigid non-planar complex surfaces and objects. Among others, a particularly promising approach to soft electronics is based on the use of organic and solution process based technologies, through the development of free-standing conformable circuits made of ultra-thin (tens of nanometers) films of various polymers^[1], directly transferrable on skin ("tattoo electronics")^[2] or other complex surfaces. In the first part of the talk will review recent achievement of our group in this field, toward future applications in personal unperceivable healthcare monitoring devices^[3], active tattoo (Figure 1.a) and ultra-conformable printed electronic systems^[4]. In the second part of the talk I'll move from 2D to 3D plastic devices, discussing the applicability of this approach in combination with two photon polymerization (2PP) technique^[5], to the direct fabrication, simple handling and seamless integration of micro-structures (Figure 1.b), toward the realization of Micro Electro-Mechanical Systems (MEMS), in the framework of the EU funded project 5D NanoPrinting^[6].

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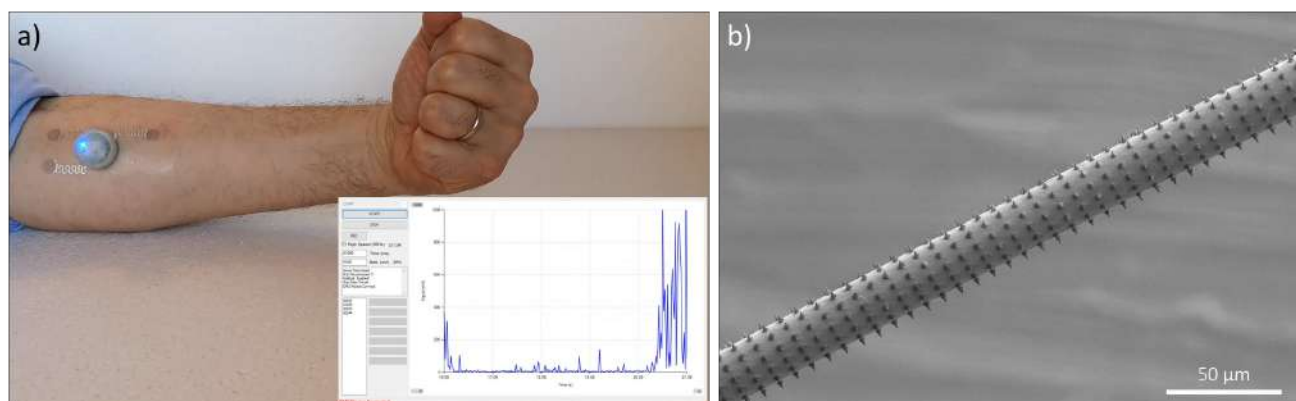


Figure 1: a) Ultrathin conformable tattoo electrodes for detection of electromyographic signals and wireless transmission. b) Example of microstructures integrated on a small diameter wire by nanometric-thin film wrapping.

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Abstract

The use of functional nanomaterials with magnetic, plasmonic and acoustic properties are appealing for introducing new functionalities to medical microrobots,^[1] in particular they enable for example the steering of the microrobots by external magnetic fields,^[2] or their visualization under scattering tissues via ultrasound or photoacoustic imaging techniques.^[3–5] Moreover, nanocarriers such as polymersomes and liposomes, which have been widely used as passive drug carriers, are here employed to decorate the surface of such medical microrobots, to increase their cargo (e.g. drugs, enzymes)-loading capacity, while providing them with specific triggering strategies that enable their function on demand.^[6–8] Additionally, as the microrobots are active devices with high thrust forces they are promising for targeted therapies aiming to reach disease sites deep in tissue.^[9,10]

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Figures

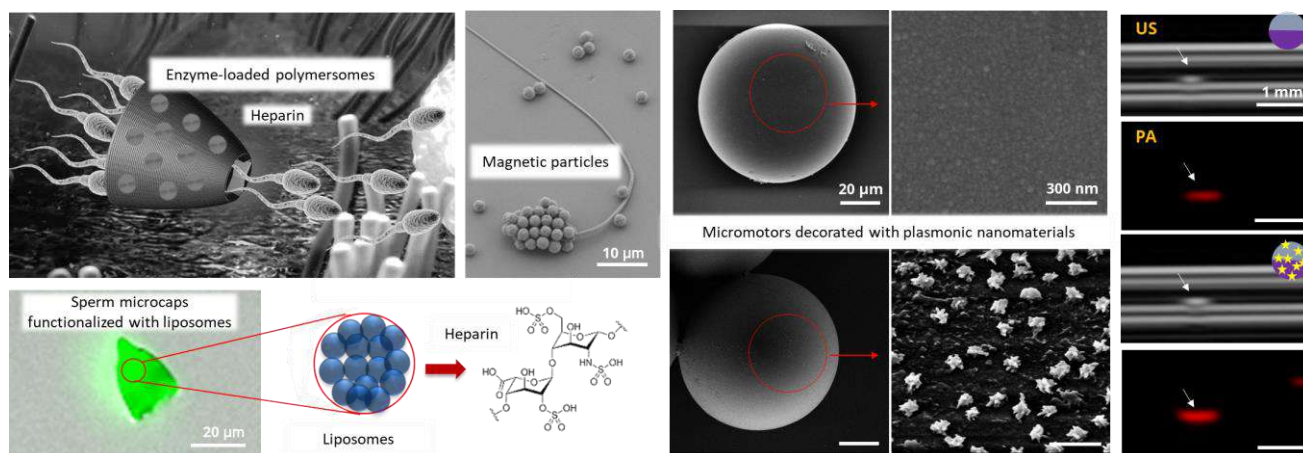


Figure 1: Various medical microrobots and micromotors functionalized with nanomaterials

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Abstract

First principles simulations are crucial in many areas of nanoscience. In electrochemistry, however, the complexity of the electrochemical environment and the presence of the external electrode potential have precluded direct application of first principles methods like DFT. We aim to overcome these barriers by utilizing recent breakthrough advances in modelling techniques that allow us to extend the use of DFT to the complexity of the electrochemistry processes.

We demonstrate how Non-Equilibrium Green's Functions (NEGF) techniques can be used to address, from first principles, the atomistic description of metal-electrolyte interfaces in the presence of an external bias applied to the electrodes. The NEGF method [1,2], implemented in the SIESTA DFT code [2,3], and commonly used to study electronic transport in nanoscale constrictions, is used here to describe the electrified solid/liquid interface, including the electronic charge redistribution induced by the external bias, and the resulting electrostatic profile. This allows us to study the structural and dynamic changes in the liquid (including the electrical double layer) and chemical reactions occurring at the electrified interface.

We will show DFT molecular dynamics simulations of aqueous electrolytes as a proof of concept for future realistic, atomistic first-principles simulations of electrochemical processes. Additionally, we explore the possibility of reaching much larger system sizes and longer simulation times by combining the DFT approach to deal with the electrodes (where the quantum-mechanical description is essential), with a molecular mechanics model for the liquid electrolyte (or part of it, not involved in the electrochemical reactions). This hybrid QM/MM approach is currently fully functional in SIESTA, allowing the simulation of realistic system sizes with a greatly reduced computational workload. The code, which offers parallelism through both OpenMP and MPI, shows an excellent parallel performance in modern HPC platforms.

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Figures

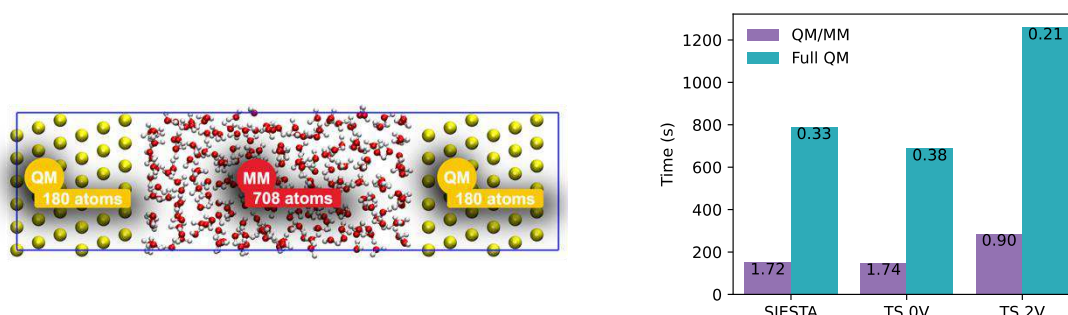


Figure 1: Left: QM/MM setup for electrode (gold) / electrolyte (water). Right: comparison of timings for QM/MM vs fully QM calculations for three MD steps for SIESTA using diagonalization (left bars), and for TranSIESTA using the NEGF formalism at $V=0$ Volt (center bars) and $V=2$ Volt (right bars). The numbers on the bars indicate the number of picoseconds per day. Data are from MareNostrum IV, using 384 cores. For this system size, QM/MM is about five times faster than a fully QM calculation.

Unraveling Secrets of Photoluminescence of Carbon Dots by Computational Chemistry

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Carbon dots (CDs) discovered in 2004 are extensively studied nanomaterials due to their applications in sensing, bioimaging, theranostics and many others. Despite the joint effort of experimental and theoretical approaches a clear link between structure of CDs and their photoluminescent properties has not been established yet. In the talk, I will introduce theoretical tools and models, which provide valuable insights into optical properties of CDs. Particularly, the spotlight will focus on a combination of classical molecular dynamics simulations and theoretical methods for the description of absorption and emission of CDs, mostly time dependent density functional theory providing valuable insights into the nature of the excited states and the source of PL. One of the objectives of this talk is to show that combining the state-of-the art theoretical approaches [1] and modern experimental techniques is very effective strategy in the photoluminescence studies of CDs.

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Nanosensors: Carbon Based Nanostructured Materials for Sensitive Monitoring of Pharmaceuticals

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A sensor is a device that detects and responds to some type of input from the physical environment. The sensor can convert the measurement into a readable signal. For electroanalytical sensor technologies, nanomaterials are mostly used for creating a biosensor, biomarker, or nanosensor. In recent years, sensor technology with its wide applications has become very popular in the biomedical and pharmaceutical areas. Sensor studies provide an overview of some of the important and recent developments brought about by the application of carbon-based nanostructures to nanotechnology for both chemical and biological sensor development and their application in pharmaceutical and biomedical areas. Nanotechnology has become very popular in the sensor fields. It is thought that the utilization of such technologies, as well as the use of nanosized materials, could well have beneficial effects on the performance of sensors. All materials are composed of grains, which in turn are made of molecules and atoms. Nanomaterials are those having grain sizes in the range of nanometers. Nano-sized materials have been shown to have a number of novel and interesting physical and chemical properties. There exist various materials of different types for fabricating nanosensors. Especially, functional carbon-based nanomaterials have become important due to their unique combinations of chemical and physical properties, extensive research efforts are being made to utilize these materials for various industrial applications, such as high-strength materials and electronics. These advantageous properties of carbon-based nanomaterials are also actively investigated in several areas of biomedical and drug assay. Electrochemical nanosensors have recently found extensive applications in pharmaceutical and biomedical industries with some advantages such as lower detection limits, wider linear response range, sensitivity, good stability, and reproducibility when compared with other sensors and techniques. Nowadays, a lot of different analytical methods are used in environmental, pharmaceutical, or clinical laboratories, and also a number of commercial point-of-care devices work using nanosensors. As the demand for smaller, faster, cheaper, and ultrasensitive qualification and quantification of samples rapidly increases, these methods provide a viable path toward the next generation of electrochemical sensors. In recent years, carbon-based nanosensors have been commonly used in pharmaceutical applications, further for real sample applications like dosage forms, human body fluids, etc.

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Using 2-dimensional materials in a 3-dimensional world: graphene composites for batteries, filters and aerospace

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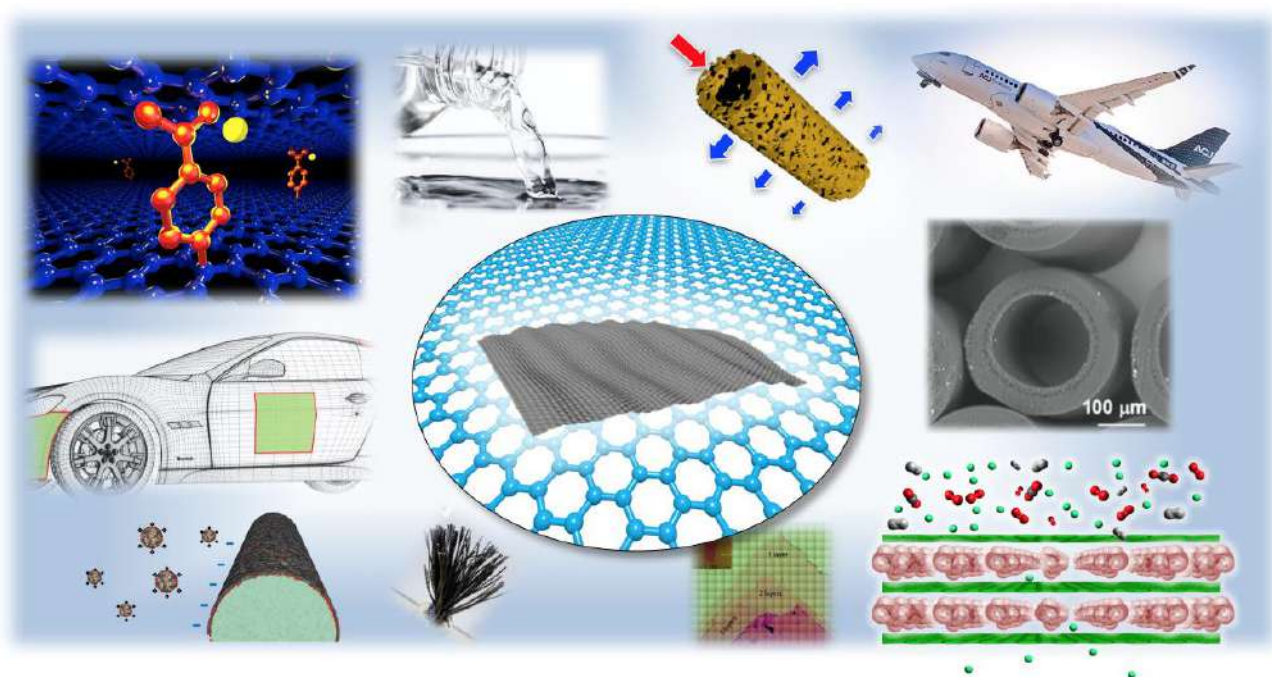
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Graphene is currently produced in tons scale as nanosheets or multilayer flakes, to be mixed in polymer composites, mainly for structural reinforcement. Such composites typically contain random dispersions of graphene in a polymer matrix, thus taking advantage only in part of the peculiar properties of graphene and of its unique 2-dimensional structure.

The development of new composites, featuring a more refined hierarchical structure and a controlled processing of graphene, would allow to exploit its properties at best, enabling groundbreaking applications; in this talk, I will describe how we process 2-dimensional nanosheets of graphene and graphene oxide in complex 3-dimensional composites using surface chemistry, electrochemistry and conventional filtration.

In this way, we produced and tested nano-composite materials in the form of foams, coatings and fibers to be used in energy storage, aerospace and water purification.



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Counting molecules, dodging blood cells: real-time molecular measurements directly in the living body

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The availability of technologies capable of tracking the levels of drugs, metabolites, and biomarkers in real time in the living body would revolutionize our understanding of health and our ability to detect and treat disease. Imagine, for example, a dosing regimen that, rather than relying on your watch (“take two pills twice a day”), is instead guided by second-to-second measurements of plasma drug levels wirelessly communicated to your smartphone. Such a technology would provide researchers and clinicians an unprecedented window into physiology and pharmacology, and could even support ultra-high-precision personalized medicine in which drug dosing is optimized minute-by-minute using closed-loop feedback control. Towards this goal, we have developed a biomimetic, electrochemical sensing platform that supports the high frequency, real-time measurement of specific molecules (irrespective of their chemical reactivity) in situ in the blood and solid tissues of awake, freely moving subjects.

Figures

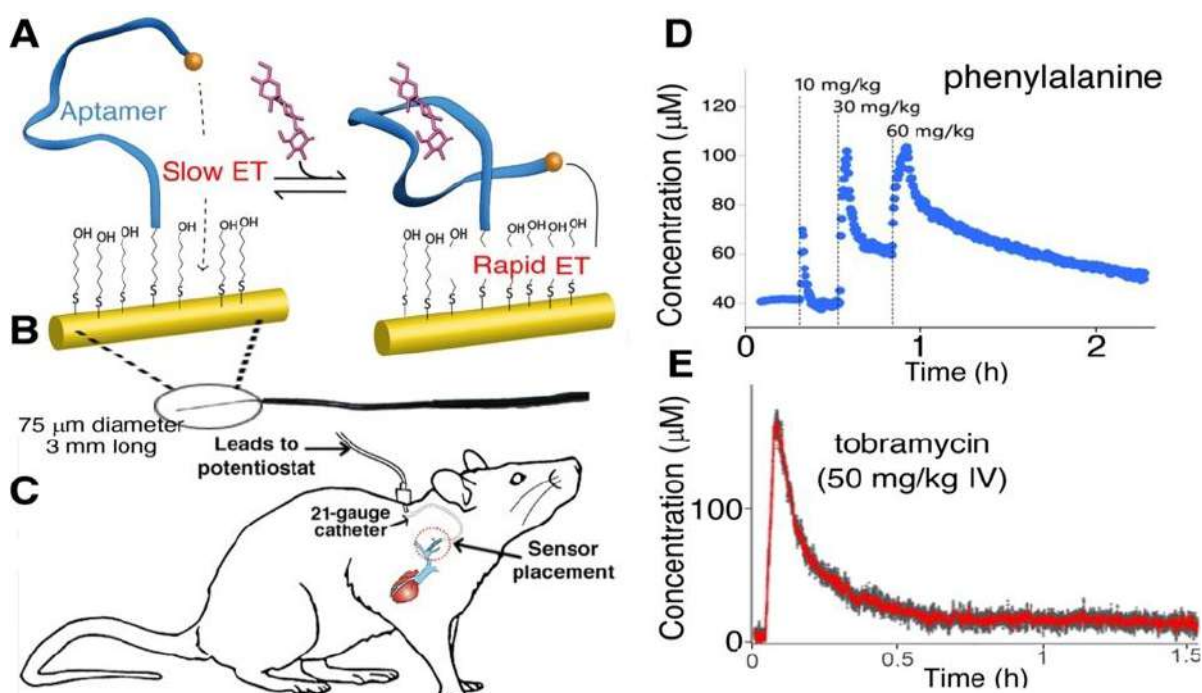


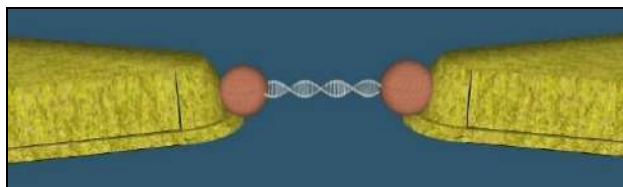
Figure 1: Electrochemical Aptamer-Based (EAB) sensors, a platform technology that relies on receptor binding, and not on the target’s intrinsic chemical reactivity, to generate a signal, are (A) comprised of an aptamer re-engineered to undergo reversible binding-induced folding. This is modified with a redox reporter and attached (via a self-assembled monolayer) to a gold electrode. The binding-induced conformational change causes a corresponding change in electron transfer rate that is easily measured using electrochemistry. (B) Bundled with its counter and reference electrodes, current intravenous EAB sensors are small enough and flexible enough to (C) be emplaced via a 21-gauge guide catheter. (D) When interrogated using square-wave voltammetry, the resulting sensors achieve excellent precision and few-second resolution. Shown, for example, are 12-s resolved phenylalanine measurements performed in the jugular of a live rat. (E) Using chronoamperometry we can push the time resolution to milliseconds; shown, for example, are intravenous tobramycin levels measured every 300 ms (red line, a 3 s rolling average).

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Abstract



The DNA double-strand recognition, as well as the ability to manipulate its structure open a multitude of ways to make DNA useful for molecular electronics. We recently reported a breakthrough in measuring charge transport in DNA (Nature Nanotechnology 2020) in a special configuration. This finding is of great importance by itself for understanding electricity in DNA in particular, and for molecular electronics in general. However, it also paves the way for the design of new ultra-sensitive detectors for DNA and RNA. Addressing these challenges is at the heart of the current pandemic as well as for early detection of cancer.

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Carbon-stabilised porous silicon nanostructures to build the next generation of diagnostic tools

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To create the next generation of diagnostic tools based on nanostructured electrochemical biosensors, tuning of the morphological features and electrochemical properties of the transducer is paramount. Our approach to design highly performing sensing devices harnesses the knowledge acquired to fabricate layers of porous semiconductors that can be carbon-stabilised and site-specifically functionalised, to adjust their electrochemical properties and biorecognition capabilities.

Key to the development of this new class of nanostructured biosensors is our work on carbon-stabilised porous silicon (pSi) [1-3]. The potential of this material for electrochemical sensing is herein exemplified by a unique carbon-stabilised pSi double-layer nanostructure fabricated via a two-step electrochemical anodisation process. [4] The pore morphological features (e.g. pore size, depth and porosity) at each pSi layer are precisely defined by simply varying the anodisation parameters. Next, different types of carbon with tailored wettability and surface chemistry are formed *in situ* on the pore walls of each layer via stepwise temperature-controlled acetylene decomposition. Double-layer structures with distinct functionalities on each layer are harnessed for site-specific modification of bioreceptors. These platforms not only feature remarkable geometrical properties, but also excellent electrochemical performance, underpinned by their fast electron-transfer kinetics, low double-layer capacitance and high sensitivity. The potential of carbon-stabilised pSi double-layer structures as novel highly performing biosensors is here demonstrated by developing a voltammetric sensor for the detection of key nucleic acid biomarkers.

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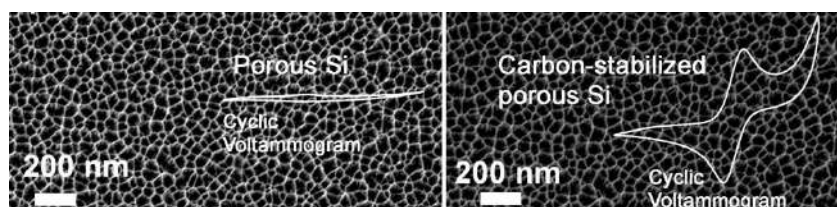


Figure 1: Scanning electron microscopy images and cyclic voltammograms of a pSi substrate prior and after carbon stabilisation.

Amorphous 2D Materials for Applications in Nanoelectronics and Neuromorphic Computing

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The fabrication and characterization of disordered materials has recently witnessed an outstanding progress leading to materials with unprecedented properties. In particular, the possibility to synthesize wafer-scale two-dimensional amorphous carbon monolayers, structurally dominated by sp^2 hybridization, has been demonstrated. This achievement has initiated a new platform of low-dimensional materials allowing to explore alternative forms of membranes with enhanced chemical reactivity which could be employed for instance in advanced coating materials [1,2].

The excellent physical properties of the mentioned materials derive from the nature and degree of their disorder which, controlled at the fabrication level, represents the key ingredient to tune their physical/chemical properties for specific target applications. In this respect, new fabrication strategies to modify the degree of disorder and a systematic theoretical characterization of the impact of the material structural quality on the ultimate performance is urgent. Even more importantly, the search for new disordered materials for novel applications appears as an extremely promising way. In this talk we present a systematic analysis of the structural, vibrational, and electronic properties of amorphous carbon monolayers as a function of the structural quality of the material. We show how disorder results in a tunable electrical conductivity and thermal properties [3]. Finally, we present the results of the newly demonstrated synthesis of a thin film of amorphous Boron Nitride showing extremely low dielectric characteristics: high breakdown voltage and likely superior metal barrier properties [4]. The fabricated material aims at replacing current interconnect insulators in the next generation of electronic circuits. We discuss the experimental setup and present the results of our calculations which have contributed to the understanding of the structural morphology of the amorphous material. We conclude discussing the resulting thermal and electronic properties [5,6] and the applications in neuromorphic computing.

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Heat capacity measurements at the nanoscale

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Heat capacity is one of the fundamental properties of matter but at the same time one of the most difficult to measure with sufficient accuracy at the nanoscale. The difficulty rises exponentially with the reduction of the mass of the sample, being measurements in nm-thick materials extremely rare and challenging. Microfabricated membrane-based nanocalorimeters working in quasi-adiabatic conditions in ultrahigh vacuum are suitable probes to provide direct access to the heat capacity of the sample and unveil dimensionality effects on phase transitions. I will show several examples of nanocalorimetric-based measurements of phase transformations in nm thick materials. In particular, size effects in the ferro or antiferromagnetic transition of thin film magnetic materials [1,2] and the anomalous transformation of highly stable organic glasses into their supercooled liquid during thermal treatments [3,4].

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Controlling the functionality of surfaces and nanoparticles with mussel-inspired approaches

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Abstract

Engineered coatings allow for control over the interface of a material and its interactions with the surrounding environment as well as for the endowment with functional properties such as chemical inertness, adhesion, biocompatibility, hydrophilicity/hydrophobicity, among others. Most of the coatings so far reported, either as a polymer or self-assembled monolayer, rely on specific chemical interactions between a given substrate and the material used as a coating. More recently, the development of substrate-independent functional thin films such as organic polydopamine (PDA) coatings and hybrid metal–phenolic networks (MPNs), have attracted widespread interest because the broad range of surfaces coated. Though, nowadays it is still challenging to predictably engineer a broad range of properties (e.g., charge, thickness, wettability, adhesion, transparency).

To overcome this challenge, in our group we have been working on different experimental approaches, ranging from the polymerization of catechols in the presence of amines (ammonia or bisamines). Our more recent results on different applications ranging from environmental to nanomedicine applications will be revised in this talk.

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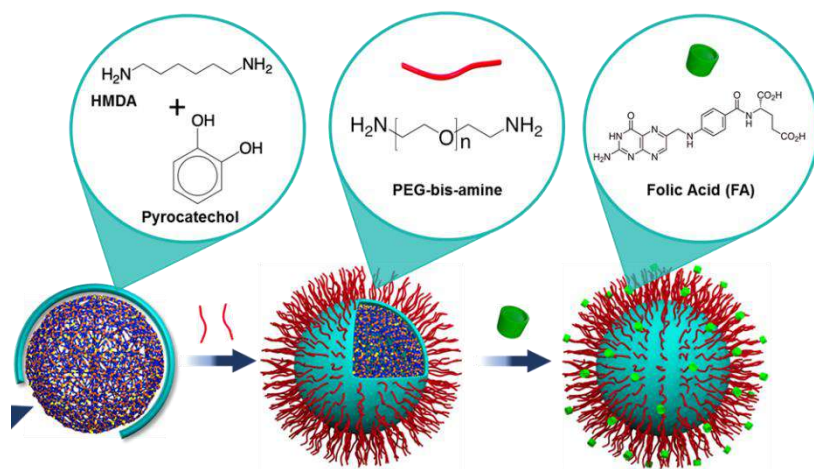


Figure 1: Representative example of application of our coatings to enhance the colloidal stability, biocompatibility and targeting of drug delivery nanocarriers

4D Nanomembrane Materials for Electronic Skin and Microrobots

Oliver G. Schmidt

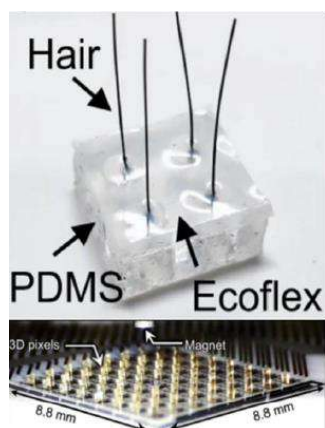
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4D materials change their shape in time. If prepared as stimuli-responsive nanomembranes on a chip surface, they are attractive for various scientific disciplines ranging from electronic skin to microrobotic systems. This talk presents the fascinating application potential of 4D materials for soft electronic skin [1], highly integrated microelectronic catheters [2] and medical and microelectronic microbots [3-5]. Particular attention will be paid to the challenge of on-board energy supply for autonomously acting smart dust microsystems [6-8].

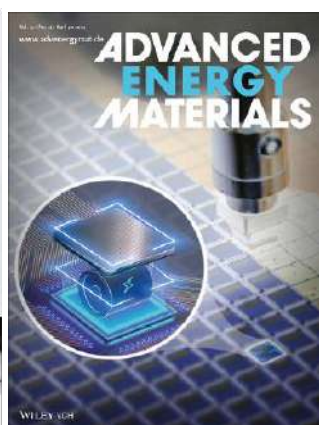
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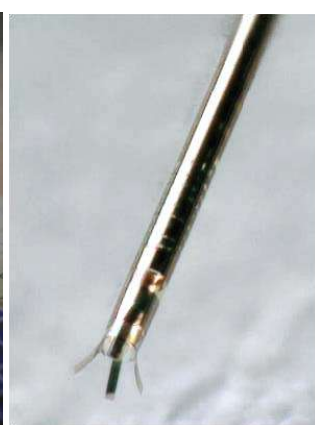
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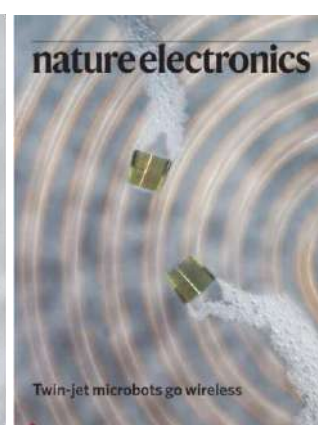
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We have developed an alternative to dye labeling for single molecule experiments: we utilize plasmonic gold nanoparticles to detect single unlabeled proteins with high temporal resolution (ms to μ s). This allows for monitoring the dynamic evolution of DNA hybridization or protein binding. The technique resolves equilibrium coverage fluctuations, opening a window into Brownian dynamics of unlabeled macromolecules. Therefore, our method enables the study of DNA or protein folding dynamics, protein adsorption processes, and kinetics as well as non-equilibrium soft matter dynamics on the single molecule level without need for labelling [1]. Recently we also used this technique to monitor the dynamics of molecules inside of the body by implanting nanoparticle doped hydrogels under the skin of hairless rats. [2,3]

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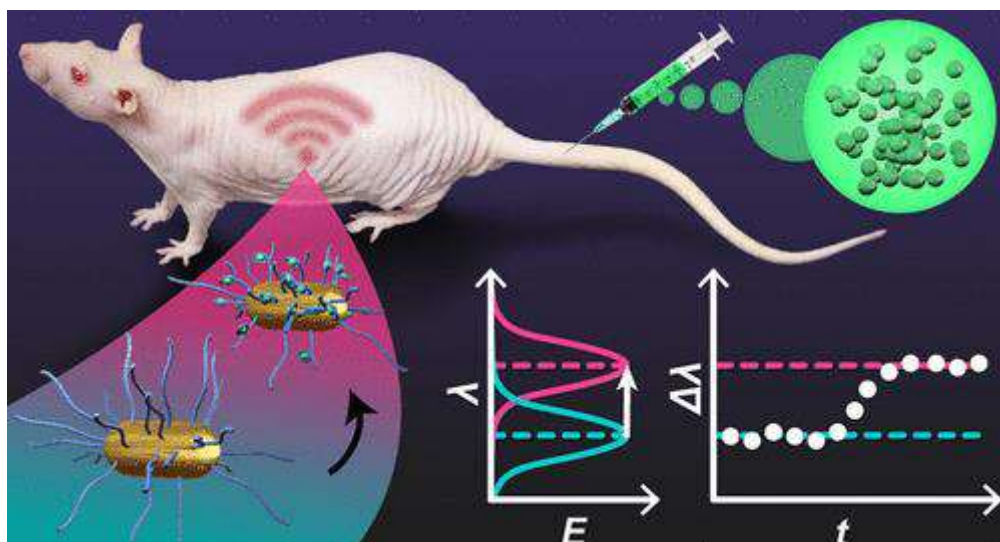


Figure 1: Implantable sensors continuously transmit information on vital values or biomarker concentrations in bodily fluids, enabling physicians to survey disease progression and monitor therapeutic success.

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The search for new state variables beyond electrons, spins and photons has turned its attention to low energy potential information carriers such as phonons.

We will report our work based on optomechanics and localization to create phonon sources based on co-located phononic and photonic crystals to confine phonons and photons in the same volume via optical and electrical driving by means of optical waveguides and surface acoustic waves, yielding a circuit based on phonons [1] which is CMOS-compatible and operates at room temperature at 2 GHz.

We will show how inherent fluctuations in critical dimensions help to localize phonons and enable phonon lasing at 6.5 GHz mediated by confined phonons modes in a slotted waveguide [2].

Finally, we will show how a phonon waveguide can be realized and characterised to establish modes in the mechanical gap (7-11 GHz) of a phononic crystal-based waveguide [3].

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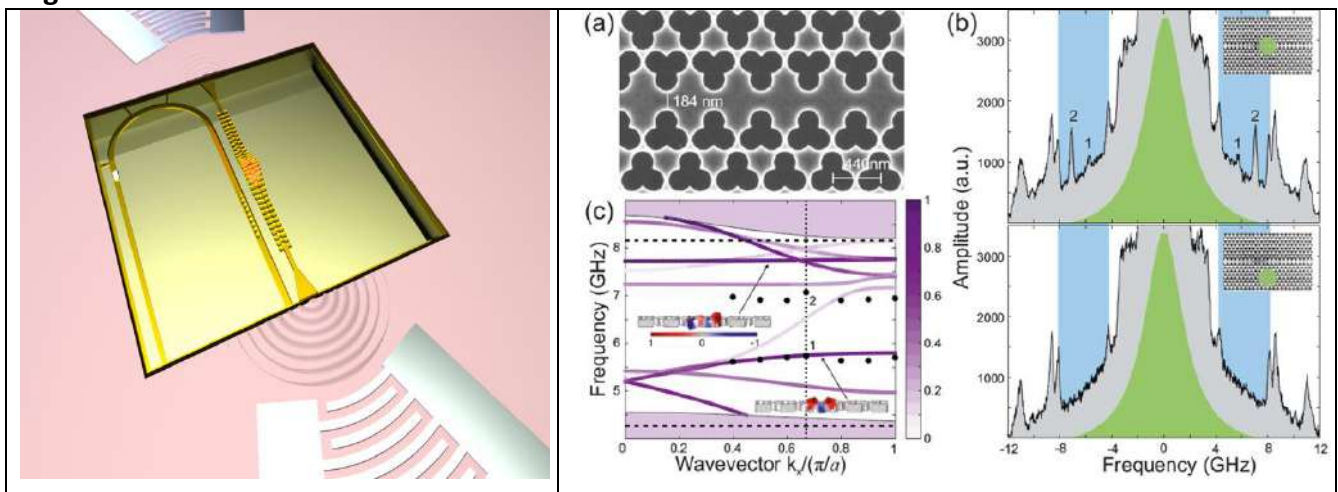


Figure 1: Left: Schematic of the phononic circuit. Right: GHz phononic waveguide. SEM of the line defect waveguide (a). BLS spectra with the mechanical band gap highlighted in blue, where 1 and 2 denote guided phononic modes (b). Band structure showing gap and guided modes (c).

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Nonlinear optical phenomena play a key role in many fundamental processes and are highly relevant for a wide range of applications, including quantum technologies, optical computing, and advanced spectroscopies. Many excellent materials are available for nonlinear optics in the visible and infrared part of the electromagnetic spectrum.

Until a few years ago, this was not the case for the terahertz regime, where only moderate nonlinearities were obtained with quantum well systems. This situation changed dramatically with the observation of highly efficient harmonic generation in quantum materials with massless Dirac fermions – charge carriers with a linear energy-momentum dispersion relation – such as graphene [1] and topological insulators [2].

In this talk, I will discuss our most recent results, obtained with a large group of collaborators, including researchers at TELBE (Germany), the University of Manchester (UK), Bielefeld University (Germany), ICFO (Spain), ICN2 (Spain), and several more. In particular, I will present ways of obtaining enhanced THz nonlinearities using quantum materials (see Fig. 1). These approaches include *a*) enhancing the THz nonlinearity of quantum materials through electrical control of the Fermi energy [3], *b*) using metal grating structures with micrometer-sized gaps that lead to local field enhancement [4]; and *c*) circumventing the saturation of harmonic generation that occurs in graphene due to heat accumulation by exploiting “Coulomb cooling” that provides enhanced electronic dissipation [5,6,7].

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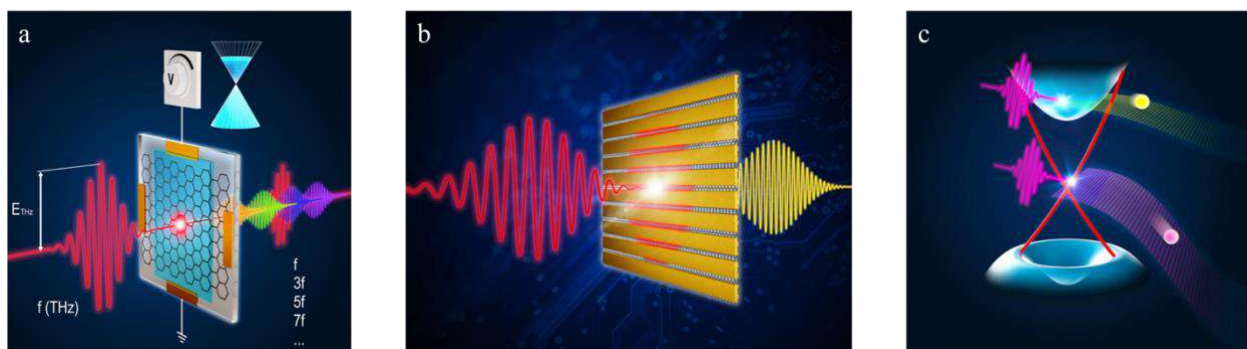


Fig. 1. **a**) Terahertz harmonic generation control and enhancement via electrostatic gating of a graphene-electrolyte system [3]. **b**) Grating-graphene metamaterial with strongly enhanced nonlinear susceptibilities due to field enhancement [4]. **c**) Band structure of topological insulator with faster cooling of surface state electrons [5,7], leading to enhanced harmonic generation [6]. All three images by HZDR.

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Label-free protein detections at a single-molecule resolution are implemented with nanometric interfaces hosting a few recognition elements. The cross-section of the interaction is low so a target protein concentration of at least nanomolar is essential. When a large millimeter-wide electronic interface is engaged, a single molecule (entity) limit of detection can be reliably reached in detecting antigens (Immunoglobulins, C-reactive proteins, spike 1, HIV p-24, ...), antibodies (anti-immunoglobulins, anti-spike 1, ...) peptides, viruses (SARS-Cov-2), bacteria (*Xylella fastidiosa*), and even DNA strands (KRAS, miR-182). This technology is called SiMoT - Single-Molecule with a large Transistor.[1] Selectivity is assured by covering the gate electrode with a large number (10^{11} - 10^{12} / cm^2) of a suitable recognition element to affinity binding of the target element.

With the SiMoT a single entity can be detected directly in a droplet (0.1 mL) of a real fluid such as saliva from COVID-19 patients, blood serum, pancreatic cysts juice, and olive saps from infected trees. Relevantly Brownian diffusion enables the entity to statistically hit the millimeter-wide interface in a few minutes.[2] Considering the footprint of a molecule on a millimeter-wide interface, it is like spotting a droplet of water falling on the surface of a 1 Km wide lake.

The applications span from a handheld intelligent single-molecule binary bioelectronic system for fast and reliable immunometric point-of-care testing of COVID-19 patients with an incidence of both false positives and false negatives of less than 1%. This means a fast (21 minutes time-to-results) and disposable immunometric test in saliva with a limit of detection of 20 zeptomolar (1+1 virus in 0.1 mL) and reliability (diagnostic sensitivity, specificity, and accuracy) of 99.2%. Meaning with the figures of merit of a PCR-based molecular test.[3] Moreover, a fast and reliable electronic assay of a *Xylella fastidiosa* single bacterium in infected plants sap is achieved, outperforming the PCR limit of quantification by at least one order of magnitude.

The phenomenon that enables this outstanding performance level was discovered in 2018.[4] While still under investigation, it is supposed to involve an amplification effect that starts from the single affinity binding event involving just one recognition antibody or complementary genic sequence. The extra energy associated only with the affinity binding locally generates a conformational change with its associated electrostatic impact, which is enough to trigger a collaborative response that propagates the change in surface potential involving at least 10^6 – 10^8 antibodies hence a very large portion of the gate area.

Future actions include deepening our understanding of the sensing mechanism and engaging in a campaign of thousands of clinical trials that will bring SiMoT beyond TRL5.

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The atomically thin nature of 2D materials promotes the design of van der Waals heterostructures by proximity effects originating from short-range interactions [1]. This designer approach is particularly compelling for spintronic devices, which harness their functionalities from thin layers of magnetic and non-magnetic materials and the interfaces between them [1,2]. On the other hand, the ability to control the generation of spins in arbitrary directions is a long-sought goal in spintronics. Charge to spin interconversion (CSI) phenomena strongly depend on symmetry. Systems with reduced crystal symmetry could allow anisotropic CSI with unconventional components, where charge and spin currents and the spin polarization are not mutually perpendicular to each other. In this talk, I will first demonstrate that proximity of a high-symmetry semiconducting transition metal dichalcogenide such as WS_2 enhances the CSI in graphene [3]. I will further show that the CSI is tunable with electrostatic gating and that the generated spin current and spin density by the spin Hall and the inverse spin galvanic effects, respectively, are mutually perpendicular to each other. Finally, I will show experimental results demonstrating that the CSI in graphene in contact with low-symmetry WTe_2 induces spins with components in all three spatial directions [4]. By performing multi-terminal nonlocal spin precession experiments, with specific magnetic fields orientations, I discuss how to disentangle the CSI from the spin Hall and inverse spin galvanic effects in this situation (Figure).

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Figure

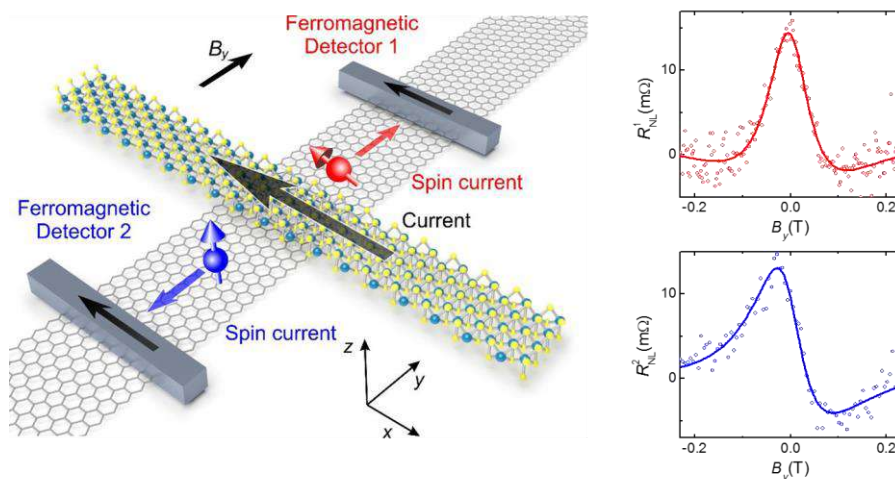


Figure: Left: detection scheme of the CSI in low symmetry structures, resulting in distinct spin accumulation on the left (blue) and right (red) ferromagnetic electrodes. Right: signals associated to such spin accumulation

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In this talk, I will present two kinds of electromechanical sensors developed in my group based on graphene, a pressure and touch sensor, and a biosensor.

NEMS pressure sensor: Graphene is an ideal membrane material for nano-electro-mechanical systems, combining low mass, high stiffness, high elasticity and high electrical conductivity. But large-scale fabrication of suspended graphene membranes has posed a challenge due to defects and wrinkles that occur during growth and transfer. We have developed a novel graphene-polymer heterostructure membrane (GPHM) which retains much of the advantages of graphene in NEMS, while providing 100% yield during fabrication processes, resulting in high performance and reliable devices. I will demonstrate pressure and touch sensors based on this GPHM technology which outperforms the current state of the art. We have recently demonstrated a route to integrating the GPMH with industry-standard process MEMS fabrication. I will also discuss a new finite element modelling package we have developed for the GPMH MEMS devices.

Biosensor: We have developed a graphene-enhanced quartz-crystal microbalance (G-QCM) chip for biosensor applications. This G-QCM chip is coupled with an in-house open source QCM platform, resulting in a low-cost, easy to use, high performance point of care diagnostic platform. We have demonstrated various immunoassay applications for this platform. In one approach, we immobilise antigens on the graphene surface to detect antibodies, in particular for membranous nephropathy, a kidney disease. In another approach, we have immobilised nanobodies on the graphene surface to detect proteins such as lysozyme. In both applications, the G-QCM sensor shows excellent sensitivity and selectivity compared to industry standard techniques.

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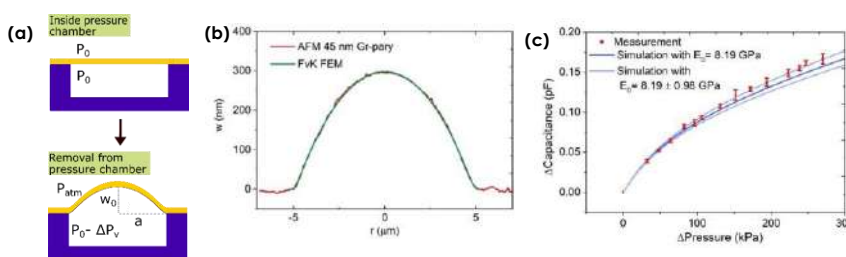


Figure 1: (a) 2-d schematic cross-section depicting the micro-blisters inflation testing procedure with a single cavity and actuating membrane with significant parameters labelled. (b) 2-d topographical line profile of inflated 45 nm thick GPH micro-blisters pressurized to $\Delta P = 116$ kPa, compared to the FEM solution to FvK equations (c) Change in device capacitance against change in external pressure compared to that predicted by FEM simulation.

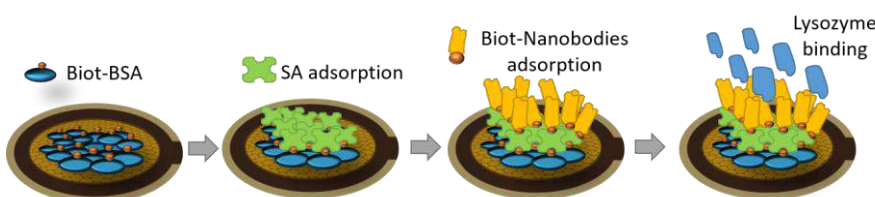


Figure 2: Sensing surface preparation for quantifying lysozyme in cow serum. The gold electrode from a QCM crystal is coated with a thin layer of GO then thermally reduced. Injection sequences are shown.

Molecular docking approach to elucidate potential genotoxic impact of copper engineered nanoparticles (CuO NP) upon red blood cells

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Abstract

Although copper-based nanoparticles (CuO-NPs) are widely used as anti-fungal and antibacterial agents and it is known that copper complexes have clastogenic effects by binding to minor and major grooves in DNA, there is no adequate information about the interaction mode and affinity of CuO-NPs with DNA [1]. In this study, docking simulations were performed to model the binding mode and interaction of CuO-NPs with its possible intracellular target, DNA, as well as to calculate its binding affinity against this target receptor. CuO-NPs significantly induced specific erythrocyte DNA damage (micronucleated cells), as well as an alteration in intracellular oxidative stress response (CAD, SOD and GST) in *Carassius carassius* used as model organism [2]. The docking results showed that the DNA damage induced by CuO-NPs could possibly be a direct damage rather than secondary ROS-induced event, that is, DNA damage induced by CuO-NPs is likely to be bimodal [3]. Ecophysiological studies on nano-bio interfaces combined with molecular docking can offer a powerful approach to better predict the effects of nanoparticles on animal and human cells and tissues.

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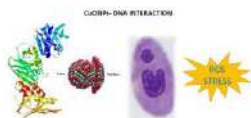


Figure 1: Copper nanoparticles-DNA interaction

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Abstract

Effective diagnostic systems with Point of Care (POC) nature, are very important in terms of diagnosis hence treatment of the patient [1]. POC systems can be defined as on-site diagnostic tests carried out at the patient bed-site using mobile devices like hand-held devices or a cart. These tests provide faster diagnosis by avoiding the need for laborious procedures and trained personnel. If the adaptation of biosensor systems to these POC diagnostic platforms is concerned, then practical, accurate, sensitive and economical biosensors must be developed. From this point of view, it is possible to say that the practical natures of electrochemical and colorimetric biosensors make them good candidates as being turned into diagnostic POC systems [2].

On the other hand, introduction of nanomaterials in diagnostic biosensing systems provides many advantages like high surface-to-volume ratio- which enables suitable surface modifications with bioactive compounds- excellent capacity, electrical conductance, good biocompatibility, localized surface plasmon resonance that results with intense visible color and selectively and sensitively altered color properties [2, 3]. For example, for electrochemical biosensors gold nanoparticles (Au-NPs) provide suitable environment for biological molecules and facilitate the reach out of electrons to the enzyme active center. On the other hand, carbon-based nanomaterials like carbon nanotubes and graphene have been widely used because they increase the electron transfer rate and provide higher surface area for the immobilization of biological molecules. Also, decoration of these two carbon-based nanomaterials with metal nanoparticles is easy and produces robust material in terms of electrochemical catalysis [1, 3].

Considering colorimetric biosensors, it has been reported that AuNPs have unique optoelectronic behavior. Also, Fe-based nanomaterials provide the necessary redox reactions in order to create color while with Au and Ag NPs it is possible to obtain intense visible color [3]. Apart from those, recently metal organic frameworks have gained considerable attention because of their surface areas and mimicking properties [4].

So, as a conclusion it can be stated that, development of effective biosensors with the help of nanomaterials, increase their effectiveness and probable usage potentials in POC diagnostic systems.

Keywords: Biosensors, Nanomaterials, POC, Nano-Diagnostic Systems, MOF,

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Best Combination of Selector Technology and Memory Element to Achieve High Density and Low Power Crosspoint Arrays for SCM Applications

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Abstract

In the area of booming in electronic components (smartphones, tablets, pc, smart home gadgets) combined with new applications (AI, Face and Speech recognition) – all generate a huge quantity of data that need to be stored efficiently and accessed fast. A better trade-off compared to what Flash and DRAM can provide is not sufficient to meet power-performance-density-cost requirements. Emerging non-volatile memory (NVM) such as PCM, RRAM, MRAM, FeRAM, can offer good option for Storage Class Memory (SCM) applications considering their speed is in the range of ~ns, their excellent scalability beyond 10nm and low power capability^{1,2,3}. To improve the memory density, NVM can be integrated in Crosspoint configuration where word lines (WL) are orthogonal to bit lines (BL) and the memory cell is placed in between the two electrodes. The main issue of this configuration is the presence of leakage or IR drop for half-selected cells with consequent degradation of the memory performance, variation of the electrical response and uncontrol of current and voltage of the cell. A possible solution consists in replacing the memory element with 1 Transistor and 1 Resistor, but the cell is mostly limited to the transistor performance and does not match well with scaling demand. Another option is to implement 1Diode-1R which has unipolar and high thermal budget, unfortunately self-rectifying cells are implemented but not mature enough. 1Selector-1R seems the best option. Selector technology (FAST, OTS, MIEC, VCB...) ^{4,5} are based on different mechanisms such as barrier engineering, threshold switching or volatile behaviour. The requirements for SCM need the selector to satisfy some parameters such as ON current density of >10MA/cm, very low leakage of pA, high selectivity>1E6, CMOS compatible processing temperature <400°C and scaling proportional to resistance element^{2,6,7}. The important task is to find the good match between NVM element and Selector. Many options are presented by different industry players such as OTS+PCM, OTS+OxRAM, OTS+RRAM, Hf-based Selector +MRAM reported in Fig.18. These options show already good performance in Mbit arrays and integrated in advanced 20nm node. The race is still open and researchers have the possibility to optimize 1S1R cell to overcome challenges such as memory wall (beyond Van Neuman - CiM, Hybrid Memory architecture) and integration from planar to vertical 3D structures (with optimized ALD process for scaled devices)⁹.

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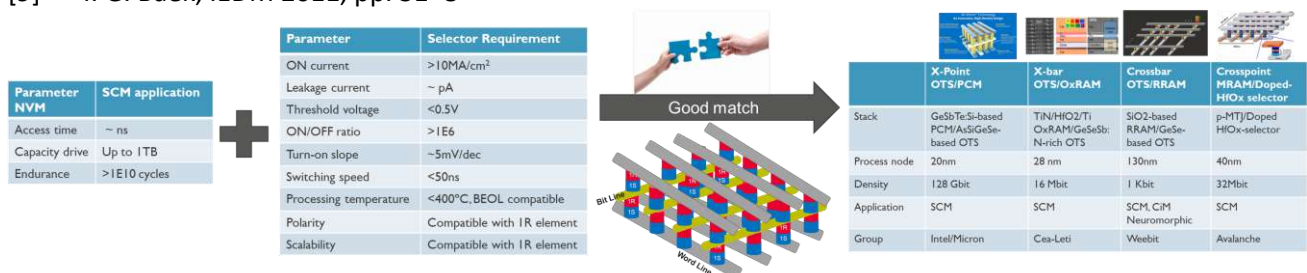


Figure 1: NVM technology and requirements in combination with Selector technology and specifications to achieve best 1S1R Crosspoint architecture towards SCM, ML and Neuromorphic applications [1-9].

Nanoencapsulation of bioactive compounds as novel strategy to improve their bioactivity and stability

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Current treatment of several diseases are often associated with drug resistance, side effects and high costs, indicating the need for more effective and less toxic therapies.

Plant bioactives have recently attracted great interest, due to their potential therapeutic effect to humans [1]. However, their therapeutic applications in general are limited since it's proven that they possess poor stability, water solubility and bioavailability, leading to decline/loss of efficiency. In that regard, nano-encapsulation of plant bioactives is a promising approach to overcome these disadvantages. The physicochemical properties of plant bioactive-loaded nanocarriers are based on the type and ratio of the nanocarriers as well as the nature of bioactives [2].

The particle size and surface charge of bioactive-loaded nanocarriers are critical parameters, as these improve physicochemical properties of bioactives and increase the membrane contact, the cellular absorption, and thereby the biological activity [3,4]. Furthermore, high nanocarrier encapsulation efficiency is crucial for addressing all concerns related to essential oil solubility and chemical stability, as well as for increasing the efficacy of bioactive-loaded nanocarriers, leading to increased therapeutic efficacy. The method of preparation, type of bioactives, vesicle composition, nanocarrier content, and storage stability was shown to impact these characteristics [4,5].

Therefore, our research was focused on development of a suitable nanoformulation for the effective encapsulation of plant bioactives. The antioxidant, antibacterial, and cytotoxic properties of plant-bioactives were significantly maintained and/or improved by their nanoencapsulation in lipid-based nanocarriers. Additionally, it has been shown that lipid-based nanocarriers are appropriate for encapsulating bioactives to increase their stability and bioavailability.

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Exotic properties of 2D materials: physics and real expectations for applications

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Abstract

The recent discoveries of exotic properties of 2D materials have opened the horizons for potential new applications that can finally project us in the Beyond CMOS realm. Indeed, 2D materials when discovered have been implemented in Moore's approach as in case of 2D used for transistors. This is not the right approach in order to achieve real advances in physics and in defining the implementation of the new roadmaps for new devices based on innovative concepts. In this contribution, we will analyse the main phenomena recently discovered such as magic angle, valleytronics and 2D topological insulators in order to understand which are the potential applications of these devices. We will analyse in a completely objective way which are the main potential implementations of these phenomena. We will perform a roadmap identifying the major turning point in each case. This analysis will allow to have a precise idea of what could be only a hype phenomenon and what could be a real game changer for specific applications.

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Electrochemical biosensing using nanochannels: from the stochastic sensing to the use of nanoporous membranes

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Selective transport in protein-based ion channels is already used in living systems for electrical signaling in nerves and muscles, being this natural behavior approached for the use of biomimetic nanochannels in biosensors. On the basis of this principle, nanopores and nanochannels-based platforms stand out from the variety of nanostructured materials, bringing new advantages for biosensor development and applications. The emerging use of arrays of solid-state nanoporous membranes has opened the way to different and versatile sensing systems ranging from electrical to optical detection devices [1].

The purpose of this talk is to give an overview on the recent trends in the use of nanochannels for electrochemical biosensing applications [2]. Some general considerations on the principles of the stochastic sensing, before focusing on the applications for DNA, protein, virus and other analytes detection will be given. Special focus will be put in recent approaches for the *in situ* monitoring of biomarkers for wound infection diagnosis as well as antimicrobial agent evaluation [3,4].

The state-of-the-art of the developed technology may open the way to new advances in the integration of nanochannels with (bio)molecules and synthetic receptors for the development of novel biodetection systems that can be extended to many other applications with interest for clinical analysis, safety, and security as well as environmental and other industrial studies and applications.

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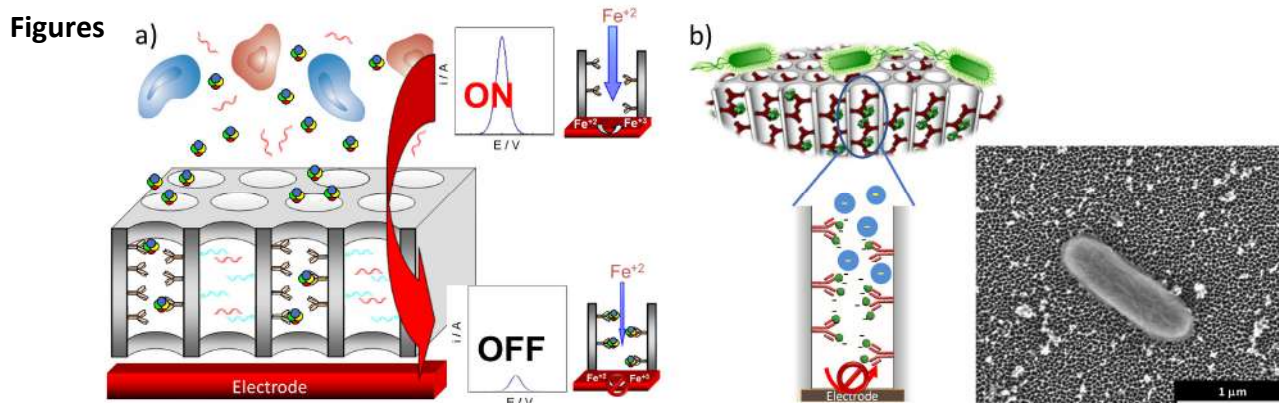


Figure 1: a) Schematic representation (not in scale) of the electrochemical biosensing strategies using nanoporous membranes, based on the concept of the stochastic sensing. b) Scheme and HRSEM image illustrating the bacteria culture on nanoporous membranes and the continuous capturing of secreted virulence factors by antibodies inside the nanochannels, leading to their steric/electrostatic blocking.

Acknowledgements

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Abstract

The recent Covid-19 pandemic proved that easy to use devices providing prompt responses concerning the presence and possibly the concentration of specific nucleic acids and antibodies are badly needed. In this occasion, lateral flow devices took the opportunity on the fly to become popular even to the man in the street, whereas biosensors lost an incredible chance. To avoid this to happen again in future, innovation is needed in the biosensor field, starting from the improvement of the amplification strategies to the development of novel bioreceptors and biosensing strategies enhancing the selectivity towards the analytical target and reliability. We provide here a few examples concerning the use of the CRISPR/CAS systems for the detection of nucleic acids [1] as well as the use of programmable Y shaped DNA nanostructures to bind specific antibodies [2]. In the first case, an easy use, rapid and low cost detection system based on a label free ssDNA immobilized on a gold electrode exploited a Cas12a protein and electrochemical impedance spectroscopy to detect the DNA of elected bacterial pathogens (Figure 1, left). In the second case, a y-shaped nanostructure created by self-assembling of three engineered ssDNA was converted into a responsive bioreceptor by modifying the three strands with two recognition elements, two redox tag molecules, and a thiol group. The reduced mobility of the nanostructure upon the interaction with the target resulted in a decrease of the electrochemical signal quantitatively related to the target concentration (Figure 1, right).

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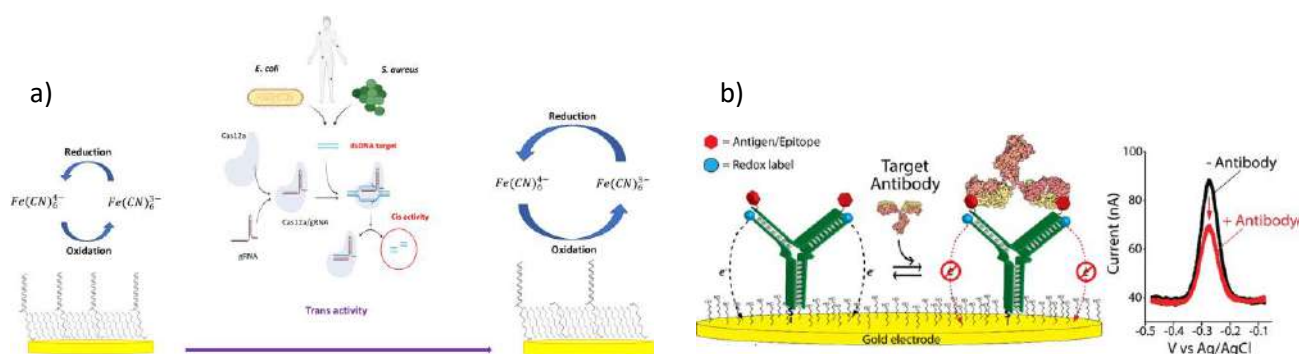


Figure 1: In the first example, the binding of the Cas12/gRNA system with the target DNA triggers the collateral activity of CAS 12, which cleaves the ssDNA on the electrode surface, improves the exchange of charges between the electrode and the solution and increases the electrochemical signal (a). In the second example, the binding of the target limits the mobility of the nanostructure and the exchange of charges with the electrode, decreasing the electrochemical signal (b).

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Integration of flexible electronics into the living system is expected for advancing medical diagnostics and therapeutics. Such devices should be seamlessly conformed to the physical and mechanical environment of living body, in which acquired biosignals are expected to be transmitted wirelessly to external device. In this regard, we envisage the development of ultra-flexible electronics for wearable and implantable applications based on polymer nanosheet technology. The polymer nanosheet shows tens- to hundreds-of-nanometer thickness close to the scale of biomembranes [1], in which various types of polymers (e.g., biodegradable polymers, conductive polymers, and elastomers) are formed into the ultra-thin structure. Free-standing polymer nanosheets showed flexible and adhesive properties derived from their ultra-small flexural rigidity ($< 10^{-2}$ nN m). In this talk, polymer nanosheet (or thin film)-based devices are introduced by combining polymer nanosheet and printing technologies with variety of unique inks [2] (Figure 1). The ultra-flexible device has been utilized as tissue-interfaced electronics to direct biosignals or functions in the design of ultra-conformable bioelectrodes for sports science [3] and plant biology [4], battery-free biosensors for glucose monitoring [5] and gas sensing [6], and implantable devices for photodynamic therapy [7] and hyperthermia therapy [8] in cancer treatment.

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Figures

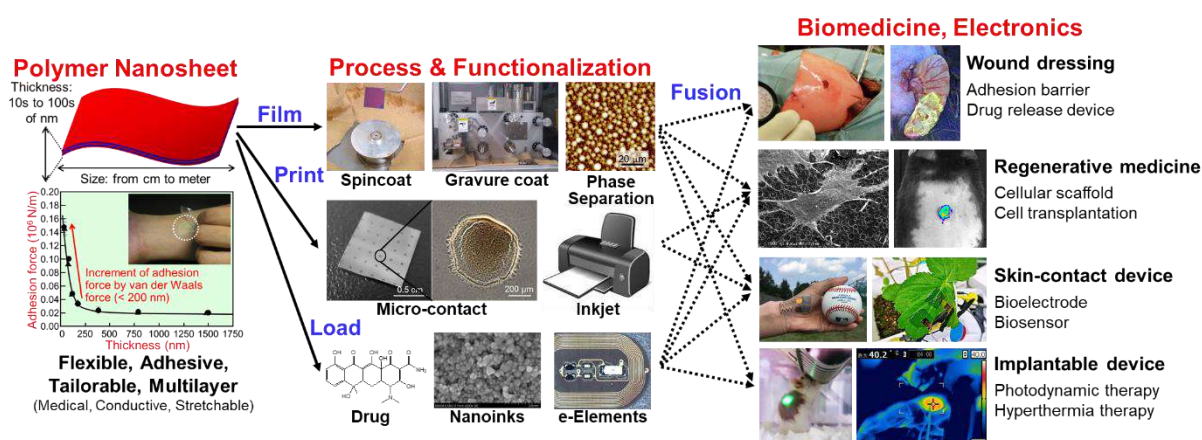


Figure 1: Ultra-flexible medical device based on polymer nanosheet technology

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Abstract

Gas and volatile organic compound detection in exhaled breath is an emerging diagnostic technique. Breath can contain thousands of such compounds, usually at ultralow levels, making it necessary to develop highly sensitive and selective detection tools. Carbon nanomaterial-based chemiresistors outperform the traditional metal-oxide sensors in terms of sensitivity at room-temperature, [1] which is convenient toward the miniaturization in point-of-care diagnostic applications. However, selectivity is a known issue still to be addressed and in the focus of current research efforts.[2] Two approaches are promising and compatible with each other to contribute substantially in the improvement of the selectivity. The first of them consists on the surface engineering of the sensing nanomaterial by including elements of known chemical affinity toward the target gas. We describe how the functionalization of carbon nanotubes with gold nanoparticles (Figure 1a) results in improved affinity toward hydrogen sulfide, a known marker of small intestinal bacteria overgrowth. A self-validation device results from the integration of multiple of such sensors in a single chip.[3] The second approach is based on the implementation of machine learning algorithms to maximize the information obtained from a single sensor. We report how its use with a graphene-based device helps to distinguish ammonia and phosphine, gases that interact similarly with graphene, by deeply analyzing their interaction kinetics (Figure 1b). [4] We predict that combining these two approaches can be a key step in the realization of novel, smart gas sensing platforms of high analytical efficiency.

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Figures

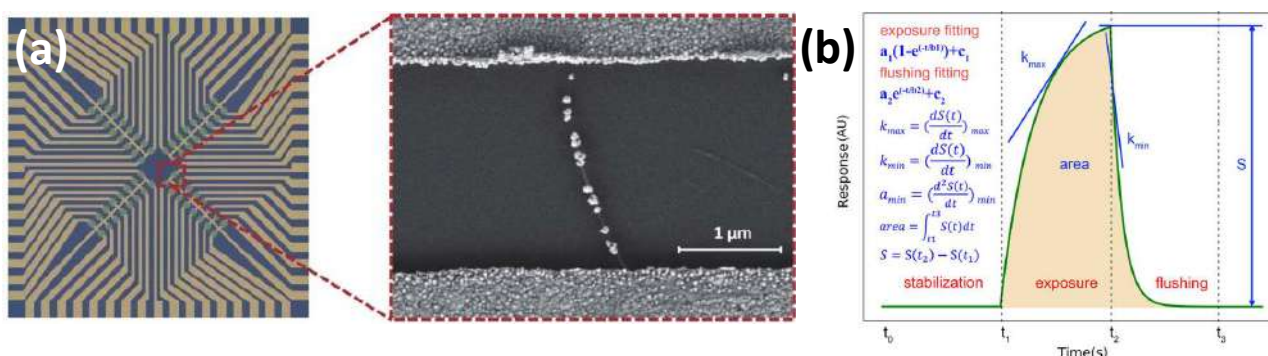


Figure 1: (a) Array of chemiresistors based on gold nanoparticle-modified CNTs. (b) Analysis of the interaction kinetics during exposure of sensors to a gas.

Stimuli-responsive DNA-Based Nanodevices programmed by Purely Entropic Linker Domains

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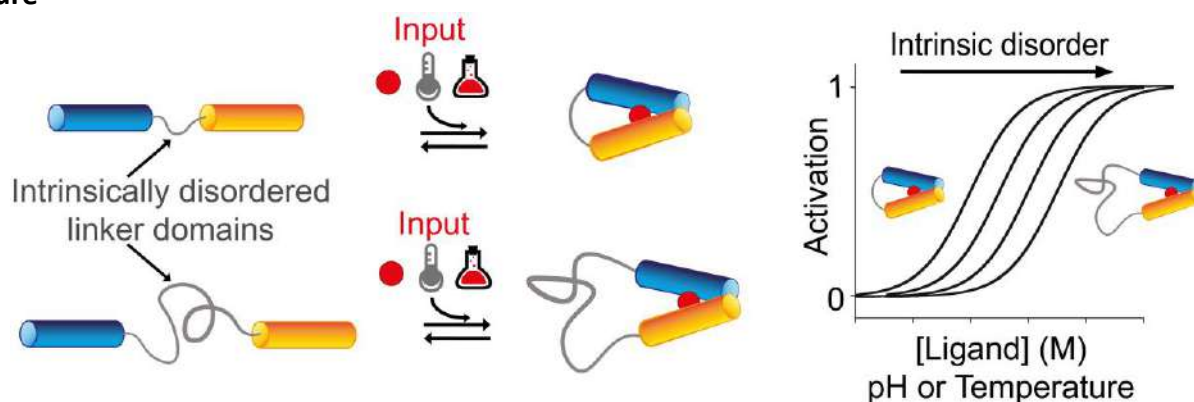
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Herein, we present a generalizable and versatile strategy to program stimuli-responsive properties of synthetic DNA nanodevices in which the capacity of the receptor to respond to a specific ligand or an environmental input (e.g., pH or temperature) can be finely modulated by controlling the entropy associated with the linker connecting the ligand-binding or pH-responsive domains.^[1,2] To do so, we have re-engineered two model DNA-based receptors and a set of pH-responsive nanodevices. Specifically, as receptors we used a triplex clamp DNA-based receptor that recognizes a specific DNA sequence and an ATP-binding aptamer; and as pH-responsive nanodevices we used the formation of an intramolecular triplex structure through hydrogen bonds (Hoogsteen interactions) between a hairpin duplex domain and a single-strand triplex-forming domain. We show that, by varying the length of the linker domain that connects the two ligand-binding or pH-responsive domains of these receptors, it is possible to: 1) finely control their affinity for their specific ligand;^[1] 2) modulate their observed acidic constant (pK_a), therefore, their pH-dependence;^[2] 3) program their thermos-responsive properties in order to release a specific molecular ligand at a defined temperature. Through mathematical modelling, thermodynamic and kinetic characterization, we demonstrate that the modulation of stimuli-responsive properties of the receptors results dependent on the total entropy associated with changes in linker length. Furthermore, the length of the linker does not affect the efficiency of the receptors during their loading/release process or binding. The possibility to rationally design stimuli-responsive DNA nanodevices using purely entropic domains can be of utility in applications such as biosensing, drug delivery, and production of smart materials in which the modulation of these systems could be obtained through a versatile, precise, predictable, and tunable approach.

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Figure



Stimuli-responsive properties of biomolecular receptors toward a specific input is strictly related to the presence of intrinsically disordered regions. With a higher entropic cost associated with the intrinsically disordered linker that connects two responsive domains, for example, a lower activation of the receptor for the same input will be observed. This mechanism is employed by Nature to dynamically control proteins function through the modulation of the entropy.

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There has been growing research interest in the development of rapid, reliable and ultrasensitive methods for clinical analysis. Among the available techniques, aptamer-based biosensing methods have shown great promise due to their high sensitivity and selectivity for the target biomolecules. Aptamers are synthetic nucleic acid ligands (single-standed DNA or RNA) that capable of binding to target molecules not only with high specificity but also high affinity. The single-stranded nature of the aptamer changes into a three-dimensional structure in the presence of the target molecule. To date, various aptamers have been developed for the detection of wide range of molecules including proteins, peptides, whole cells and drugs⁵. Our studies are aimed to carry out applications of these nanobiosensor systems in combination with certain bioreceptors (i.e. antibodies, aptamers) for detection of variable biomarkers in real biological samples for further possible development of point-of-care diagnostic tools.

Electrochemical aptasensors provide sensitive, fast response, low cost, miniaturized and easy to handle systems to obtain excellent point of care (POC) platforms. In recent years, a prompt development of nanotechnology and a better understanding of nanoparticle structures and properties have enabled their use in different areas of biosensors for diagnosis and monitoring of not only diseases but also drug discovery, food analysis and quality control. Among all nanomaterials, graphene oxide (GO) is one of the most attributed materials for opening new possibilities in the development of next generation biosensors due to its unique properties, such as high electron transfer rate, high affinity for specific biomolecules, thermal stability, water solubility, large specific surface area, exceptional elasticity and rigidity. On the other hand, transition metal oxide nanoparticles of iron, titanium, manganese, zirconium, cobalt, nickel and their composites offer promising features in the field of electrochemical and biosensing. Transition metal oxide nanoparticles of different shapes and structures have been synthesized using various techniques. These metal oxide nanoparticles possess good electrical and photocatalytic properties because of their size, shape, stability and larger surface area.

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Tunable Tamm Plasmon Resonance based on Nanoporous Anodic Alumina Photonic Crystals

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Abstract

Hybrid materials were designed by gold coating on porous nanostructures to create a metal/dielectric interface at which surface modes of electromagnetic field propagation can be generated [1]. The creation of resonance Tamm optical states in gradient index filters based on nanoporous anodic alumina (NAA-GIFs) was investigated. The NAA-GIFs were fabricated using a sinusoidal pulse-like anodization technique [2-4] that produces slight periodic modulations of the nanopores in the one-dimensional photonic alumina crystals (1D-PCs) obtained. The influence of the structural properties of 1D-PCs [5] and the thickness of the gold layers coated by sputtering on reflectance spectra were analyzed. The main photonic features of the fabricated samples were presented and discussed. The controlled nanofabrication of these novel structures allows obtaining better quality factors than in similar photonic nanostructures and the Tamm resonance spectra are narrower than the photonic bands themselves (**figure 1**). This gold-NAA photonic crystal structures open new opportunities for use as bio-sensors and optoelectronics devices.

Acknowledgments

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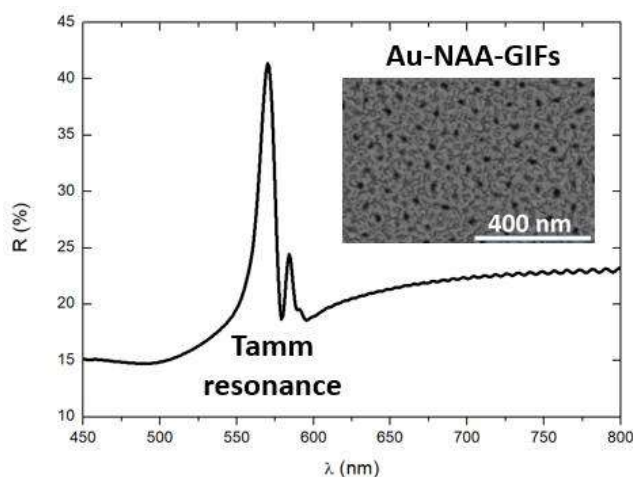


Figure 1: Reflectance spectrum of NAA-GIF coated with gold (Au-NAA-GIF) showing the characteristic dip corresponding to a Tamm resonance signal. Top view of Au-NAA-GIF (inset).

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Abstract

The design of highly efficient and sustainable electrocatalysts for water splitting is a key issue for alternatives to conventional carbon-based energy sources. Hydrogen and oxygen evolution reactions (HER and OER) needs to be optimized in proper electrolytes with fast kinetics and efficient material utilization. Indeed, very different electrocatalytic performances appear in literature and without an appropriate investigation of mass activity and overpotential a fair comparison is unmanageable. Nanotechnology could help in boosting water electrolysis still the stability remains an open issue. Here, we will review recent progress in low-cost nanostructures of transition metal oxides (NiO, WO₃, CuO, ZnO) for improving HER and OER in acidic and alkaline conditions. Decoration with mono or bimetallic nanoclusters will also be discussed. Well established metrics (overpotential, TOF, Tafel slope) will be used to asses solid and comparable electrocatalytic performances of nanostructures. Physically based models will be proposed to explain catalytic activity with respect to electronic energy bands of semiconductors. WO₃ nanoneedles with optimized hexagonal/monoclinic phase junctions shows HER overpotential of 170 mV for 10 mA/cm² in acidic electrolyte [1]. NiO microflowers, composed of very thin sheets (20 nm thick) intertwined like petals of a desert rose, exhibit an overpotential of only 314 mV at current density of 10 mA/cm² under alkaline conditions, with promising intrinsic activity of catalyst (Tafel plot as low as 40 mV/dec and turnover frequencies of 0.01 or 6.98 /s⁻¹ for bulk or redox determination, respectively) [2]. NiO nanoplates decorated with ultralow amount of Pt nanoclusters show a HER overpotential of only 66 mV at current density of 10 mA/cm² in alkaline media. A cell for water electrolysis fully based on Ni nanostructures shows a low potential of 1.57 V to afford a current density of 10 mA/cm² and a good long-term stability [3].

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Figures

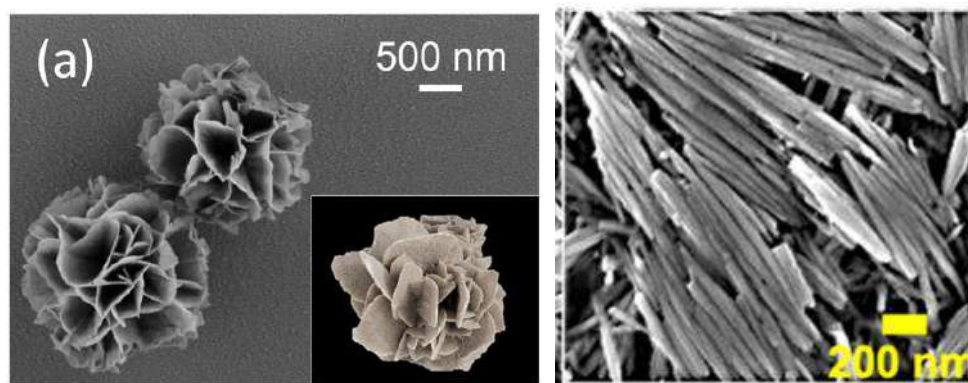


Figure: [left] NiO microflowers dispersed on GP (desert rose in the inset). [right] Bundles of WO₃ nanoneedles.

Wide-field surface plasmon microscopy: a new tool for ultrasensitive analytics of natural and artificial nanoparticles as well as for nanoelectrochemistry

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Abstract

The recently developed wide field surface plasmon microscopy (WF-SPRM) is a power tool for ultrasensitive analytics of large analytes (nano- and submicroparticles of natural and artificial origin, for example, viruses, exosomes, liposomes, polymeric or inorganic nanoparticles) as well as for investigation of electrochemical processes at the level of single nanoparticles [1-3]. In both cases the method allows one to follow up to a million of nanoparticles on the sensor surface simultaneously thus providing statistically reliable data for analysis with so high resolution. The first part of the talk will include a short review of analytical application of this approach including a quantitative detection of engineered nanoparticles in very complex media. Further, an application of WF-SPRM for nano electrochemistry will be discussed. It includes an identification of nanomaterials using their electrochemical dissolution [4] or conversion as well as a comprehensive investigation of initial stage of electrochemical nucleation [5]. In the latter case it provides a non-intrusive monitoring of formation and grow of each single nano-nucleus independently on the macroscopic electrode surface. It gives growth kinetics of each nucleus independently, time dependence of their surface density and their mutual localization. The current transients, calculated from the analysis of optical data, correspond quantitatively to the independently measured experimental current-time dependences and allow one to distinguish diffusion and reaction limited growth kinetics for each individual nucleus and time moment.

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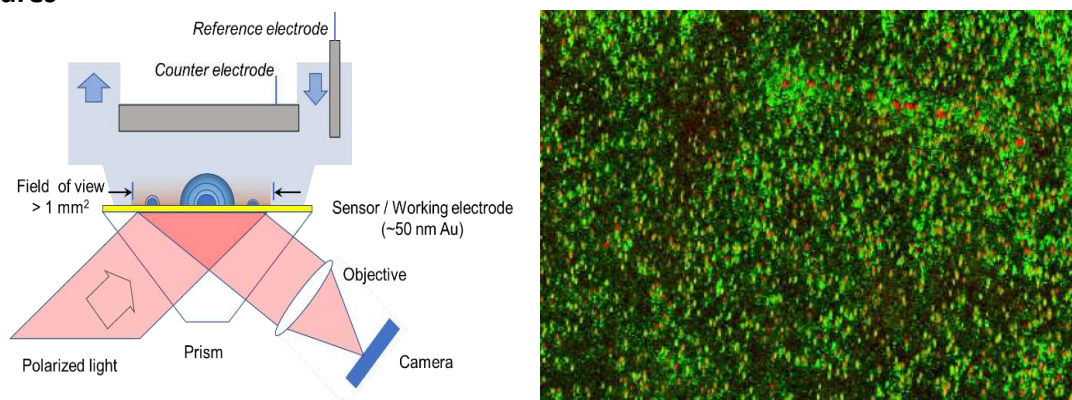


Figure 1: Schematic view of wide field surface plasmon microscopy setup (left) and the map of the nuclei growth (right) where the time of nuclei appearance is indicated by shades of green and the average growth rate is indicated by the shades of red.

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Abstract

The paradigm shift ongoing in rapid diagnostics field requires novel tools to succeed. Traditional methods, such as ELISA and Lateral flow tests using monoclonal antibodies, are well established although having shortcomings. Next generation of immunodiagnostic platforms, including immunosensors, should meet the requirements of high sensitivity, specificity, multiplexing potential, stability, reproducibility, low prize and easy-to-use. Especially the development of a multiplexed assay for many different analytes with varying detection ranges in a single sample has turned out to be challenging.

Recombinant antibodies are small antibody fragments discovered in most cases from antibody libraries displayed on bacteriophages by utilising *in vitro* selection and screening methods. Different antibody formats from single-domain nanobodies to larger Fab-fragments differ in size from ca 2.5 x 4 nm to 3 x 7.5 nm, respectively. Current trend of miniaturization of diagnostic systems increases the demands for surfaces with very high binding capacity. Nanosize recombinant antibodies, which can be tailored for site-specific and oriented immobilization, meet these demands. Antibody engineering can be applied to e.g. improve binding properties or create fusion proteins aiming at further optimization of the immunodetection.

The presentation gives an introduction to recombinant antibodies and their potential to tackle the challenges in future immunodetection of analytes from different application fields. Examples of the utilization of the Fab-fragments in sensitive and specific rapid diagnostic platforms are presented.

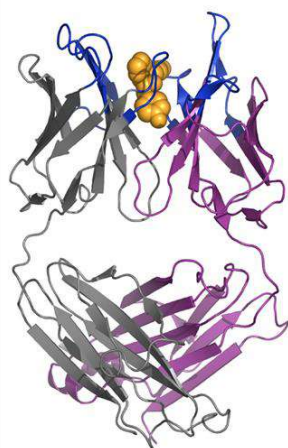


Figure 1: Recombinant antibody Fab fragment contains the intact light chain (grey) and two domains of the heavy chain (magenta) of a monoclonal antibody. Three complementary determining regions (CDR loops in blue) of light and heavy chains create the antigen-binding site responsible for the specificity and affinity of the binding. Target molecule is marked with yellow. (Figure made by Tarja Parkkinen, University of Eastern Finland)

Liquid Plasma as Processing Tool for Nanotechnology

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Abstract

Recently, research on liquid plasma gained importance due to novel applications in Nano, environmental and medical technologies. Especially in nanotechnology it has a huge potential for novel nanomaterial production or nanoparticle coating for nanocomposites and also for environmental applications. The medical applications for killing bacteria and viruses cannot be neglected especially in pandemic times. The other potential is also for production of agricultural application for nitride production as fertilizer.

Plazmatek company designs and sells liquid plasma systems for sterilization of water, for nanoparticle production, and also for environmental purposes. Plazmatek also produces vacuum plasma systems for coating and deposition of nanoparticles and also nanocomposite production and nanoparticle coating systems and Nanoparticle production systems.

In this talk the liquid plasma production systems will be discussed and potential applications will be given.

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Abstract

Nanobioengineering utilizes many alternatives to assemble materials at a nanometer-scale size in the frontier of different areas, with new unique properties regarding their bulk material counterparts. It also searches for new or existing (bio)materials, understanding their interactions and providing new functionalities for new products and unexpected applications. In health care, nanobioengineering offers outstanding opportunities to design diagnostic and therapeutic tools. For example, nanobioprobes and nanobioconjugates may provide a convenient real-time diagnosis of diseases closer to the patient and opportunities for more efficient drug delivery and targeted therapeutics concerning conventional technologies.

This talk will discuss nano-bioengineered material-based functional platforms developed in our group to diagnose and treat diseases. The first part will highlight new approaches regarding nanobiosensors to detect viral infections and their discrimination among related viruses [1,2,3], including nanobiosensors for SARS-CoV-2 detection [4, 5, 6]. The second part will cover strategies for encapsulating therapeutic agents into functionalized nanoparticles -photosensitive [7] or not [8]- for site-directed specific intracellular cargo delivery; and photosensitive micromotors for enzyme protection and dynamic substrate degradation [9]. Overall, the talk will demonstrate nanobioengineering's enormous potential for tackling real-life problems in today's world and highlight their opportunities for multiple clinical diagnostic and therapeutic applications.

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In-plane time-of-flight photoconductivity of two-dimensional materials and their composites with organic semiconductors

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Photoconductivity of two-dimensional materials (2DM) is highly sensitive to the environment due to enormous ratio of their surface to thickness [1]. Photoconductivity measurements of 2DM thereby promise superior performance in sensing applications compared to bulk materials [2]. Frequently, submicron-size flakes of 2DM are obtained using various methods, which have potential of large-scale production. More, blending them with organic semiconductors (OS) introduces new material functionalities [3]. In order to fully understand charge transport in thin layers of 2D flakes, electronic properties of the microscopic environment at the interfaces between individual flakes and/or between a flake and an OS molecule must be considered in addition to the inter-flake charge transport [4]. These interconnecting segments drastically change the overall charge transport characteristics, as was thoroughly studied in graphene/organic semiconductor composites. Here we present recent results of in-plane time-of-flight photoconductivity (TOFPC) measurements of thin films of MXene (Ti_2C_3) flakes and of quasi-two-dimensional conjugated polymers. Due to high sensitivity of TOFPC, we were able to distinguish the samples exhibiting nondispersive, or dispersive transport of photoexcited charge carriers. In the case of samples exhibiting non-dispersive charge transport, charge carrier mobility as high as $200 \text{ cm}^2/\text{Vs}$ was detected. This surprisingly high mobility is atypical for spin-coated thin films comprising interconnected 2DM nanoparticles. In fact, by using unique TOFPC method, we can discover high-mobility pathways, which can be formed in an interconnected network of these materials. More, by tuning the excitation photon energy, TOFPC can be used to explore transport of hot charge carriers through non-equilibrium states, which exists at higher energy levels.

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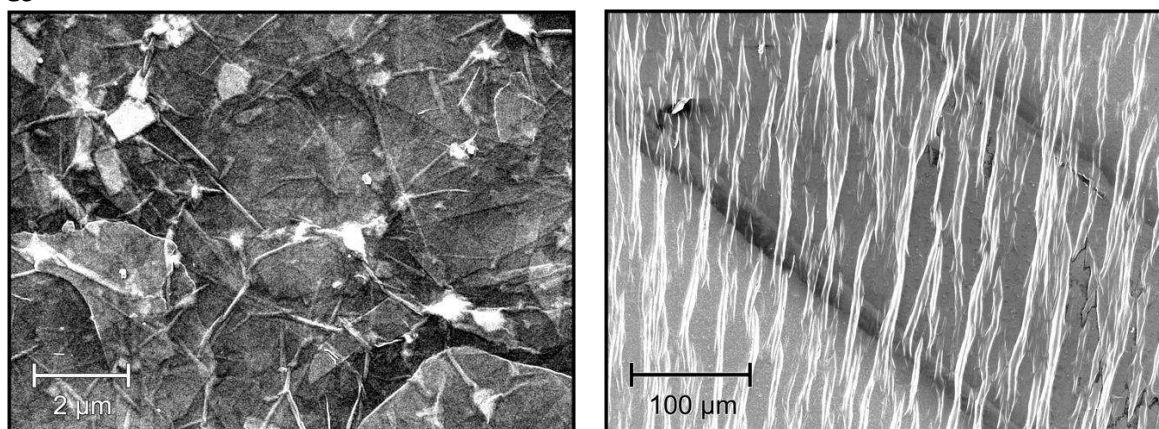


Figure 1: Time-of-flight photoconductivity measurements were performed on thin-films of interconnecting MXene flakes (left) and on thin-films of quasi-two-dimensional conjugated polymers (right). Scanning electron imaging reveals the microscopic morphology characterized by grain boundaries and wrinkles.

Control of the composition of the grafted organic layer by diverting the reactivity of aryl radicals

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Aryl radicals derived from aryl diazoniums during their electrochemical or spontaneous reduction on the electrode surface at the electrode potential about 0 V/SCE in aprotic or aqueous solution, in general, are able to attack the material surface and create a polyphenylene layer. [1] However aryl diazonium salts that contain two methyl substituents in the ortho position to the diazonium group, 2,6-dimethylbenzodiazonium salt, generate 2,6-dimethylphenyl (2,6-DMP) radicals that are unable to react with electrode surface due to their steric hindrance. These highly reactive radicals are prone to abstract hydrogen atom from the solvent, acetonitrile or methyl amine that enabled the generation of cyanomethyl or aminomethyl radicals that are attached on the electrode surface, see figure 1. [2] Therefore, by diverting the reactivity of aryl radical one can change the composition of the grafted layer. 2,6-DMP radicals are also able to remove halogen atoms from alkyl iodides and bromides solutions in acetonitrile and form highly reactive alkyl radicals that tether electrode surface with alkyl moieties. [2,3]

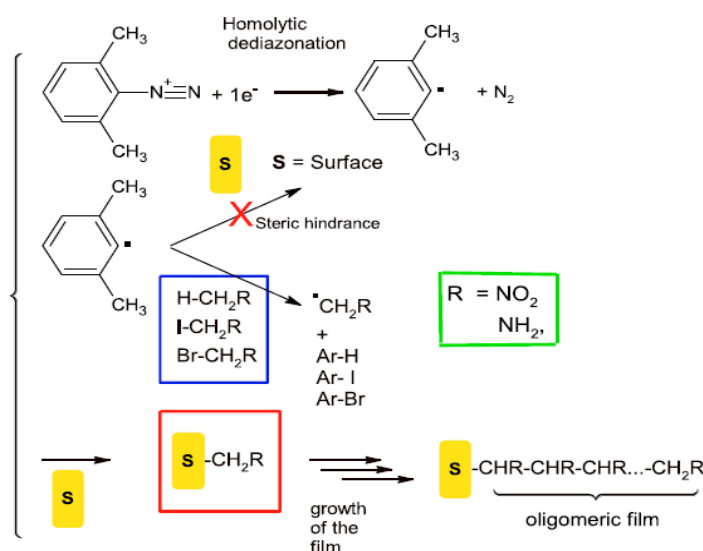


Figure 1: Grafting through C-H, C-I, C-Br activation with a sterically hindered aryl radical obtained by reduction of the 2,6-dimethylbenzen diazonium salt.

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BioPoC: A Novel Biosensing Technology Based on Responsive Polymers and a Low-Cost Transducing Technology for Point-of-Care Applications

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Abstract

Medical diagnostics sector is relying on affordable, hand-held autonomous devices incorporating smart integrated biosensing interfaces that enable clinical analysis with minimal technical expertise, end-user intervention and resource requirements. Crucially, the development of simple yet reliable transducing technologies affording true advantages over well-established electrochemical, potentiometric, or optical detectors in the analysis of non-treated complex biological matrices is expected not only to provide convenient solutions to the most contemporary demands in decentralized health-care systems but also to facilitate the translation of global health-care strategies into practice.

In this response, our group has developed a novel enzyme-based biosensing technology, we call it “BioPoC”, for the determination of biomarkers in undiluted urine. “BioPoC” biosensing technology is demonstrated by using pH responsive free-standing membranes or pH responsive polymer coated paper-based biosensing surfaces for the determination of urinary urea and creatinine. The biosensing surfaces, after their modification with urease or creatinine deiminase, respectively are sandwiched between patterned conductive strips and spacers, thus creating an inbuilt dosing well and a vertical microfluidic channel. “BioPoC” biosensing technology relies on the measurement of the time required the original electric resistance between the conductive strips (R_{∞}) to become finite (R_{finite}) because of the specific, enzyme substrate-triggered degradation of the polymer and the ensuing vertical flow of the sample, which thus allows an ionic type electrical bridging between the conductive strips [1]. Based on a smart assembly with three conductive strips onto a SIM card, and through a wireless communication with a Bluetooth microprocessor-controlled time and electric resistance measuring circuits, the device manages an automatic on/off (addition of the sample/end of the measurement) function for measuring the polymer degradation time via electric resistance measurements between the conductive strips, calculations, and the display of the results [2]. The different version of the “BioPoC” devices were successfully applied to the determination of urinary urea and creatinine.

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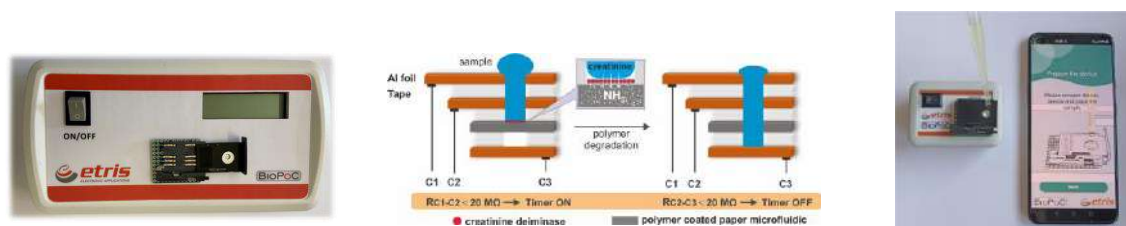


Figure 1: “BioPoC” devices. (Left) Standalone device. (Middle) Simplified representation of the biosensor buildup. (Right) Smartphone paired SIM card-type integrated device.

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Metallic and photoluminescent nanoparticles (quantum dots and carbon dots) have drawn great attention over the last decades due to their potential applications in bioimaging or (bio)sensing. However, most of the conventional synthetic methods are limited due to the complexity of controlling size distribution and crystalline properties, thus making very difficult to achieve good reproducibility, which is crucial for analytical purposes. Microfluidic technology, based on the most common materials employed for miniaturization (glass, silicon or polymers), has been proposed to overcome these difficulties. Microfluidic platforms allow experimental variables such as temperature, flow rate and reagent concentration to be varied and controlled in a rapid, reproducible and precise way, which results in more uniform particles. The Sensors and Biosensors Group in the UAB has been working for more than ten years in the development of microreactors for the synthesis of colorimetric [1] and photoluminescent nanoparticles [2-4] based on the Low-Temperature Co-fired Ceramics technology (LTCC). This technology, based on green tapes, shows some very interesting advantages for this purpose such as high chemical and thermal stability. Moreover, the technology enables the construction of multilayered systems, which can integrate other mechanic, electronic, fluidic components and sensors in a single device without the need of sophisticated facilities and a rapid prototyping reduces significantly the cost and production time. Different developed automatic microreactors, which integrate heaters, temperature sensors, microfluidics, optical windows and which allow the possibility of the in-situ optical control of the synthesis variables will be reviewed, taking emphasis on the characteristics of the obtained nanoparticles and their applications [5,6].

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Figures



Figure 1: Example of the follow-up of the synthesis of carbon dots for heavy metals detection

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Chemical sensors are an enabling tool across many industries, including the largest ones such as energy, transport, and construction. Low-cost, high performance sensors, especially ones compatible with flexible substrates, are becoming increasingly important with the development of mobile gadgets and wearable devices. Here we show chemical sensors produced in a facile way from inexpensive materials. The sensors, made of liquid-phase exfoliated (LPE) 2D materials deposited on a substrate with Langmuir-Blodgett assembly, are made with an inexpensive process that can be applied to any substrate, including flexible ones. The sensors that we make from graphene are more sensitive to humidity than ones demonstrated with CVD graphene [1], with up to 30% change in sheet resistance upon exposure to water vapor. The LPE graphene sensors are also ultrafast, enabling applications such as real-time respiration monitoring and touchless finger proximity detection [2]. We also demonstrate chemiresistive sensing of nitric acid vapour, ozone gas, and CO₂ [3] with the same films. Using thin sheets of LPE PtSe₂ we show NH₃ and NO₂ gas detection with unprecedented 200 ppb and 15 ppb detection limits, respectively.

We also present our latest results on sensors of physiological parameters made of laser-induced graphene (LIG). Such graphene is readily and quickly obtainable, and can be made into various sizes and shapes. We use LIG on different polymer substrates to produce flexible wearable sensors of heartbeat and respiration.

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Figures

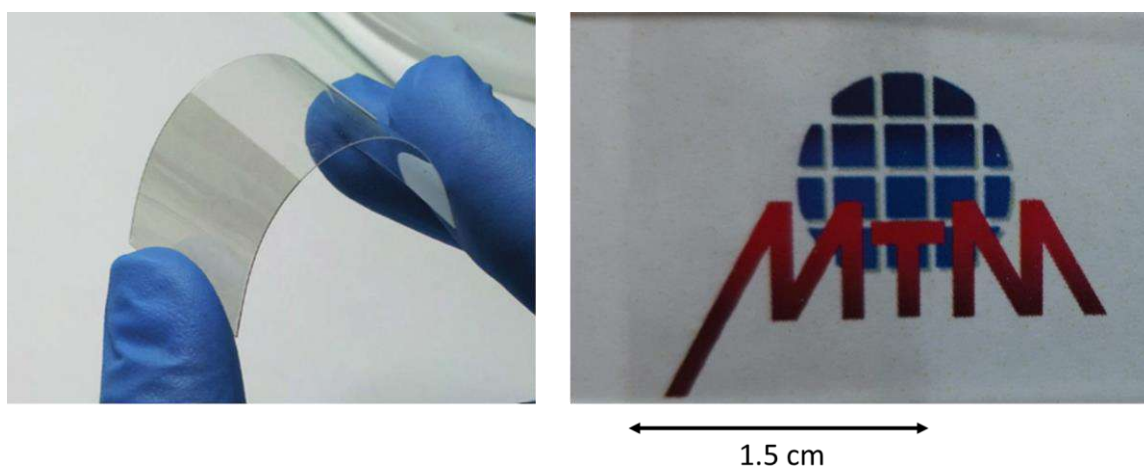


Figure 1: Large area, thin graphene film on flexible substrate for transparent conductors and sensing.

StretchBIO - Photonic nanosystem for continuous two-dimensional Stretch monitoring of fresh tissue Biopsies

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Tissues biopsies are widely used in diagnosis and monitoring of diseases. However, they are often difficult to obtain and require surgery. In this EU project we aim to enable easily obtainable microscale biopsies to be analyzed for mechanical deficiencies. It has been established that tissue mechanics play a major role during tissue development, normal function, and diseased conditions [1]. Normal tissue elasticity is essential to support physiological tissue functions. On the contrary, numerous diseases proceed with a chronic loss of tissue elasticity inducing a progressive impairment of physiological functions [2]. A good example is lung cancer solid tumors, which present remarkable stiffness. Recent in vitro and in vivo studies [3] have reported several links between tissue stiffening, tumor progression and reduced drug delivery. There is, thus, an urgent need to early identification of tissue stiffness and apply therapeutic approaches that can rescue normal tissue elasticity. In this work a novel approach of developing a compact photonic nanosystem for measuring the in-plane forces applied to the microbiopsies will be presented. Our approach is based on a two-dimensional force sensor nanosystem with the ultimately aim of continuous ex-vivo monitoring of mechanical effects of drugs on living tissues for its use in personalized cancer therapeutics. The basic principle of the nanosystem is shown in Figure 1. It is formed by a photonic crystal, consisting of a complex nanopillar array (Figure 1a), in which one or more nanopillars are laterally deflected (Figure 1b) by in-plane forces exerted by the living tissue on the tips of the nanopillars. During the presentation, the whole nanosystem will be presented, pointing out its innovative properties and describing the actual development state of its different components.

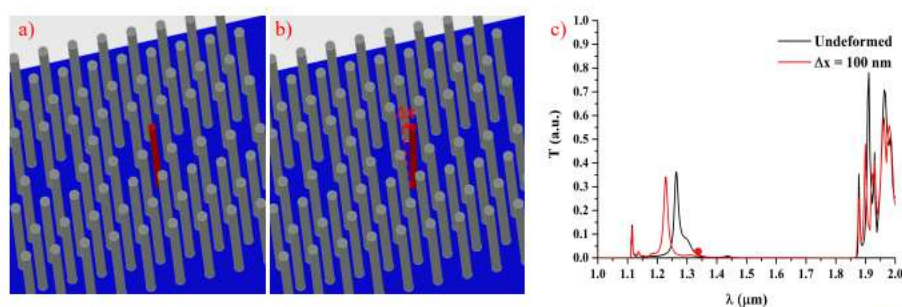


Figure 1: The nanosystem sensing approach: a) one undeflected narrower nanopillar (red) in a nanopillar matrix (grey); b) deflection of the red nanopillar upon exertion of an in-plane force; c) simulation of light transmission through the structure of undeflected (black) and deflected (red) nanopillars of figures a) and b), showing a clear shift in the resonance peak at $\lambda=1.28 \mu\text{m}$.

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Liquid Plasma as Processing Tool for Nanotechnology

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Abstract

Recently, research on liquid plasma gained importance due to novel applications in Nano, environmental and medical technologies. Especially in nanotechnology it has a huge potential for novel nanomaterial production or nanoparticle coating for nanocomposites and also for environmental applications. The medical applications for killing bacteria and viruses cannot be neglected especially in pandemic times. The other potential is also for production of agricultural application for nitride production as fertilizer.

Plazmatek company designs and sells liquid plasma systems for sterilization of water, for nanoparticle production, and also for environmental purposes. Plazmatek also produces vacuum plasma systems for coating and deposition of nanoparticles and also nanocomposite production and nanoparticle coating systems and Nanoparticle production systems.

In this talk the liquid plasma production systems will be discussed and potential applications will be given.

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Surfactants can be used in the construction of voltammetric sensors to improve and enhance the function of the electrode in terms of selectivity, sensitivity, improving electron transfer, [1] etc. In particular, the formation of molecular films on the electrode surface with a specific orientation enable the immobilization of other compounds by expanding the use of surfactants in the field of electrochemical sensor [2]. A new voltammetric immunosensor has been studied for the determination of ferritin based on the principles of biological cognition, antibody-antigen response combined with nanotechnology, and the advantages of electrochemical detection strategies. A thin layer of trimethyl-tetradecylammonium ion (TTDA) is used on the electrode surface (GCE / CPE) to better immobilize ferritin antibodies (FeAb). The surfactant forms a dense layer with a positive charge on the solution, which enables the fixation of the carboxyl groups of the antibody providing a stronger and more stable bond between FeAb and the electrode surface. The electrodes were characterized by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). Experimental conditions such as surfactant amount, pH, scan rate, immobilization time, support electrolytes are studied and optimized to obtain better analytical performance parameters. The immunosensor is calibrated by calculating the current reduction and expressing it as a function of the corresponding ferritin concentration [3]. The dependence is observed to be linear up to the concentration of 0.6 mg / L ferritin ($R^2 = 0.9992$), and the sensitivity more than 2 times higher than the bare GCE. Quantitative analysis of $RC\% = f(C_{\text{ferritin}})$ in equilibrium measurements was used to calculate the binding/affinity constant of the immunological reaction, respectively. The double reciprocal coordinates was used for data linearization [4] and the binding constant resulted in the order of 10^9 , indicating a specific reaction. The analytical application of the modified immunosensor was studied in relation to the determination of ferritin in the spiked human serum sample. Recovery of ferritin addition resulted within 87% to 125% for immunosensors constructed into the GCE / CPE surfactant-modified platform.

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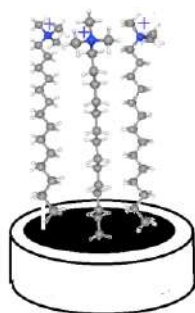


Figure 1 Schematic dense layer with positive charge onto GCE surface

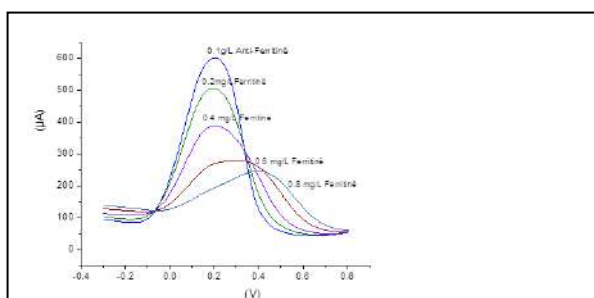


Figure 2 Typical DPV signal of immunosensor in different concentration of ferritin

Elastic composite photo-chromatic sensors with micro and nano mixed valence inorganic fillers

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Abstract

Two types of sandwich polyazulene-composite thin films are in focus of this research. Distinguishable changes between pure polyazulene and composite associate their in-situ cyclic voltammetric measurements revealing shifting and appearance of extra oxidation/reduction effects as well different current jumps involved in each polymerisation process. Post syntheses FTIR measurements show the existence of extra bands located at 772 cm^{-1} , 946 cm^{-1} , 1568 cm^{-1} , along with those belonging to the polymer and the inorganic fillers. Under a bias of 3V, polyazulene films respond better to white (5500 K) and red (623 nm) light, followed by amber (590 nm) and blue (460 nm) light, with the highest response for white light. Targeted tuning of the inorganic filler composition, substituting two sulfur positions in the structure of $\text{In}_5\text{S}_3\text{Se}_2\text{Cl}$ with selenium, leads to a sandwich composite polymer with reverse photo-switching response compared to polyazulene film (fig. 1). Polyazulene thin film displays negative intensities upon amber light illumination and positive ones for green and red light. The sandwich composite film of polyazulene- $\text{In}_5\text{S}_3\text{Se}_2\text{Cl}$ display positive intensities upon these three monochromatic lights, while the sandwich composite film polyazulene- $\text{In}_5\text{SSe}_4\text{Cl}$ reacted oppositely to polyazulene film toward the selected illumination wavelengths.

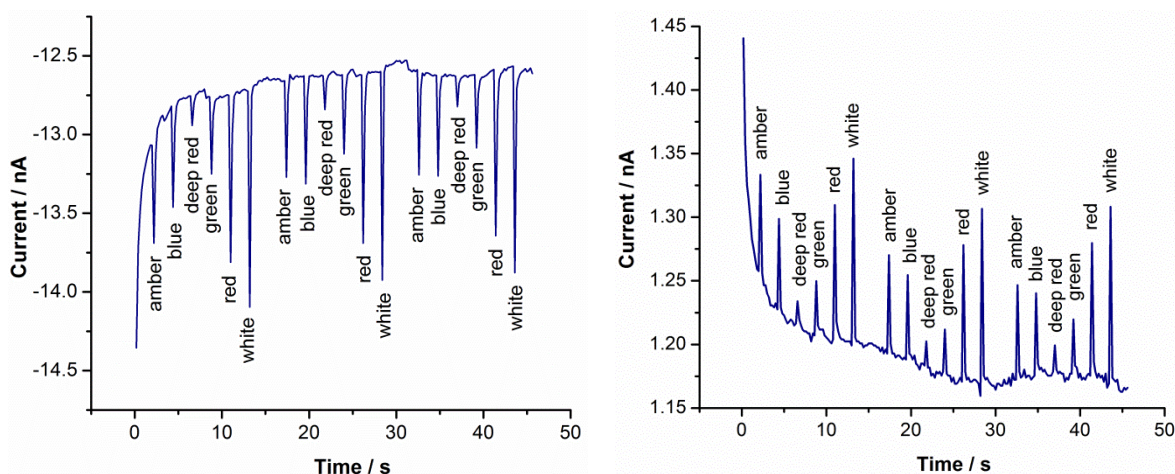


Figure 1: I-t curves recorded upon pulsed monochromatic light (exposure time of 0.01 s) with a frequency of 1000 Hz and density power of 70 mWcm^{-2} , in absence of bias for: (a) polyazulene film, (b) sandwich composite film polyazulene- $\text{In}_5\text{SSe}_4\text{Cl}$

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Graphene paper (G-paper) is a paper-like material possessing high flexibility and large surface area; it can be shaped in different geometries, featuring a high electrical conductivity (*ca.* 10^5 Sm^{-1}), tuneable surface chemistry and mechanical stability even after hundreds of thousands bending times [1]. We recently proposed the use of G-paper for the realization of electrochemical devices (named GPE) on flexible plastic and textile supports (Fig. 1) [2]. They were applied in the enzymatic detection of lactate in sweat, featuring higher selectivity with respect to commercial, carbon-based screen-printed electrodes (C-SPE and Gr-SPE); this performance is obtained thanks to the activation of electrocatalysis towards NADH oxidation, afforded by oxidized moieties naturally present on the electrode surface.

The properties of G-paper can be tuned by inclusion of various components in the material. In particular, we tested the electrocatalytic properties of G-Paper after the inclusion of graphene oxide (GO) to activate the electrochemical oxidation of H_2O_2 , and those of electrode platforms after functionalization with Prussian blue for H_2O_2 reduction. This allowed us to expand the application spectrum of the G-paper based platforms toward the realization of wearable biosensors for the detection of various biomarkers. As an example, we will show the performance in the detection of glucose, using glucose oxidase as mediator on the electrode surface.

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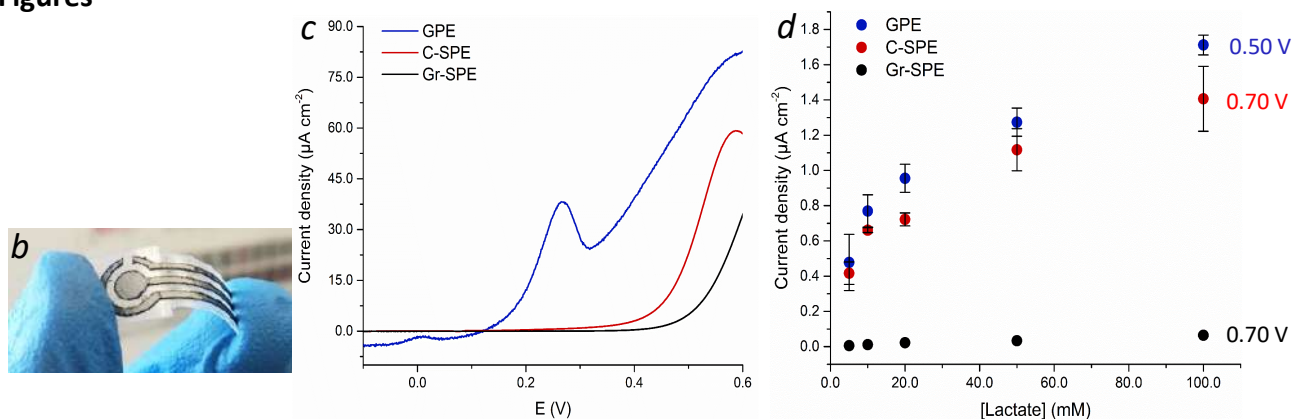


Figure 1: G-paper based electrodes on *a*) cotton and *b*) PET; *c*) Voltammetric signal (blue line) recorded at 1.0 mM NADH (0.1 M PBS, 0.1 M KCl) in comparison to commercial devices (red and black lines); *d*) calibration plot of lactate in sweat at GPE (blue dots) in comparison to commercial devices (the different potential chosen for these experiments reflects the voltametric behaviour shown in *c*).

Nanoparticle-aided Radiotherapy with Immunotherapy using smart biomaterials in cancer treatment

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Abstract

Cancer today is the main cause of death worldwide and metastasis accounts for over 90% of all cancer associated suffering and death, and arguably presents the most formidable challenge in cancer management. The main techniques involved in the cancer treatment are the Radiotherapy (RT), chemotherapy and Immunotherapy. Although these methods and especially RT have made significant advances in the last decades, there is still a significant amount of cancer patients experiencing toxicities on normal cells, cancer reappearance and deadly metastasis. A new method using nanoparticle-aided radiotherapy (RT) where gold nanoparticles can amplify damage to cancer cells during radiotherapy, generating neoantigens that can serve as a cancer vaccine powering cytotoxic immune system T-cells to kill both local and metastatic cancer is presented. The combination of RT with the Immunotherapy (anti-CD40) can further boost local and metastatic tumor cell kill, with minimal damage to healthy tissue. Biodegradable polymers are used as payload for targeted, concentrated and controlled delivery of nanoparticles and immunotherapeutics into the tumor volume, over time. The multifunctional properties of metallic nanoparticles (MNP) related to their physic-chemical properties and biocompatibility make them very suitable for applications both in diagnosis and therapeutic treatment.

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Chirality is a prominent characteristic of natural systems [1,2]. It is an impressive characteristic of asymmetric structures, allowing to explain two non-superimposable mirror-image forms, *enantiomers*, of a structure. Investigation of these asymmetric structures is crucial to understand processes occurring in living organisms that act commonly in an enantioselective manner [1,3]. Enantiomers of chiral species in pharmaceuticals or food additives can display different effects on living organisms [4]. Therefore, new effective methods and/or (nano)materials are required to explain the chiral recognition of chiral substances. Chirality has also been considered to be a crucial topic in nanotechnology and inherently chiral or chiral-modified stereospecific nanoparticles have been mostly used in the field of chiral sensors. Metallic nanoparticles, carbon nanotubes, organic and inorganic quantum dots, graphene and related materials, metal-organic frameworks (MOFs), and so forth are employed as innovative chiral sensors. With the recent advances in nanomaterials, great effort has been devoted to the development of miniaturized analytical platforms such as paper-based optical sensing platforms [5]. Taking advantage of the nanomaterials, in this talk, trends in nanomaterials-enriched chiral sensors/platforms that can be used as convenient signal probes to discriminate enantiomers of chiral molecules are overviewed.

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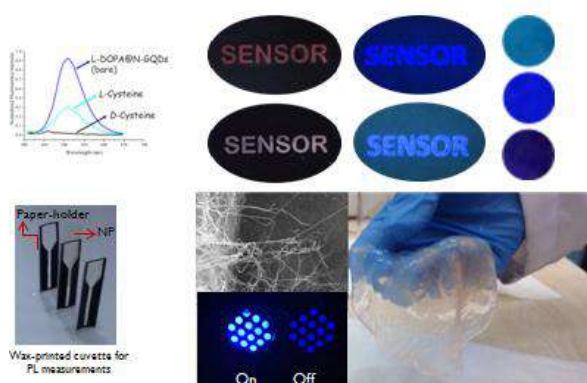


Figure 1: Nanomaterials-enriched nanopaper-based optical chiral sensors

Lysozyme Responsive Prolonged Dual Anti-glaucoma Drug Deliverable Nanocomposite to Manage Intraocular Pressure

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Abstract: The designing of highly efficient and biocompatible nanocomposites with multifunctional delivery and tracking characteristics is noteworthy for clinical and therapeutic applications. Herein, we report the delivery of anti-glaucoma drugs, latanoprost (LP) and Timolol (TM) under an enzymatic stimulus, lysozyme (Lyz) with novel chitosan (CS) - graphene quantum dots (GQD) nanocomposite. The LP-TM caged CS-GQDs nanocomposite was well characterized through extensive spectral, morphological, particle size, and zeta potential studies along with cytotoxicity assays against human corneal epithelial (HCE) cells. The prolonged delivery of the drug was observed for 72 hours in the presence of lysozyme. Further, AO/EB staining and biocompatibility assays further proved excellent cell viability of >80%. ¹H-NMR spectral studies confirm the release of drugs through the hydrolysis of 1,4-glycosidic bonds of chitosan, and mucoadhesive investigations confirm the prolonged residence feature of composite. Besides, an *ex-vivo* test, HET-CAM assay, and histopathological studies prove the non-irritancy of the as-prepared dual drug-loaded nanocomposite upon the exposure of 5 minutes. These findings justify the further utility of novel CS-GQDs caged drug nanocomposite for preclinical investigations and for fabricating medicated soft contact lenses to treat glaucoma.

Keywords: Chitosan, Drug delivery, Graphene quantum dot, Lysozyme, Latanoprost, Timolol

Graphene-enabled printed, flat-flex reference electrodes for in operando monitoring Li-ion battery parameters

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Abstract

To reach climate neutrality, a total installed battery storage capacity worldwide of TWh-scale is foreseen for end of this decade.[1] In this context, Li-ion batteries (LiBs) are playing a major role in several markets, including battery electric vehicles, plug-in hybrid electric vehicles and portable/mobile electronics.[2] Beyond the need for high energy density, high power density and cost effectiveness, the quality-reliability-lifetime (QRL) and safety are crucial requirements for specific end-use applications of current battery systems and cells.[3] Research and development efforts are therefore considering the integration of sensing components into battery cells, so that their output data can be used by advanced Battery Management Systems (BMSs) to monitor, through *in operando* and real-time modes, the key parameters of a battery cell, providing accurate estimates for states of charge, health, power, energy and safety cell indicators, along with other early-failure indicators.[3] This, in turn, should enable the BMS to implement corrective actions to protect the cell and battery systems from degradation phenomena and undesired electrochemical side-reactions, preventing dangerous effects, like thermal runaway events and consequent battery fire, and even guaranteeing possibly battery reuse in second-life applications.[4] In this talk, we will report the recent progress on the development of reference electrodes to monitor separately the anode and cathode potentials, avoiding the latter to reach critical thresholds that initiate irreversible cell failures. Meanwhile, reference electrodes can be used to monitor the electrochemical behaviour of each half-cell through non-invasive electrochemical impedance spectroscopy measurements. A special focus will be dedicated to the graphene-enabled printed, flat, and flexible reference electrodes, directly deposited onto the cell separator in form of thin film (without using any metallic current collector).

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Multifunctional biomimetic nanoparticles-induced hyperthermia improves survival in a human glioblastoma multiforme orthotopic mice model: A pilot study

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Glioblastoma multiforme (GBM) is the most common and deadliest form of brain cancer.¹ Current standard-of-care for GBM includes maximal safe surgical resection, radiation, and chemotherapy with temozolomide (TMZ). However, the highly invasive and resistant GBM nature prevents an effective tumor regression after therapy, causing significant neurologic morbidity and mortality, resulting into a mortality rate close to 100%.² just these data describe the urgent need for current treatment improvement and for new complementary therapies.

In light of this, applying magnetically-responsive nanoparticles to formulate anti-GBM therapies can be a powerful tool to both increase the bioavailability and the selectivity of pharmacological agents targeting the brain tumor microenvironment and to perform hyperthermia treatments.³ In particular, superparamagnetic iron oxide nanoparticles (SPIONs) can be exploited in the development of smart drug delivery systems, as “bio-magnetics switches”, owing to their capability to produce heat under the exposure to an external alternating magnetic field (AMF).⁴

In this work, lipid-based magnetic nanovectors functionalized with the peptide angiopep-2 encapsulating TMZ and SPIONs (Ang-LMNVs@TMZ) have been efficiently exploited in an *in vivo* approach to promote a cytotoxicity effect to human glioblastoma by the synergistic action of the chemotherapeutic drug loaded into the nanocarrier ([LMNVs]=24 mg/[TMZ]=0.98mg /kg weight mice; injection volume = 3 μ L) and the cell sensibilization in response to the local heating ($H \times f$ = $4.2 \cdot 10^9$ A/ms, t = 30 min, 3 consecutive days, 24 h after Ang-LMNVsTMZ intratumoral administration). Obtained data on orthotopic U87MG human glioblastoma tumor-bearing nude mice evidenced an effective suppression of the tumor growth, and a significantly improved medium survival time after Ang-LMNVs@TMZ + AFM treatment (75% of the subjects are still alive at the end of the study), suggesting the suitability of the proposed nanoplatform for the GBM treatment.

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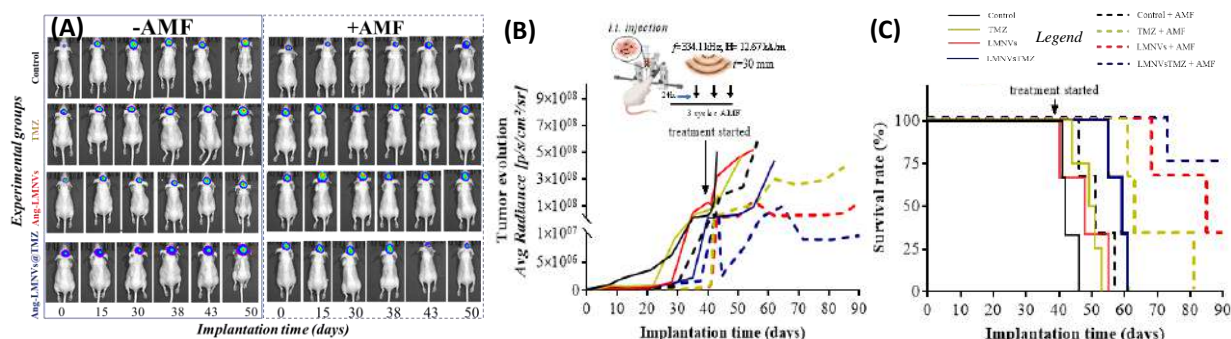


Figure 1: (A) *In vivo* bioluminescence images of orthotopic U87MG-Luc human glioblastoma tumor-bearing nude mice at different time points following tumor implantation. (B) Tumor evolution measurement by quantification of the luminescence levels of mice in each group using the IVIS system. Data are presented as mean ($n = 3-4$ mice/group). (C) Mice survival rate for each experimental group ($n = 3-4$ mice/group). Treatment schedule is also shown; data are expressed as % survival vs. time.

Which is superior for the absorption of the Lindane pesticide, graphene or graphene oxide? Experimental and DFT investigation

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Graphene and graphene oxide are intriguing materials with numerous applications, including adsorption, formulation of the composite materials, sensors, photovoltaics . . . [1-3]. In this study, graphene oxide is synthesized by reducing graphene oxide (with ascorbic acid) employing the well-established Hummers method, which may be summed up as the controlled treatment of graphite flakes with potassium permanganate in concentrated sulfuric acid. Combining FTIR and UV-VIS spectroscopy, the produced materials are characterized.

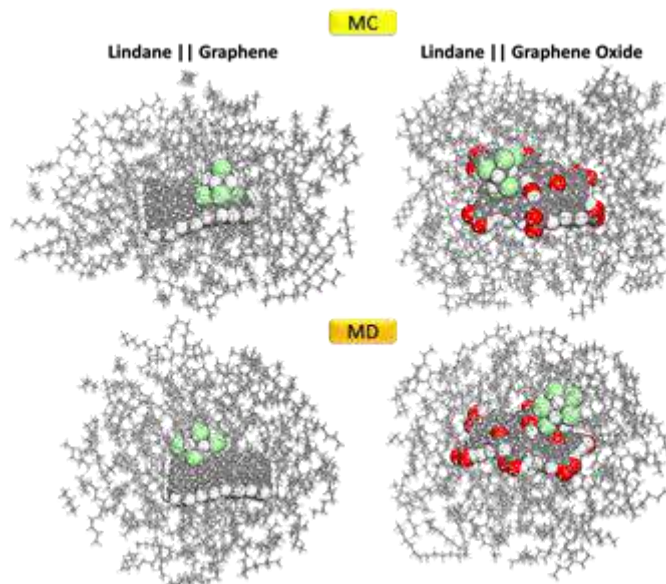


Figure 1: The final Molecular Dynamic (MD) and Monte Carlo (MC) geometries for Lindane adsorption onto Graphene and Graphene Oxide.

Lindane is adsorbed from hexane using a solution of concentration ranges from 25 to 500 ppb with a constant mass of 15 mg graphene or graphene oxide as adsorbents. The GC-ECD was used to determine the adsorbed concentration of Lindane. These materials have exceptional absorption characteristics. Graphene can remove up to 92.5 % of Lindane from hexane solution, whereas graphene oxide can remove up to 56.1 %. To gain a better understanding of the nature and adsorption energetics for the Lindane's interaction with the two adsorbents, quantum and molecular mechanics-based computations were undertaken (Figure 1).

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Abstract

In the last decade, atomically thin capillaries made from 2D materials have created a wave of new research especially in hydrodynamics and mass transport properties of fluids [1,2]. Van der Waals assembly of 2D materials to make capillaries, such as graphene, molybdenum disulphide and hexagonal boron nitride has already been achieved, but require highly sophisticated environments and nanofabrication techniques such as e-beam lithography, dry etching, and photolithography, and are very time consuming as we make one device at a time [1,2]. Herein, we are presenting an unique and novel nano-fabrication process to prepare 2D channels with well-defined geometries in a scalable manner. This technique demonstrates the fabrication of 2D channels from different naturally occurring layered materials such as graphite, metal oxides and sulphide, transition metal dichalcogenides, and phyllosilicates have been prepared in mass production, but in a shorter period. In addition, this method can be applied to prepare 2D channels from different 2D nanosheets such as graphene, molybdenum disulphide and hexagonal boron nitride through Van der Waals assembly. Moreover, this process holds advantages in making 2D channels of different dimensions and shapes with angstrom-scale precisions, alongside of the reduction of time and fabrication cost. The construction of these 2D channels will open doors to upscale production of nanofluidics devices, which can greatly impact studying and understanding the fundamental properties of fluids in confined geometries.

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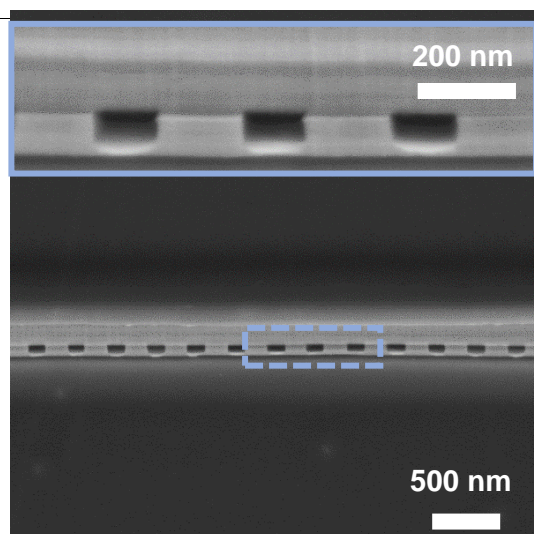


Figure 1: Cross-sectional scanning electron microscopy image of 2D channels fabricated by our method.

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Small molecule (SM) detection has gained increasing interest in the last years in various areas of science and technology. Understanding the fundamental mechanisms of binding kinetics in molecular biology, as well as accurate and rapid diagnostics of contamination in environmental, health, agriculture, and food control, demand for new methods of detection of molecules with sizes less than 1 kDa. Among the small molecules, drugs, pesticides, and toxins are of particular interest.

A number of aptasensors have been demonstrated to be highly specific to SMs due to strong binding with designed aptamers. The graphene-based aptasensors provide a low-cost, scalable, and highly sensitive technology for detection of small molecules [1]. While the general principle of graphene-based biosensors has been investigated, the understanding of microscopic effects is still challenging for SM detection. While SMs are more than 10 times smaller than aptamers, the main effect on graphene properties modulation may lay in the electrical and structural interactions of aptamer and graphene.

In this work, we have developed the aptasensors based on the spectral phase interferometry [2] and graphene field-effect transistors [3] for real-time detection of mycotoxin molecules. We have investigated the optical and electrical changes in graphene during detection of the increasing concentrations of ochratoxin A (OTA). The insight of the principle of aptamer reconfiguration and its interaction with graphene upon binding of the OTA molecules is discussed (Figure 1a). The high sensitivity and reproducibility of the sensors have been demonstrated (Figure 1b).

This work was supported in part by the IPANEMA project, which received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N° 872662.

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Figures

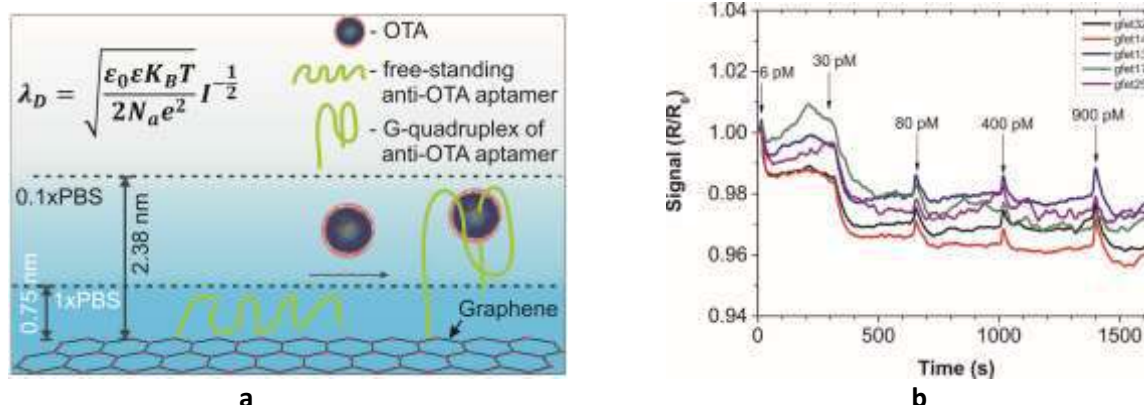


Figure 1: (a) Hypothesized mechanism of anti-OTA aptamer target-induced reconfiguration close to graphene channels with different ionic strength. (b) Time course of response of an array of five GFET sensors under increasing OTA concentration in 1xPBS.

Application of nanostructured carbon based voltammetric sensors for antibiotics analysis in real matrixes: pharmaceutical tablets, milk and environmental water

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Abstract

The antibiotics represent one of the most important therapeutic classes, with a huge impact on the human health. Since, World Health Organization has endorsed a global action plan on antimicrobial resistance, recommending an urgent improvement in the surveillance of the antibiotics use [1,2]. There is a need for the development of sensitive sensors, with low-cost and easy preparation to determine antibiotics in different matrices samples. The present study shows the effect of nanostructured materials (mineral- Rutile; metal- Au/np; and carbon nanomaterials- multi walled carbon nanotubes and graphene oxide), used alone or combined with other (nano)materials, into bulk modification of carbon paste electrode CPE for detection of β -lactam (penicillin) and macrolide (azithromycin) antibiotics, using voltammetric techniques: CV, SWV and DPV. In optimal condition modified sensors resulted with a good analytical performance toward tested antibiotics compared with bare CPE, indicating a good compatibility of nanomodifiers into CPE electrode. Satisfactory results were found in the analysis of real samples and good recoveries were obtained by applying the standard addition method to spiked river water, pharmaceutical tablets, and milk samples.

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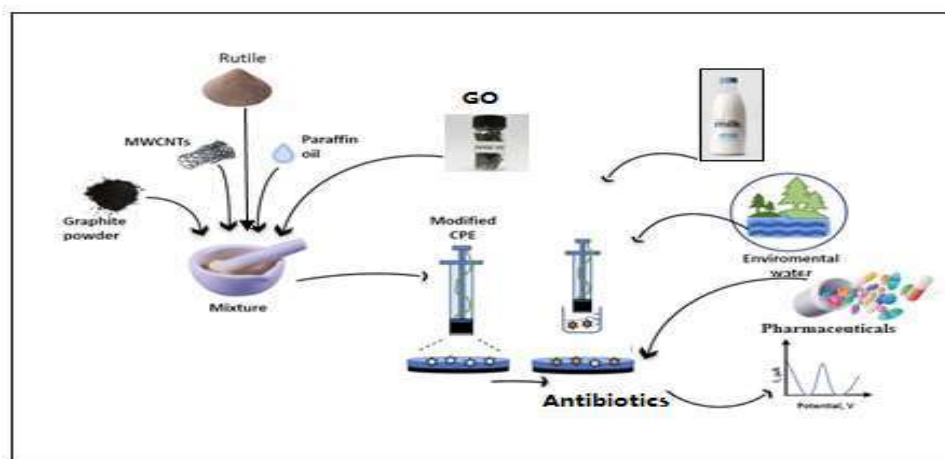


Figure 1: Schematic preparation of nanostructured carbon based sensors for antibiotic detection

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There has been extensive research in order to bring reduced graphene oxide (rGO) to printed and flexible electronics. While originally preparation techniques relied on chemical reduction of graphene oxide (GO) and the use of solvents to promote the transfer of rGO to the substrate, recent developments have simplified the process and made it more convenient. By using a laser, GO can be selectively patterned and transferred onto virtually any substrate in dry conditions, including paper. [1] The interest of paper lays upon the fact that it is an excellent material to accomplish the requirements that make a point-of-care biosensor, due to it being cheap, easy to transport and moreover it can be easily modified with bioreceptors. Therefore, laser-reduced graphene oxide (rGO) electrodes transferred onto nitrocellulose were fabricated and integrated in order to merge the beneficial features of both materials within a platform with potential application in disposable biosensors.

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Hepatic steatosis, being present in approximately 25% of the adult population, represent the world's most common liver disease [1]. The liver is a pivotal player in lipid metabolism, being responsible for the synthesis, redistribution, and utilization of lipids. Liver lipids synthesis is finely tuned by a large variety of enzymes and hormones and an alteration in this process may lead to the onset of liver steatosis [2]. Liver steatosis can lead to liver injury, fibrosis, inflammation, and cardiovascular disease that can even cause the death of the patient [3]. Antioxidant molecules have gained attention as a potential tool to treat hepatic steatosis thanks to their involvement in lipogenesis and regulation of oxidation processes such as lipid peroxidation [4]. Some of the tested compounds include polyphenols, carotenoids, and glucosinolates [4]. Polydopamine nanomaterials and in particular polydopamine nanoparticles (PDNPs) have received attention in recent years mainly due to their high biocompatibility, organic chemical nature that grants them biodegradability, and a relatively high antioxidant capacity granted by the polyphenols rich surface of PDNPs [5]. In this work we tested the possibility to employ PDNPs as a potential therapy for hepatic steatosis. In particular, we tested PDNPs on an in vitro model of hepatic steatosis obtained through the treatment of Hep G2 cells with oleic acid and assessed the ability of PDNPs to act on lipid accumulation and cell viability.

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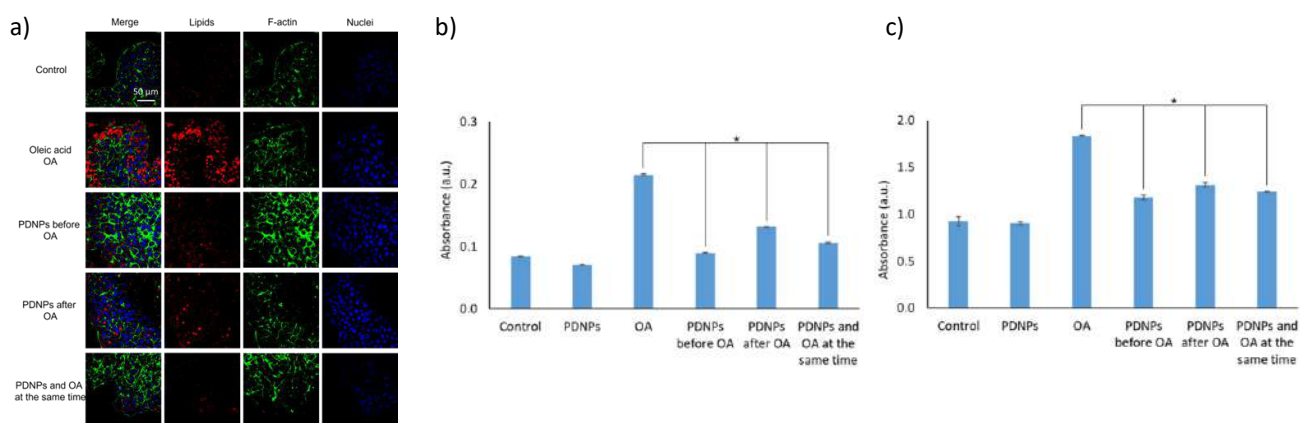


Figure 1: a) Confocal imaging acquisitions of lipid accumulation in Hep G2 cells at various conditions (from left to right merge, in red lipids accumulation, in green F-actin, in blue nuclei); b) & c) respectively, results of Total Cholesterol and Triglyceride assays performed on Hep G2 cells at various conditions.

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The academic and industrial community have devoted and are currently devoting important efforts to diagnose diseases quickly, easily and with a low cost. Biosensors have an important role in this direction, since they can swiftly detect biological compounds at the point of care. An increasingly popular method to fabricate biosensor is inkjet printing, reducing the cost and fabricating devices with high reproducibility out of the cleanroom. In this context, the use of consumer printers to fabricate biosensors have been widely explored in the last years. However, a pre-treatment of the substrate surface using a coating material or/and a primer solution typically needs to be performed. A method to potentially avoid it and tune the ink adhesion properties, is to heat up the substrate surface during the printing. Therefore, in our work we designed and fabricate a heater to dry the printed ink in real-time, during the printing. We optimized the design of the heater using finite element modelling and we printed it with a conductive silver nanoparticles (AgNPs) ink by an EPSON XP1500. Temperature measurements demonstrated that the heater surface could reach up to 95 °C, this value was limited by the heater substrate. With the use of the heater, placed inside the printer, AgNPs electrodes were printed onto several flexible substrates such as PET, Kapton and paper, without the need of a coating material and/or a primer solution application. Microscopic images showed the difference between the process with and without the heater. Furthermore, the heater itself is produced by the same printer, thus allowing for its acquisition and installation at no cost.

Acknowledgements

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Nanobiosensing architectures for the detection of β -1,4-Galactosyltransferase-V colorectal cancer biomarker

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β -1,4-Galactosyltransferase-V (β -1,4-GalT-V) is a glycosyltransferase that glycosylates high-branched N-glycans. Colorectal cancer (CRC) tumor cells overexpress this glycosyltransferase concerning normal cells and release it into the body fluids [1]. Conventional methods such as immunoassays and liquid chromatography-based methods enable the determination of the β -1,4-GalT-V accurately but have limitations, including the use of sophisticated and centralized laboratory equipment and skilled personnel. Thereby, there is a need for the detection of β -1,4-GalT-V at the point of care.

Electrochemical biosensors allow overcoming the challenge of β -1,4-GalT-V glycoprotein detection. These biosensors enable the affordable and accurate detection of the analyte at low concentrations, with high specificity, in simple formats, and with rapid response [2]. We developed bare and nanostructured electrodic architectures to detect the colon cancer biomarker β -1,4-GalT-V by electrochemical impedance spectroscopy (EIS) and electrochemical capacitance spectroscopy (ECS). Both biosensors use an antibody immobilized onto the electrode surface, which recognizes the analyte by biochemical affinity [3]. The resultant biosensors were highly specific for the β -1,4-GalT-V, whose response was linear from 5 to 150 pM ($r^2 = 0.993$), with a limit of detection (LOD) of 7 pM, for the bare architecture. We further enhanced the sensitivity toward the glycosyltransferase detection in a linear range from 50 to 400 fM ($r^2 = 0.994$) and lowered the LOD 350-fold down to 20 fM for the nanostructured architecture. Therefore, we report ultrasensitive biosensing interfaces that could be used as a label-free approach to detect and quantify β -1,4-GalT-V at clinical relevance concentrations and quantify it in raw human serum samples, thus holding considerable potential for determining this cancer biomarker and other proteomic cancer-related biomarkers.

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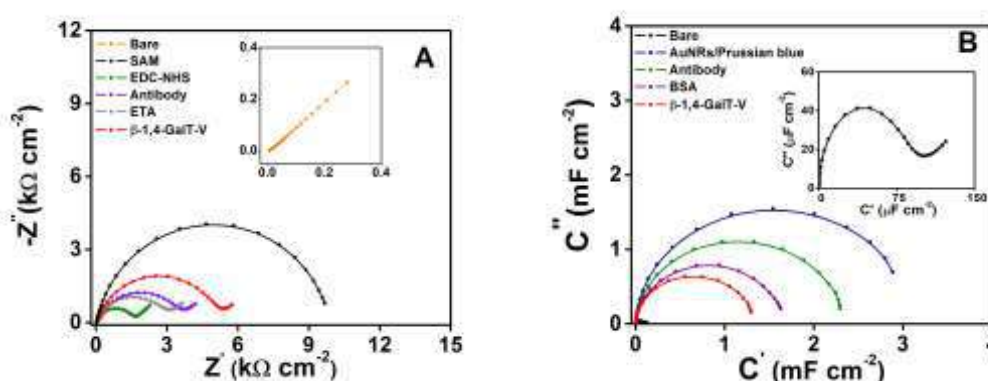


Figure 1: Nyquist plots of the development of the biosensors. (A). Impedimetric biosensor (B). Capacitive biosensor.

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Global developments demand for fossil free, renewable energy solutions. The hydrogen energy cycle through water splitting by electrolyzers and electric power generation by fuel cells can provide a sustainable solution for energy consumption and storage. In order to increase the accessibility of hydrogen energy systems, the cost efficiency is tackled by development of platinum-free electrocatalysts such as nickel-based alloys. The catalytic reactions in focus are hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR), which, in absence of platinum group metals (PGMs), are investigated in alkaline media. The electrodeposition of Ni-based alloys from aqueous media allows for the synthesis of well-defined nanostructures of thin films with increased efficiency at HER with respect to dense thin films due to their nanoporosity [1]. In this work, Cu-Ni alloy films are electrodeposited within a wide compositional range by simple modification of the deposition potential. The addition of a block copolymer in the electrolyte results in the spontaneous formation of polymeric micelles. In this way, the so-called micelle-assisted electrodeposition yields a homogeneous mesoporosity independent of composition, with a pore size of approx. 10 nm (Figure 1). HER is evaluated by linear sweep voltammetry in 1 M KOH as a function of the composition. The study is complemented by common characterisation such as SEM/EDX, XRD, and XPS. In addition, it was determined that although the pore size of 10 nm leads to high efficiencies at HER due to high surface-to-volume ratio, higher pore size may be advantageous for the electrocatalytic activity. A high-molecular weight block copolymer was developed for the generation of larger micelles in order to obtain larger pore sizes. As a result, electrodeposited Ni films using this polymer do not only show larger pores up to 600 nm, but the porosity is also very obviously interconnected as demonstrated by SEM imaging. Most importantly, the efficiency at HER in alkaline media is significantly improved with respect to the 10 nm pore size.

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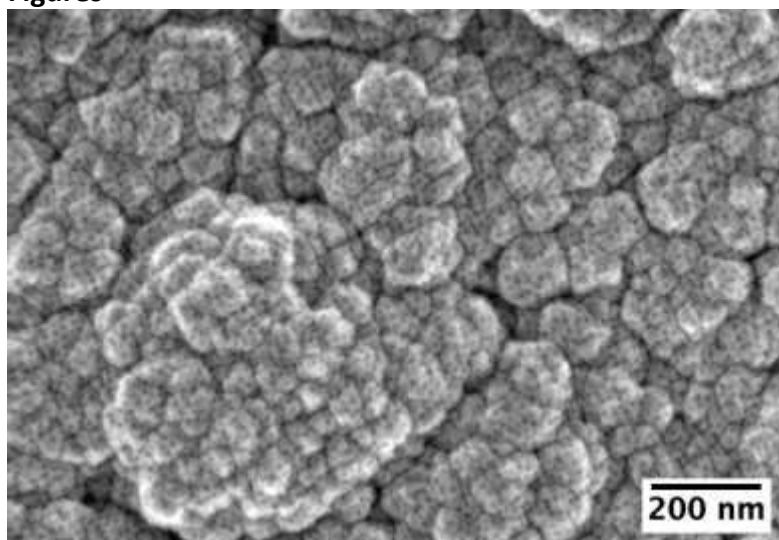


Figure 1: SEM micrograph of a mesoporous Cu₆₈Ni₃₂ alloy thin film produced by micelle-assisted electrodeposition.

Polydopamine nanoparticles-based hyperthermal chemotherapy for the treatment of liver cancer

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Polydopamine (PDA) is a polymer synthesized by the self-polymerization of dopamine monomers; during the polymerization process, spherical nanoparticles are obtained (PDA NPs) [1], the characteristics of which can be easily tuned by tailoring the synthesis parameters: in particular, size can be altered by changing the ammonia/dopamine molar ratio [2]. PDA NPs have been attracted the interest of researchers because of their interesting properties; in particular, they own high drug encapsulation capacity, easy and versatile surface modification through their catechol, imine, and amine groups, and ability to convert the near-infrared (NIR) radiation into heat, as well as strong antioxidant capacity [3]. In our study, considering their mentioned excellent properties, PDA NPs have been proposed to be exploited as anti-cancers agent *via* hyperthermia through remote NIR excitation. In order to let them acquire a stronger cancer therapeutic activity, PDA NPs have been loaded with a chemotherapeutic agent, sorafenib (SFR-PDA NPs), specifically effective on liver cancer. Representative scanning electron microscopy (SEM) and transmission electron microscopy (TEM) images are reported in Figures 1A-D, and show highly uniform and spherical nanoparticles. The excellent colloidal stability of the nanovectors, evaluated through ζ -potential assessment (Figure 1E), has been demonstrated by values of -46.7 ± 0.3 mV (PDA NPs) and -33.5 ± 0.7 mV (SRF-PDA NPs). Eventually, considering the data obtained after irradiation (performed for 10 min) with a single-mode NIR laser (808 nm), a consistent temperature increment from 37°C to 54°C was observed (Figure 1F). Altogether, these results encourage further *in vitro* investigations on liver cancer models in order to arrive closer to their clinical applications.

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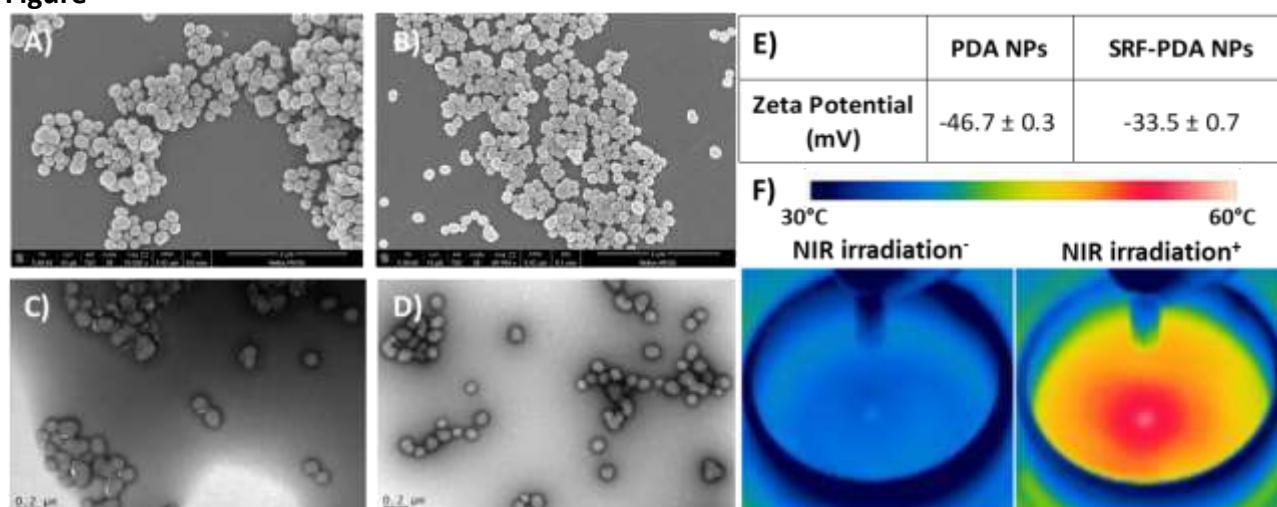


Figure 1: Characterization of PDA and PDA-SRF NPs. Representative scanning electron microscopy (SEM) and transmission electron microscopy (TEM) images of PDA (A and C) and PDA-SRF NPs (B and D). ζ -potential measurements (E) and thermo-images of an aqueous dispersion of NIR-stimulated PDA NPs (F).

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Abstract

Phenylketonuria (PKU) is a hereditary autosomic-recessive metabolic disease that inhibits the metabolism of the amino acid phenylalanine, and it has been diagnosed after birth through bacterial inhibition assay, a well-established screening method for newborn babies since 1963.[1] Its accumulation in blood, urine, and other tissues, can cause seizures, intellectual disabilities, and other mental disorders if not adequately assessed through diet and periodic visits to an assigned PKU clinic.[2] Fast, robust, sensitive, and user-friendly tests are desirable for better monitoring of phenylalanine levels in PKU patients to improve their lifestyles. Herein, we present a Point-of-Care aptamer lateral flow biosensor in a strand displacement format and gold nanoparticles (AuNPs) as an optical label for phenylalanine determination in a buffer sample, allowing the determination of mild hyperphenylalaninemia, mild PKU, and classic PKU. In this work, we conjugated AuNPs to a short nucleic acid sequence complementary to a region of a previously reported aptamer that recognizes phenylalanine and printed the complex as a first line.[3] When a buffer sample containing phenylalanine reaches the aptamer, the competition displaces the AuNP conjugate and the decrease of the optical signal in the first line is measured. As the AuNP conjugate flows through the lateral flow strip, they are captured by a complementary sequence in a second line, causing the appearance of a second measurable signal. The assay is completed in 20 minutes and has a limit of detection of 50 μ M, which is the standard phenylalanine concentration in healthy patients' blood.

Acknowledgments

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 825694. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. The European Union cannot be held responsible for them.

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Nanotechnology, an exceptional opportunity for the sustainable economic development

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Waste accumulation in the environment has unfortunately become an accompanying problem for Albania since the early 1990's. As in other European countries, the reduction of waste accumulation has been based so far on the limited implementation of the principles of integrated waste management. But time is telling that the reduction of waste accumulation requires above all the development of effective strategies to shift the paradigm of used materials from wastes to resources, where waste could become a valuable input to another processes, where products could be repaired, reused or upgraded instead of thrown them away.

Waste management according to the European Circular Economy Package of four amended directives, is seen so far as the most credible process, able to guarantee sustainable economic development if implemented in the largest part of the world, especially where the productive and economic activity is more dynamic. In this frame, producers in Albania and all around the world see scientific research in the field of nanotechnology and the new findings and the concrete applications in the economy related to nanotechnology, as an opportunity that will help addressing the many challenges that humanity is facing to achieve sustainable economic development. Nanotechnology is therefore one of the biggest expectation that we, the entrepreneurs, have towards scientists, the academic world and other relevant factors.

As far as "Circular Economy" is concerned, we think that nanotechnology will strongly influence the extraction of raw and auxiliary materials. The new innovative applications of nanotechnology will enable us to have a high efficiency in the use of these materials as well as energy, air or water that are needed in this process. Consequently, the impact on the environment will be much greater decreases, especially CO₂ emissions.

We are hopeful that nanotechnology will help to re-dimension the process of mechanical and chemical recycling of waste, and especially plastic waste, in both size and efficiency. The method of chemical recycling of plastic waste that comes from human activity (post user), although still in experimental stage, promises radical changes to the challenges we face today including "marine liter". We are interested on the use of nano-additives to improve the properties of recycled plastics, on the fundamental aspects of colloid stabilization. Furthermore, the contribution of nanotechnology to the fabrication of effective catalysts for the depolymerization of plastics into the constituent monomers is very interesting.

Finally, we are open to cooperate, support the requests of the community of academic researchers who will work to make, adapt their scientific discoveries in instruments applicable in industrial technologies.

A rational approach to tailor Au-IrO₂ nanoflowers as colorimetric labels for lateral flow assays

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Lateral flow assay (LFA) is regarded as an ideal screening tool and is widely used in clinical diagnostics due to its simplicity, rapidity, user-friendliness and low cost^{1,2}. In particular, during the COVID-19 pandemic, colorimetric lateral flow assay (especially gold nanoparticles based LFA) has demonstrated its convenience and superiority in personal home use³. However, lateral flow assay shows relatively low sensitivity due to short reaction time and insufficient sample processing (i.e. sample matrix colour interference). The application of nanoparticles with higher extinction coefficient (stronger light absorption capacity) is the most direct and simplest way to improve the sensitivity of lateral flow assay. Following this strategy, we rationally optimize the synthesis of gold and iridium oxide nanoflowers (Au-IrO₂ NFs) referring to De Freitas and co-workers' work⁴ with modification by increasing the concentration of reduction reagent (2.5 mM sodium citrate) and decreasing reaction time. Specifically, we were able to rationally control their size (from 155 nm to 53 nm in diameter) in order to guarantee an optimal flow along the different pads of a LFA. Then, thanks to their superior plasmonic behavior (compared to standard AuNPs), we could achieve an 8-fold lower limit of detection (down to 1.7 ng/mL) for human immunoglobulin G (human IgG) than standard LFAs (13.5 ng/mL). And the Au-IrO₂ NFs based lateral flow assay can specifically identify the human IgG among various IgG from other hosts. Meanwhile, the Au-IrO₂ NFs based LFA showed acceptable recovery for detecting human IgG spiked in human serum (human IgG depleted). Therefore, due to their optical and redox properties, bioconjugation capabilities, and the synergic combination of the individual components, Au-IrO₂ NFs appear as potential candidates for the next generation of optical LFAs.

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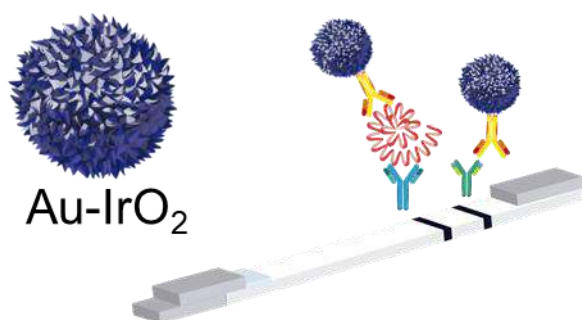


Figure 1: Scheme of Au-IrO₂ nanoflowers based lateral flow assay

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Abstract (Calibri 12)

Roxadustat (Figure 1) is an orally used antianemia drug for the treatment of renal anemia. Renal anemia is caused by a deficiency of erythropoietin, a protein that helps formation of red blood cells. Roxadustat increases the stability of HIF in the kidney by inhibiting the enzyme prolyl-hydroxylase, which activates hypoxia (lack of oxygen) inducible factor (HIF). Thus, it undertakes the treatment of anemia by causing an increase in erythropoietin production [1, 2]. Chromatographic and spectroscopic studies of roxadustat are available in the literature, but electrochemical studies have not been found yet. Electrochemical methods can be preferred because of their advantages over other methods such as low cost, low solution consumption and shorter analysis times. In this study, the electrochemical behavior of the roxadustat drug in aqueous media was investigated in various buffer solutions. The oxidation mechanism has been tried to be clarified by pH and velocity scanning studies. After the optimization of the method, calibration studies were carried out in the determined pH 5.3 acetate buffer solution and validation parameters were examined.

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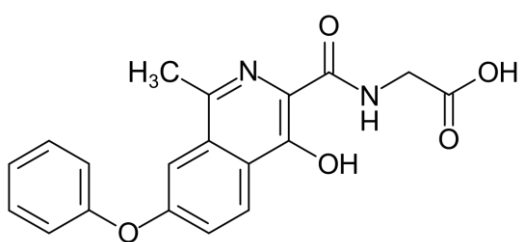


Figure 1: Chemical structure of roxadustat

Role of aluminum in nanostructure and strength of cement hydration phases

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This research work is about the influence of various aluminum species on the nanomolecular structure and strength relationship of cement hydration phases.

The aluminum species and their corresponding amounts were studied by ²⁷Al MAS NMR technique. The technique has found out three Al species in cementitious samples: four-coordinate Al(IV), five-coordinate Al(V), and six-coordinate Al(VI) species [1, 2, 3]. The results show that an even more pronounced increase in the sample's polymerization degree of C-(A) S-H (C-S-H containing Al) phase is observed through the addition of alumina-based pyrogenic oxide. Based on this technique we have been able to know the amount and location of Al which is of major importance for the electrostatic cohesion and durability of the cement paste.

Keywords: ²⁷Al MAS NMR, Aluminum sites, C-(A) S-H phase, Cement hydration.

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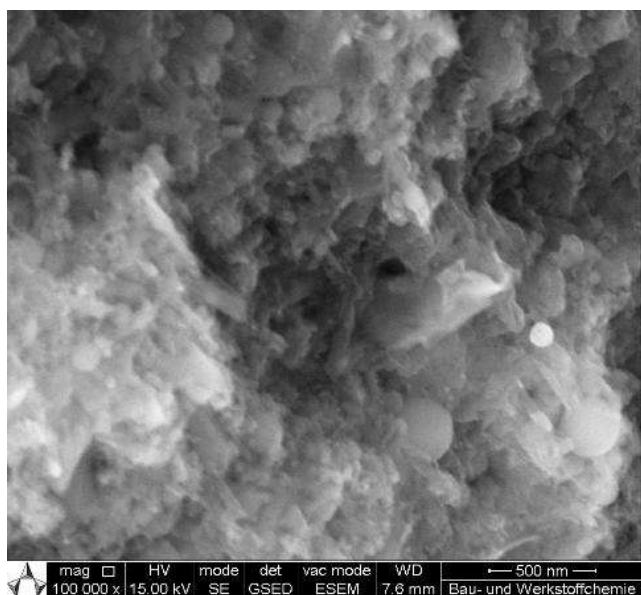


Figure 1: SEM images (100000x) of Ultra high performance concrete with Pox (UHPC)

ORR study of a Pt-free catalyst with RRDE, SECM and SECCM, from macro to nano scale measurements

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The hazardous pollution caused by burning of fossil fuels has put the well-being of the whole globe in jeopardy and yet they still account for 80% of energy production worldwide, generating the need for alternative energy sources. Electrochemical energy conversion devices are a promising option for green energy supply, although the challenge associated with electrocatalysis have caused increasing complexity in the materials and systems, demanding further research and insights. Electrocatalytic materials needed for key reactions in Fuel Cells such as Oxygen Reduction Reactions (ORR) are the main problematic in the field. The synthesis of noble-metal-free electrocatalysts is vastly encouraged, however the unambiguous determination of their electrocatalytic activity is just as crucial. In this work, we study a non-precious catalyst based on multi-walled carbon nanotubes (MWCNT) for its ORR activity, with macro, micro and nano scale laboratory techniques, respectively Rotating Ring Disc Electrode (RRDE), Scanning Electrochemical Microscopy (SECM) and Scanning Electrochemical Cell Microscopy (SECCM). Hence, unravelling crucial information about the catalyst and emphasizing the power of nano-scale single entity measurements.

Figures

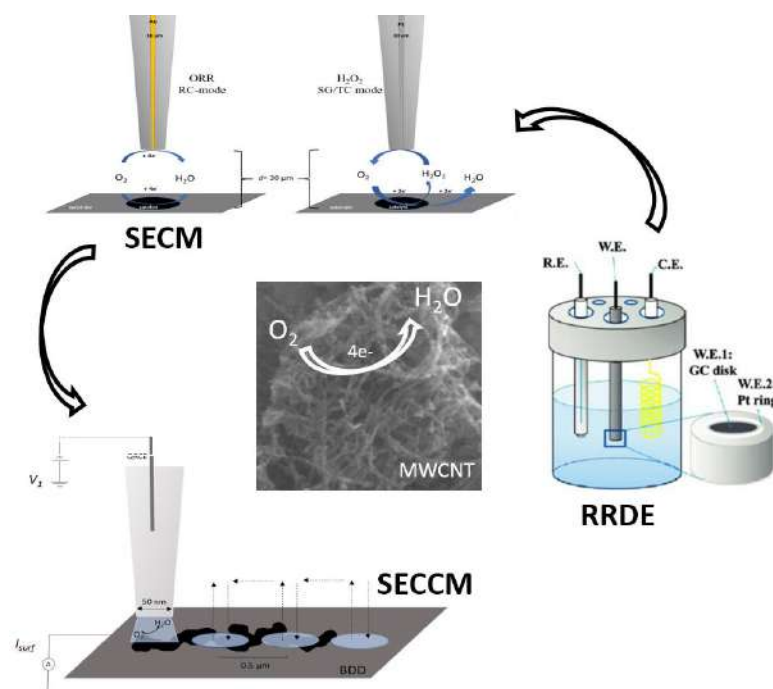


Figure 1: RRDE, SECM and SECCM investigation of a MWCNT-based catalyst for its ORR activity

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Printed sensors, both on flexible substrates and directly on the skin, have been shown to have great potential for developing wearables and point-of-care devices. For this reason, integrating sensors by printing methods into already developed mussel-inspired membranes as artificial skin for tissue regeneration is of great interest not only for sensing on the skin, but also for treating wounds.

However, printing on delicate materials such as artificial skin presents many challenges, especially when a common desktop printer is used. To print on these materials, they must be dry, making them fragile and brittle. Due to this, some of the inside components of the desktop printer, like the rollers and wheels for dragging the paper can easily damage and eventually break them apart.

This work presents the comparison, advantages, and disadvantages of printing on the mussel-inspired membrane using a Dimatix (Fujifilms DMP 2800 series) research grade printer and an Epson XP-15000 desktop printer. As a case study, the resistivity obtained from the inks has been compared and its possible application for the construction of RF antennas as well as for a temperature sensor on the skin.

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Figures

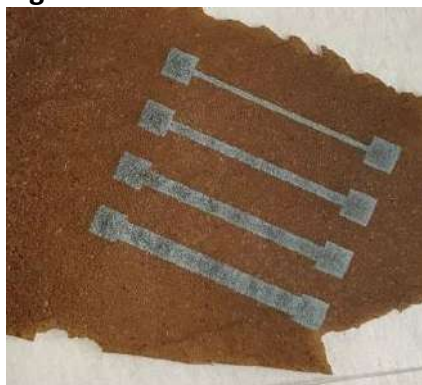


Figure 1: Silver tracks printed with Epson printer on the mussel-inspired free-standing membrane

Acknowledgements

The ICN2 is funded by the CERCA program/Generalitat de Catalunya and supported by the Severo Ochoa "Centers of Excellence" program, grant SEV-2017-0706 funded by MCIN/AEI/10.13039/501100011033. This work was supported by grant RTI2018-098027-B-C21 funded by MCIN/AEI/10.13039/501100011033 and by ERDF – "A way of making Europe". Also, it has been financed by the Severo Ochoa Seed Funding for Emerging Topics 2021 Program. GM acknowledges the Fundación Carolina for the Doctoral Scholarship granted under the program "Doctorado 2020". PBD is particularly grateful to the São Paulo Research Foundation (FAPESP) for the award of a post-doctoral scholarship (Grant no. 2021/14732-0).

Challenges and Possible Approaches to Molecular Imprinting for Nanobiosensing of Small Molecules

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Abstract

In various applications, from biomedicine to environmental monitoring and nanobiosensing, molecularly-imprinted polymers (MIPs) have shown their potential as customizable synthetic receptors capable of distinguishing large and small molecules with high molecular specificity. Biorecognition elements, such as antibodies and enzymes, have shown inherent problems with temporal stability and can be denatured under extreme conditions [1]. MIPs, however, are more robust in complex media, have better long-term stability, and a more straightforward and reproducible fabrication procedure. However, there is a scarcity in the literature of papers investigating the quantitative analytical capabilities of MIPs in real-world applications. There are still several factors that must be addressed before MIPs-based biosensors can be commercialized [2,3]. The most critical challenge that needs to be addressed in MIPs development is to study the binding interactions between monomers and between the monomer and the template in a porogenic solvent, which must form a spontaneous and stable template-monomer complex. In this project, we study the ionic form of kynurenic acid, as a model small molecule template, in several matrices, along with its complexation with o-phenylenediamine. Additionally, further studies encompass an adaptation of the MIP layer onto nanomaterial-based electrodes, due to their ease of tuning and fabrication. MIPs have been shown to possess higher sample loading capacities, sensitivity, and selectivity for small molecules than conventional immunoassays [4,5], which makes them interesting in quantitative small molecule biomarker detection.

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Acknowledgments

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Abstract

Nature has inspired the development of artificial nanosystems in which different stimuli promote the switching between equilibrium and out-of-equilibrium states. Those based on the photochromic effect have been widely studied because they allow the spatiotemporal switch of state. To mimic photochromic nanosystems, the scope of this study includes the synthesis of photochromic amphiphilic copolymers and their self-assembly in well-defined polymersomes suitable for encapsulation of hydrophobic and hydrophilic cargoes. First, photochromic amphiphilic copolymers were synthesized by the one-step nucleophilic addition of amine-containing 4-aminoazobenzene (AZO) and amine-PEG3-Biotin (biotin) moieties onto a poly(ethylene-alt-maleic anhydride) (PEMA) backbone, i.e., AZO-PEMA and biotin-AZO-PEMA. The synthesized copolymers contained residual carboxylic acids as hydrophilic groups, AZO moieties as photoswitchable chemical hydrophobic groups, and biotin moieties as a protein-binding ligand and hydrophilic groups. Then, both amphiphilic copolymers were self-assembled in nanopolymersomes with the in-situ encapsulation of cargoes of different molecular nature: (i) molecules as methylene blue (MB) and ferrocene (Fc), (ii) the enzyme horseradish peroxidase (HRP); and (iii) inorganic platinum nanoparticles (PtNPs). These polymersomes were highly stable with a high cargo-retention efficiency even for weeks. The ability of AZO-based polymersomes to isomerize upon ultraviolet (UV) irradiation at 365 nm was employed to change the permeability of polymersome bilayer by switching polarity from a nonpolar *trans*- to a *cis*-azobenzene with increased polarity. This conformational transition in the bilayer promoted selective permeability. Small hydrophilic molecules such as MB can be released while nanometer-sized cargoes such as HRP and PtNPs remain in the polymersomes' hydrophilic core. However, small substrates can penetrate the polymersomes bilayer, yielding photochromic nanoreactors. The AZO-based polymersomes demonstrated the potential to switch permeability and could find applications to cargo release and off-on reactions.

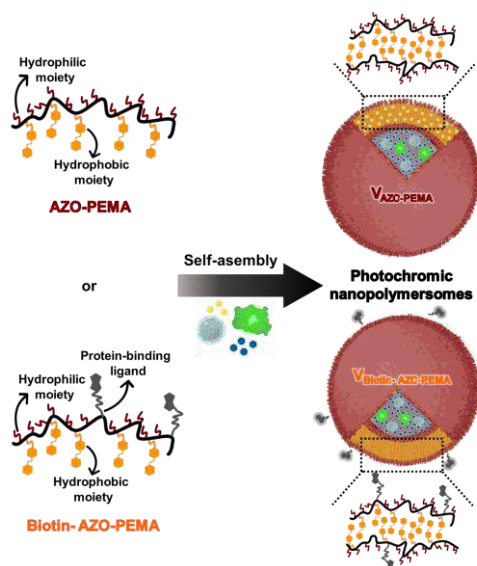


Figure 1. Schematic representation of photochromic nanopolymersomes.

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Molecularly imprinted polymer on glassy carbon and graphene surface for electrochemical detection of Isoproturon

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Molecularly imprinted polypyrrole (MIP) film containing isoproturon (ISO) were made first onto glassy carbon (GC) and then on pure electrochemical graphene deposited on polystyrene. The electrochemical preparation procedure included two steps: electropolymerization of pyrrole performed by cyclic voltammetry and chronoamperometry where ISO template molecules were successfully trapped in the PPy film. After the electrochemical extraction of the template, the PPy film acted as a MIP for the selective recognition of ISO whereas the non-imprinted polymer (NIP) film, made in the same conditions except for the presence of targeted molecule, did not exhibit any interaction. ISO-MIPPy films made on GC electrodes were found to selectively detect ISO. Its limit of detection (LOD) in milli Q water, achieved via square wave voltammetry was as low as $0.5 \mu\text{g L}^{-1}$, whereas in real water samples it was found to be $2.2 \mu\text{g L}^{-1}$. In a second part, an original method for elaboration of 100% graphene electrodes has been developed. It is based in electrochemical exfoliation of graphene at negative potentials in a single step and then the electrodes were prepared by temperature compression of graphene on a polystyrene substrate. Electrochemical properties of these electrodes were evaluated using redox probes. XPS, Raman, IR methods and four-point probe conductivity measurements are used to finely characterize the surface chemistry and nanostructure of graphene electrodes. Finally, the electropolymerization of ISO-MIPPy films has been successfully carried out onto graphene and their potential for the determination of ISO in water has been demonstrated.

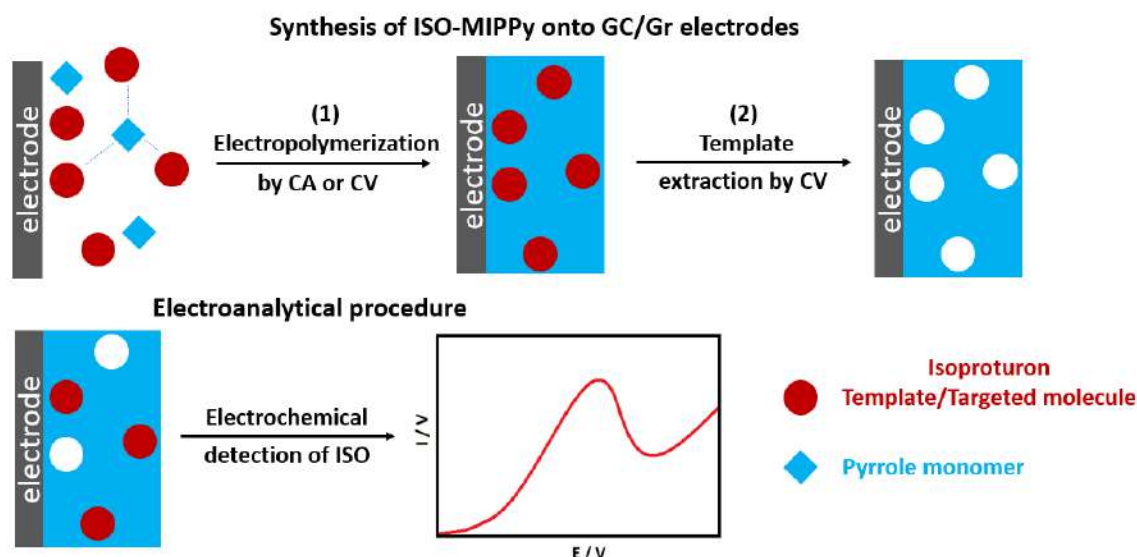


Figure 1: Schematic representation of the procedure used for the preparation of ISO-MIPPy films onto GC and Gr electrodes, including two steps: 1) electropolymerization of MIPs by CA and/or CV, and 2) the CV extraction of ISO molecules. Both electrodes were tested for electrochemical detection of ISO.

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Trastuzumab-functionalized piezoelectric nylon-11 nanovectors as an innovative tool in cancer therapy

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Nanotechnology suggests the exploitation of biocompatible and biodegradable nanovectors for the enhancement of bioavailability and targeting of drugs [1]. In this context, an innovative approach has been recently proposed in cancer nanomedicine based on the use of nanomaterials that can remotely respond to external stimuli such as ultrasound [2]. Piezoelectric nanomaterials, featuring the capability of converting mechanical energy into electricity, present great potential in cancer therapy. Nylon-11, a polyamide bioplastic, presents satisfactory piezoelectric properties [3] never exploited in biomedicine so far: here, we propose the use of trastuzumab-modified nylon-11 (Tmab-nylon-11) nanovectors to improve the therapeutic outcome in cancer neoangiogenesis treatment, by exploiting an indirect electric stimulation mediated by the mechanical excitation of the nanoparticles: this stimulation in fact affects cell fate by enhancing drug release or/and regulating the invasion and migration pathways [2,4].

Nylon-11 nanoparticles were prepared by a simple anti-solvent method. Trastuzumab (Tmab) was conjugated to the nanoparticles, after reducing the antibody molecule by using 1,4-dithiothreitol (DTT), by exploiting the cysteine residues of the antibody and the 1,2-distearoyl-*sn*-glycero-3-phosphoethanolamine-N-[maleimide(polyethylene glycol)-2000] (DSPE-PEG-Mal) on the particles. Successful binding was confirmed by sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) and bicinchoninic acid (BCA) assay. The morphological characterization of the particles was assessed using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The biocompatibility of the Tmab-nylon-11 nanoparticles was tested on human brain capillary endothelial cells (HCMECs). Statistical analysis was carried out by using analysis of variance (ANOVA) followed by Fisher's *post-hoc* test.

SEM and TEM imaging suggest the formation of spherical-shaped nanoparticles. SDS-PAGE and BCA assay show the presence of the antibody on Tmab-nylon-11 nanoparticles. Dynamic light scattering (DLS) measurements show a size of nylon-11 and Tmab-nylon-11 nanoparticles of 193.9 ± 3.5 nm and 182.1 ± 0.9 nm, respectively (Figure 1A). After synthesis, the particles were stored at 4°C, and the long-term stability has been monitored using DLS and ζ -potential measurements. Finally, the biocompatibility data showed that the particles are well tolerated by HCMECs up to 250 $\mu\text{g/mL}$ after 24 h of incubation (Figure 1B).

Concluding, piezoelectric nylon-11 nanoparticles were successfully synthesized by a simple anti-solvent method and decorated with trastuzumab to improve therapeutic efficiency. The obtainment of biocompatible, stable, and monodisperse polymeric piezoelectric nanoparticles is the first step towards innovative approaches in cancer nanomedicine.

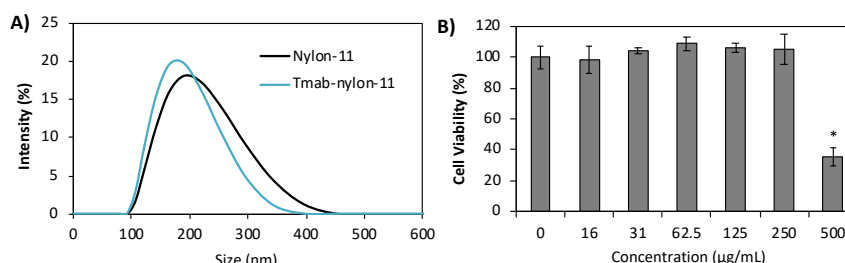


Figure 1: A) Size distribution of the nanoparticles. B) Biocompatibility results for Tmab-nylon-11.

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Au/Fe nanoreactors to directly generate ROS in water for environmental remediation and therapies

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Abstract

Reactive oxygen species have been widely studied and industrially used due to their applications in various environmental and biomedical areas. ROS can be generated *via* the Fenton reaction, which generally requires high hydrogen peroxide (H₂O₂) concentration, UV light, and acidic conditions. Here, we present galvanic Fe/Au nanoreactors that can directly generate ROS in water at neutral pH without the need for any additive. The electrochemical nanoreactors are based on anisotropic Fe/Au layers deposited in a semi-shell fashion on mesoporous silicon oxide nanoparticles. The bimetallic coating has been designed to enable the *in-situ* production of H₂O₂ and Fe²⁺ in water by exploiting the different work functions and electrochemical potential of the metals, thereby triggering the Fenton chemical path for ROS production. In this study, as proof of concept, we analyzed the degradation and mineralization of the dye methylene blue and the antibiotic tetracycline. The degradation was monitored by spectrophotometry at pH7 and it was correlated with Total Organic Carbon (TOC) analysis. The analysis showed a very fast degradation of the contaminants within the first 15 min of the reaction. This reactivity was achieved with a very low concentration of nanoreactors (i.e., 20 µg/mL). In addition, the nanoreactors were applied for the ROS generation in the vicinity of cancer cells *in vitro*, showing a substantial viability reduction even when the nanoreactors were located 100 µm away from the cells. In conclusion, the *in-situ* generated hydrogen peroxide (H₂O₂) at the Au semi-shell surface produced efficient •OH *via* the Fenton reaction catalysed by the Fe²⁺ ions released from the Fe semi-shell layer. Therefore, these nanoreactors are a new highly effective route to produce fast local oxidations without the need for any chemical additive.

Keywords

Nanoreactor,
Reactive Oxygen Species,
Fe,Au

Probing temperature-responsivity of pNIPAM microgels by super resolution microscopy and numerical simulations

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Abstract

Super resolution microscopy can observe microgel morphologies at the nanometer scale and monitor their response to temperature changes in situ, which opens exciting opportunities to design and precisely control the behavior of microgels for various applications [1]. In this context, direct stochastic optical reconstruction microscopy (dSTORM) is a well-established tool used to investigate colloidal systems e.g. poly(N-isopropylacrylamide) (pNIPAM) microgels [2].

When performing advanced microscopy experiments, interactions between the particle and the environment are vital. Often microgels are deposited on a substrate since they have to remain still for several minutes during the experiment. This study uses dSTORM and molecular dynamic (MD) simulations to investigate how individual microgels anchored on hydrophilic and hydrophobic surfaces change morphology with temperature. Super resolved images of individual microgel particles at different swelling stages are analyzed, and we obtain their density profiles numerically and experimentally. The results suggest that the anchoring parts of the microgel stick to the surface as the temperature increases. We find the experimental data and the MD simulations in excellent agreement. Our study is essential to establish a high-resolution monitoring technique as a platform for investigating more complex systems, where molecules of interest can be encapsulated in the microgel network and controllably released with temperature.

Keywords: super resolution microscopy, dSTORM, interface, pNIPAM microgels.

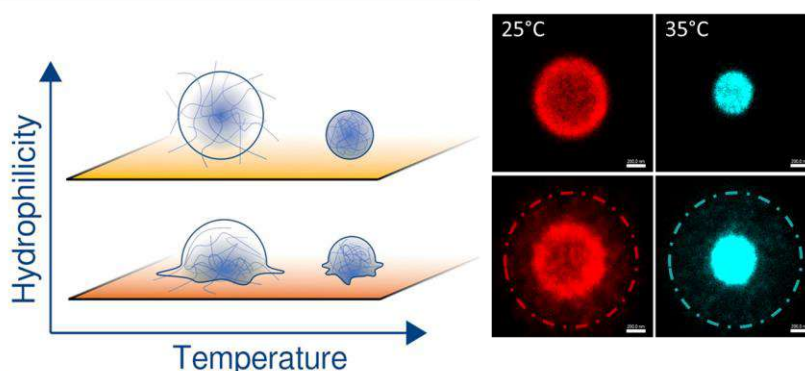


Figure 1: Schematic representation (left) and averaged dSTORM images (right) of microgels below and above LCST (left to right) and at two different surface treatment (bottom to top).

Acknowledgements: The authors acknowledge funding from H2020 Marie Curie Actions of the European Commission (ITN SUPERCOL, Grant Agreement 860914)

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Study on the distribution of ground level PM concentrations of urban air in most frequented places of Tirana City

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In Albania, reliable data and information on air quality in urban areas in most cases is fragmentary or lacking.

This work presents data regarding particulate matter, PM 1, 2.5, 4 and 10 as well as TSM for the city of Tirana. Tirana has undergone a dramatic demographic growth. During the last 25 years the population of Tirana has quadrupled. Construction has been rapid and, in most cases, chaotic and unstudied. Vehicle fleet in Tirana, in 2020, reaches up to 249.396, 47% of them are more than 11 years old. As a result, the created environmental pressure has been very high. Vehicles, construction sites and non-compliance with environmental standards has created serious problems in urban air quality. Studies suggest that long term exposure to fine particulate matter may be associated with increased rates of chronic bronchitis, reduced lung function and increased mortality from lung cancer and heart disease. It is also reported that long term exposure to air pollution increases the severity of Covid-19. In the city of Tirana it is surprising that the most popular places, such as cafes and restaurants, are those located along roads and intersections, where city traffic is extremely heavy. The obtained results show high values of PM concentration, exceeding several times the values recommended by WHO. It was observed that in cafes and restaurants located along the streets with low traffic, but where vegetation (tall trees) and buildings were present, PM values were up to 10 times higher than maximum recommended level by WHO. The higher values can be explained due to isolation of air masses from trees and buildings, thus preventing air flow, leading to high PM values. Measurements performed immediately after rain showed very low PM concentration, all below the maximum allowable limit. Meanwhile, on days without rain, even during the early morning hours 3:00 to 5:00, when car traffic is very low, PM 2.5 in all locations exceeded 2 to 8 times the maximum recommended value by the WHO (10 µg/m³→). The city of Tirana needs a strategy that will aim to improve air quality. Correlating the frequency of various health problems, such as heart attacks, cerebral haemorrhages, bronchitis and Covid-19 etc. to PM values would be a very important information to reach useful conclusions.

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NextGenMicrofluidics: low-cost. modular Lab-on-a-Cartridge devices for public health and food safety monitoring

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Current and emerging challenges to public health and food safety, due to infectious disease outbreaks, new toxins and rising antibiotic resistance, coupled with environmental change and shifting consumer habits and preferences have stressed the need for low-cost and reliable diagnostic tests that can be widely-implemented at the Point-of-Need or Point-of-Care. In an attempt to address this demand, and within the context of the H2020 NextGenMicrofluidics project, we have focused on the development of portable devices that combine microfluidics-based cartridges made by injection-molding with structured sensor foils produced on a large scale and cost-efficiently by roll-to-roll (R2R) procedures. The modular design of the cartridges, consisting of reaction chambers and reservoirs carefully-selected from a design library allows for a plethora of biochemical and molecular assays to be undertaken, while detection multiplexity is achieved through the utilization of probe microarrays, spotted onto appropriately-functionalized polymer sensor foils. The latter also serves as a waveguiding element, where a sensitive TIRF (total internal reflection fluorescence) readout is realized. Furthermore, liquids are moved within the cartridge by integrated electrochemical micropump, making PCB-based fluidic actuation obsolete. To showcase the capabilities of these devices, the multiplexed detection of the genetic material of SARS-CoV-2 as well as Influenza A (both H1N1 and H3N2 strains) is demonstrated, while for food safety, the combined detection of antibiotics and Aflatoxin M1 in milk with the use of aptamers acts as the target application. The elegant combination of the aforementioned advances and innovations in assay development, sensor foil fabrication and biofunctionalization, cartridge design and fluidics actuation act as a paradigm shift in the development of portable biosensing platforms and will significantly aid towards both disease management in the general population as well as safeguarding food safety and quality in the challenging times to come.

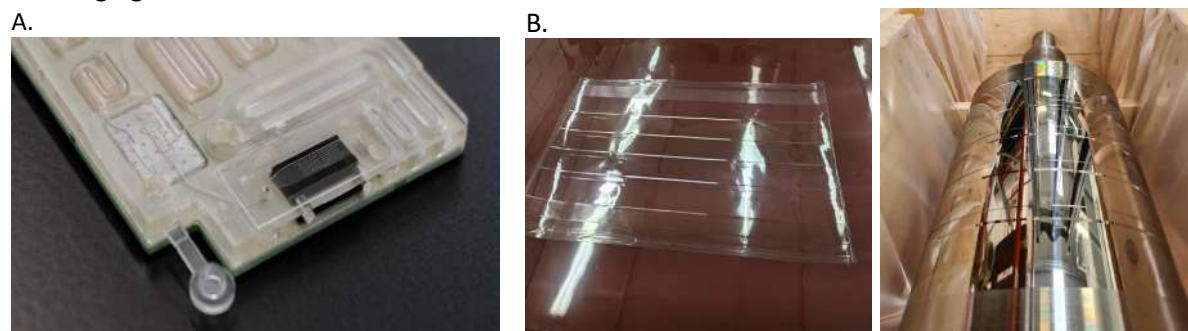


Figure 1: A) Prototype cartridge with probe-spotted sensor foil, B) Structured sensor foil with in-coupling and out-coupling optical structures for TIRF-based detection (left) and the roller used to fabricate the master shim for sensor foil fabrication by R2R Extrusion-coating (right).

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Abstract

Metal complexes and metal nanoparticles are being widely explored in nanotechnology with a remarkable use in biomedicine and cancer therapy. Up to date, an increasing number of papers report the beneficiary effects of Au and Cu particles in several biological application ranging from diagnostics to therapeutics including infectious diseases and cancer. However, on the other side the application of metal complexes and nanoparticles has been challenged by the accompanying risks such as genotoxicity, cytotoxicity and immunotoxicity. Side effects are promotion of ROS activity, induction of DNA breaks and apoptosis. It has been noted that size of the metal particles, time of exposure, concentration and type of administration are the key characteristics that should be taken into account to minimizing the undesirable side effects. This study explores the potential risks of causing DNA breaks upon treatment with heavy metal complexes and nanoparticles. We have used amphibians as a model organism to investigate the induction of DNA breaks upon treatment with copper (Cu) complexes and gold (Au) nanoparticles respectively. In addition to *in vitro* and *in vivo* assays, we have performed an *in silico* approach in order to predict the level of toxicity for each compound.

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Preparation of An Efficient and Selective Sensor Based on Carbon Electrodes Modified with TiO₂ Nanoparticles and Carbon Nanomaterial's for Macrolide Electrochemical Quantification

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The tetragonal (rutile) nanostructures of TiO₂ have attained immense significance due to their large active sites, electronic states, superior electrode performance, stability and conductivity. Metal oxide NPs as a multicomponent material combined with carbon material has pointed with several advantages to which we have proposed novel TiO₂ NPs using carbon ink as bulk material to prepare screen printed carbon electrodes as an electrochemical sensor for quantification of macrolides, specifically Azithromycin (AZM) and Erythromycin (ERM). Azithromycin (AZM) is one of the top prioritized antibiotics which are used by humans at high concentrations; lastly it is one the most used antibiotic to treat patients with COVID-19 infection, where the side effects and waste produced by antibiotics to human and environment is causing significance damage. There over, there is much need to develop a sensitive and selective method for the determination of AZM using flexible modified screen-printed carbon electrode (SPCE). Additionally, using different carbon nanomaterial's such as MWCNT and CNPL as a modifier were done studies for electrochemical activity of macrolides. Characteristic analysis like SEM analysis was performed to determine the physical and surface properties. Cyclic voltammetry and differential pulse voltammetry (DPV) analysis determined prepared TiO₂ NPs/SPCE electrode has a low limit of detection (LOD) of 0.93 μM with a limit of quantification (LOQ) of 3.1 μM , sensitivity of 7.36 $\mu\text{A } \mu\text{M}^{-1} \text{ cm}^{-2}$ (S/N = 3) and with a linear range of 0.05–50 μM towards determination of AZM. The prepared sensor has specific selectivity with high reproducibility and stability through real sample monitoring in human urine and water samples to present environmentally friendly strategy in determination of Macrolides.

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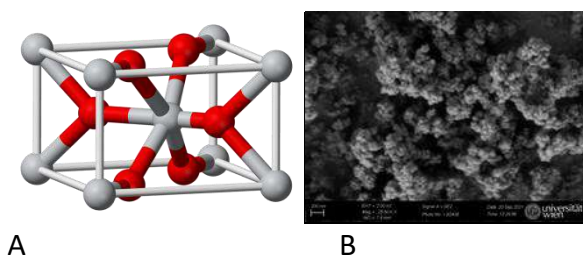


Figure 1: (A) Rutile (TiO₂) 3D structure (B) SEM images of TiO₂ NPs

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We discuss our recent progress [1-4] in atomistic modeling of a broad range of nanostructures. We start with alloyed quantum dots and inspect the role of alloy randomness that triggers the optical activity of dark excitons. We show that this process is mediated by two mechanisms: mixing dark and bright configurations by exchange interaction (Fig. 1), and the equally important appearance of nonvanishing optical transition matrix elements that otherwise correspond to nominally forbidden transitions in a nonalloyed case. Next, for 2D-like nanostructures with no alloying – so-called crystal phase quantum dots – we show that coupling between two sections of wurtzite leads to the formation of quasi-molecular hole states that may have an unusual antibonding character. Last but not least, we demonstrate that the same computational tools can be used to simulate STM images of dopants in silicon.

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Figures

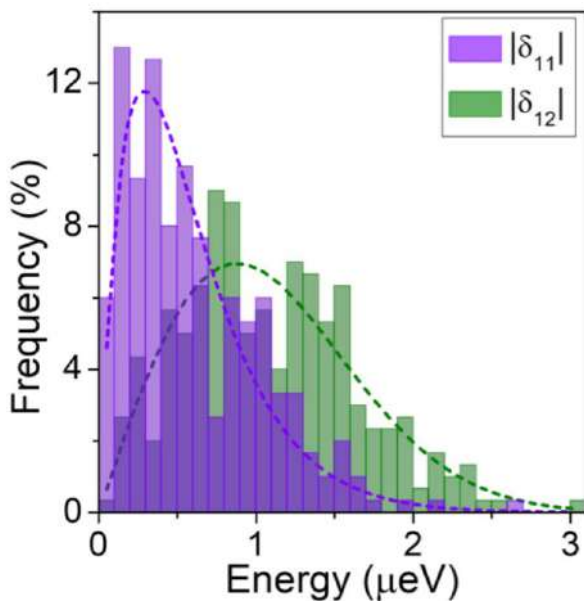


Figure 1: Histogram of absolute values of dark-bright exciton mixing exchange integrals [1] for an ensemble of 300 alloyed quantum dots calculated using atomistic tight-binding method.

Wearable and fully printed microfluidic nanosensor for sweat rate, conductivity, and copper detection with healthcare applications

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Wearable sensors and biosensors, also known as wearables, have been of great interest due to their applications in sports, well-being, and health monitoring. A wearable is ideally non-invasive and one of the most common samples is sweat, being the simplest in composition, abundant, and containing many biomarkers for pathologies and the general well-being of the subject [1]. Amongst the many biomarkers in sweat, heavy metals (HMs) such as copper have an important role as a biomarker of rheumatoid arthritis, coronary heart disease, Wilson's disease, and liver cirrhosis [2,3]. Nevertheless, several issues such as sampling conditions, sweat rate normalization, reliable continuous monitoring, and typically expensive fabrication methods still need to be addressed in sweat analysis with wearables. In this work, we propose an all-printed wearable system composed of: a) an inkjet-printed microfluidic part for the active sampling by reverse iontophoresis and measurement of the sweat volume/rate, b) a screen-printed carbon electrode (SPCE) for the copper electrochemical detection and its concentration normalization with the sweat rate, and c) a flexible wearable potentiostat transmitting the data wirelessly to a smartphone. The copper sensor showed a limit of detection of 396 ppb, a linear range up to 2500 ppb, a sensitivity of 2.3 nA/ppb, and resilience to interference tested in artificial sweat. Furthermore, the conductivity and volume integrated sensors allow for the normalization of the copper concentration on the base of the sweat rate. Lastly, the sweat absorption by a sponge in contact with air at the outlet of the device allows to empty of the microchannel (with the sweat in the sponge evaporating); thus, permitting the reuse of the device over time, pursuing the continuous monitoring concept.

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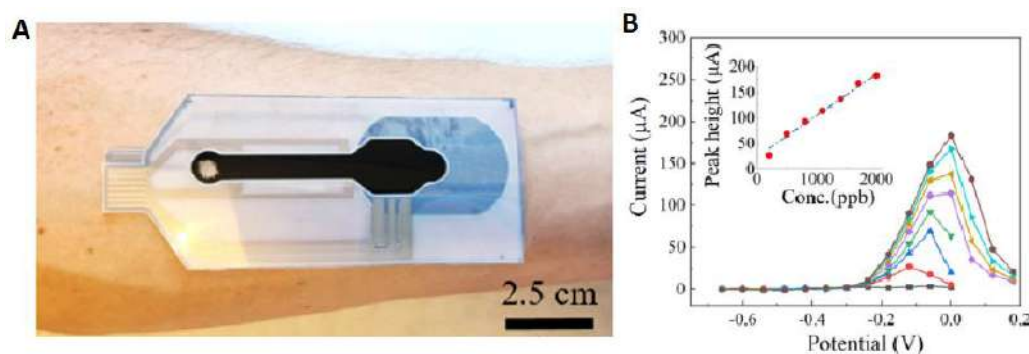


Figure 1: A) The assembled device applied on the forearm of the skin and B) the voltammograms of the printed microfluidic device on the flexible potentiostat and mobile phone system

Graphene Oxide as an effective adsorbent for (2E, 5E)-2,5- Bis(4-methoxybenzylidene) cyclopentanone

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Graphene oxide (GO) has attracted the interest of many scientists because of its extraordinary properties, not only because it possesses a large surface area, but also has many oxygenated polar groups (-hydroxyl, -epoxy, -carboxyl). Graphene oxide is evaluated as an adsorbent for the organic molecule such as (2E, 5E) -2,5-bis (4-methoxybenzylidene) cyclopentanone dissolved in organic solvent such as acetonitrile. The functional groups in GO were characterized by using an FTIR spectrometer. The concentration of the organic molecule after adsorption is analyzed using ultraviolet-visible spectroscopy.

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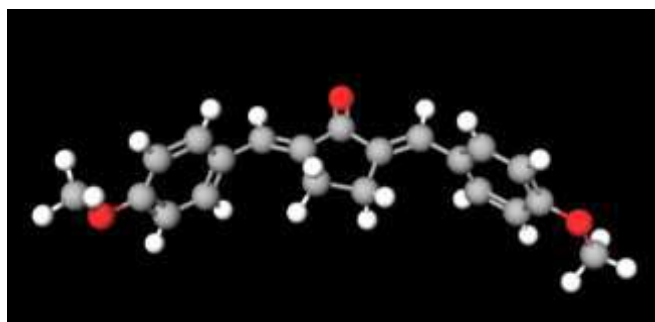
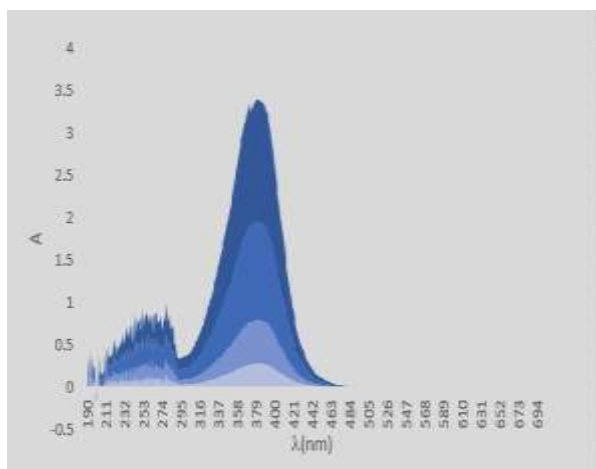


Figure 1: UV –VIS spectrum of (2E, 5E) -2,5-bis (4-methoxybenzylidene) cyclopentanone in organic solvent such as acetonitrile.

Figure 2: Structural formula of (2E, 5E) -2,5-bis (4-methoxybenzylidene) cyclopentanone

Ab Initio investigation of chemically modified Carbon Nanocones via aryldiazonium salts as a promising mild steel corrosion inhibitors

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Corrosion products are produced when industrial metals, such as iron, interact with an aggressive environment containing corrosive species such as chloride ions and oxygen, hence lowering the lifespan of the materials. Diverse vital industries [automotive, structural engineering, aerospace, oil and gas (energy), etc.] sustain significant corrosion-related losses. Corrosion inhibitors continue to be the simplest and most effective method for controlling the scale of this process [1-3].

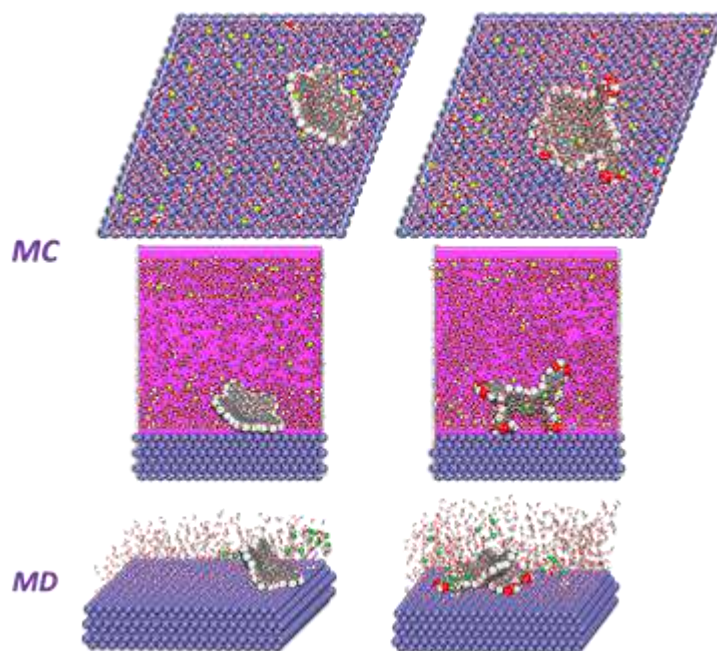


Figure 1: MC and MD poses of the lowest adsorption configurations for the Carbon Nanocones (CNCs) inhibitors in the simulated corrosion media on the iron surface under Periodic Boundary Condition (PBC) model.

Carbon Nanocones (bare and grafted by caboxyphenyl groups) were examined as corrosion inhibitors for mild steel in hydrochloric acid-containing aqueous corrosion medium in an effort to uncover new untapped potential inhibitors. The adsorption of Carbon Nanocones onto the Fe (1 1 0) surface was examined using Density Functional Theory (DFT), Monte Carlo simulation (MC), and Molecular Dynamics simulation (MD). On a molecular level, the obtained results revealed the adsorption capacity, geometry, and adsorption energies of Nanocones on the Fe(1 1 0) interface.

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Flow-injection amperometric determination of ranitidine after derivatization producing 2-methylfuran cation as an electroactive compound

Liridon Berisha

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Abstract

The new developed method for the electrochemical determination of ranitidine is optimized in flow injection analysis. Through the derivatization of ranitidine in an acidic environment with sodium nitrite, deaminating ranitidine and forming the electroactive species 2-methylfuran cation, it was possible to determine ranitidine at a lower potential at the glassy carbon paste electrode modified with anionic surfactant sodium dodecyl sulphate (SDBS). At optimized conditions such as pH, operating potential, flow rate, SDBS concentration, the method has an application in the concentration range from 1 to 600 mg/L ($R^2=0.996$) and LOD 1.3 mg/L. The determination of ranitidine with the new method in tablets and ampoules has been carried out successfully and the results are within the confidence limits with 95% reliability compared to the reference method with HPLC.

Keywords: Ranitidine, Surfactant, Flow injection system, Glassy carbon paste electrode.

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Abstract

In the last decade, atomically thin capillaries made from 2D materials have created a wave of new research especially in hydrodynamics and mass transport properties of fluids [1,2]. Van der Waals assembly of 2D materials to make capillaries, such as graphene, molybdenum disulphide and hexagonal boron nitride has already been achieved, but require highly sophisticated environments and nanofabrication techniques such as e-beam lithography, dry etching, and photolithography, and are very time consuming as we make one device at a time [1,2]. Herein, we are presenting an unique and novel nano-fabrication process to prepare 2D channels with well-defined geometries in a scalable manner. This technique demonstrates the fabrication of 2D channels from different naturally occurring layered materials such as graphite, metal oxides and sulphide, transition metal dichalcogenides, and phyllosilicates have been prepared in mass production, but in a shorter period. In addition, this method can be applied to prepare 2D channels from different 2D nanosheets such as graphene, molybdenum disulphide and hexagonal boron nitride through Van der Waals assembly. Moreover, this process holds advantages in making 2D channels of different dimensions and shapes with angstrom-scale precisions, alongside of the reduction of time and fabrication cost. The construction of these 2D channels will open doors to upscale production of nanofluidics devices, which can greatly impact studying and understanding the fundamental properties of fluids in confined geometries.

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Figures

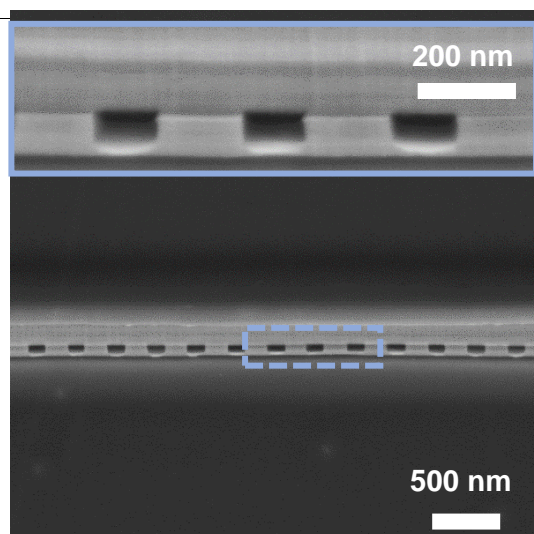


Figure 1: Cross-sectional scanning electron microscopy image of 2D channels fabricated by our method.

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Recently, wireless strain sensors capable of exploiting structural colors have attracted interest in new emerging applications such as robotics or composite materials monitoring [1]. Many approaches for mechanically tuning color using photonic crystals and plasmonic nanostructures have been reported and are fabricated typically using two techniques: the first one is self-assembly [2] and the second one is soft lithography [3].

In this work we study alternatives to obtain an affordable fabrication process for the nanostructured strain sensors. Laser interference lithography is used to obtain the original master with periodicity of the nanostructure easily tunable between 200 nm and 800 nm. From this master, multiple nanostructured films are obtained by thermal Nano-Imprint-Lithography on PVC. In order to maximize the optical response of those film a metallic layer is added by evaporation. These nanostructured labels are glued to metallic specimens and tested on a test bench (Fig 1). We have demonstrated experimentally that deformations down to 1% can be measured analyzing the optical response of those labels (Fig 1).

This development is focused on its applications on structural health monitoring of H₂ storage and aeronautic composite components

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Figures



Figure 1: Insert caption to place caption below figure (Calibri 11)

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Abstract

Nanopore sequencing technology (MinION, Oxford, UK), and its applications in basic and applied research have undergone significant growth since Oxford Nanopore Technologies (ONT) provided the first nanopore sequencer, MinION, in 2014 [1,2]. This technology relies on a nanoscale protein pore, or 'nanopore', that serves as a biosensor and is embedded in an electrically resistant polymer membrane [1]. Being a low-cost, accurate, fast, and easy in-situ handling technology, its' application for detecting and characterizing known and undescribed plant pathogens in different plant species and crops has gained a lot of space in agricultural research. The big advantage of such innovative technology resides in the supremacy of multiple detection and characterization of many pathogens and in a reduction of expenses of posting the DNA in foreign laboratories to perform the analysis, as well as the time of obtaining the sequences.

The ONT sequencing as a tool in plant virology has been relatively slow despite its promise in more recent years to yield large quantities of long nucleotide sequences in real - time without the need for prior amplification. Here, we present a protocol using the ONT Flongle platform that was applied on mini-dsRNA templates extracted from a range of symptomatic ornamental plants that could be used to search for new unreported pathogens for domestic surveillance of plant samples. The results of the ONT's application on dsRNA templates, compared with those obtained from total nucleic acid templates extracted from tissues of the same plants, as a valid diagnostician's toolkit that, together with the integration of high-throughput sequencing technology, showed to be a highly reliable and validated plant virus diagnostic method for known and unknown virus detection, as well as for other types of plant pathogens. The existence of these novels and previously reported viral entities in the tested plant material was ascertained through the application of nanotechnological diagnostic methods, *i.e.*, qPCR, TaqMan PCR, LAMP in our laboratories (IAMB, Italy; and NanoAlb, Albania) and afterward registered in NCBI database.

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Tailored electrochemical nano-immunosensor for anti-p53 autoantibodies based on cerium oxide doped PEDOT

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Abstract

Nano-immunosensors have the potential for the rapid, sensitive, and specific diagnosis of diseases such as cancer by detecting related biomarkers even at early stages, for instance, by detecting anti-p53 autoantibodies (aabs) produced by the individual's immune system against tumor-associated antigens several months or even years before the onset of clinical symptoms of the disease [1]. In this context, a novel and simple label-free electrochemical nano-immunosensor was developed for the selective and specific detection of anti-p53 aabs [2]. The immunoassay combined the extraordinary conductivity of poly(3,4-ethylenedioxythiophene) (PEDOT) electropolymerized *in situ* on screen-printed gold electrodes (SPAuE) and the direct functionalization of small cerium oxide (CeO_2) nanoparticles embedded in the polymeric matrix with p53 antigen. The individual nanostructures and each step of the nano-immunosensor architecture were extensively characterized in chemical, physical, and electrochemical properties by DLS, ELS, TEM, EDX, UV-Vis, FT-IR, XRD and electrochemical techniques. Under optimal conditions, the nano-immunosensor selectively and specifically detected anti-p53 aabs by differential pulse voltammetry at clinically relevant concentrations in less than 1 h, with high sensitivity and a limit of detection (LOD) of 3.2 pg mL^{-1} and with a shelf life of four weeks. Overall, the biofunctional nanocomposite-based immunosensing system assembled on SPAuE demonstrated excellent analytical performance even in spiked human serum samples, contributing to future ultrasensitive detection systems for cancer-related biomarker screening.

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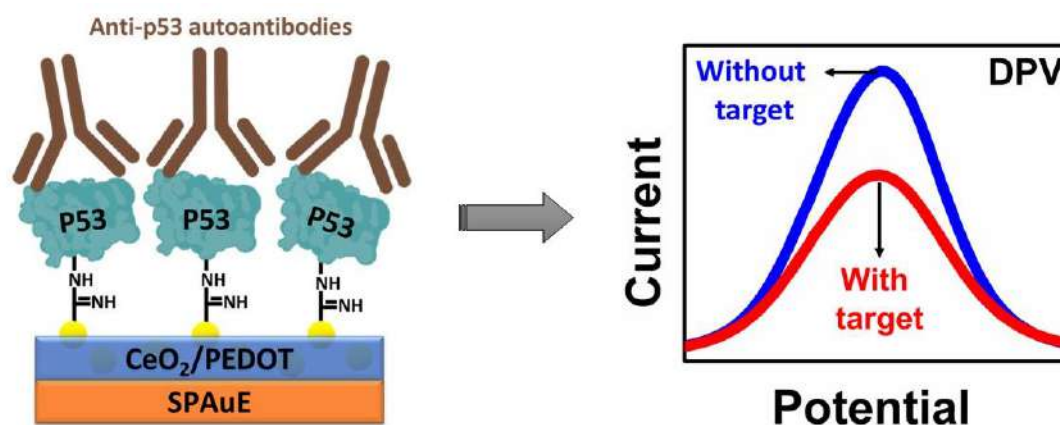


Figure 1: Scheme of CeO_2 -doped PEDOT-based nano-immunosensor for detection of anti-p53 autoantibodies by DPV using PBS 1X pH 7.4 solution containing $5 \text{ mM } [\text{Fe}(\text{CN})_6]^{3-/4-}$ as a redox mediator.

A Multiplexed Nanobiosensor for the Detection and Classification of Anaemia

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Anaemia is a blood-related disease affecting people of all ages, genders, and ethnicities. It is caused by the reduction of the number of erythrocytes or haemoglobin concentration in blood, resulting in a deficiency in oxygen transport. Anaemia is often a symptom of other diseases which can make its diagnosis difficult [1]. Anaemia can be classified into different phenotypic groups, such as: haemolytic, microcytic, macrocytic, hypochromic, and Iron Deficiency Anaemia (IDA), among others [2,3]. These have different causes and treatments and can be identified by measuring the levels of different biomarkers in patients' blood. Diagnosis of anaemia types requires knowledge of haemoglobin concentration, red blood cells' physical parameters (size, shape, volume, etc), as well as serum iron and serum ferritin concentrations [2,3]. Current methods for anaemia diagnosis rely on blood analysis and a complete haemogram; which are time-consuming, require expensive equipment and trained personnel. Herein, we are developing a point-of-care microfluidic, multiplexed biosensor based on nanotechnology detection techniques for the diagnosis and classification of anaemia through the evaluation of the previously mentioned parameters. This point of care biosensor will be user-friendly, fast, and less invasive, requiring only a small drop of blood. Additionally, it could serve as a screening and monitoring tool for other disease states in which anaemia is a symptom.

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The present paper reports an inside look into the synthesis of different doped TiO₂ photocatalysts supported on zeolite or graphene, in order to obtain surfaces able to inactivate and eliminate COVID-19 by photocatalysis under UV-A [1]. Throughout various combinations of raw materials and their amounts, eight different nanocomposites of metal-doped titanium dioxide coupled with graphene or zeolite are synthesized to investigate their photocatalytic properties [2]. By using concrete specimen molds, concrete cubes are obtained and a nanocoating of photocatalytic thin-films is applied. SEM-EDX analysis was performed for all photocatalytic composites. Physical-chemical characterization of the raw materials, like fly ash and zeolites, is conducted by using SEM, XRD, and XRF [3].

Keywords: Photocatalysts, COVID-19, Antiviral activity, Concrete cube, Nanocoating.

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Figures

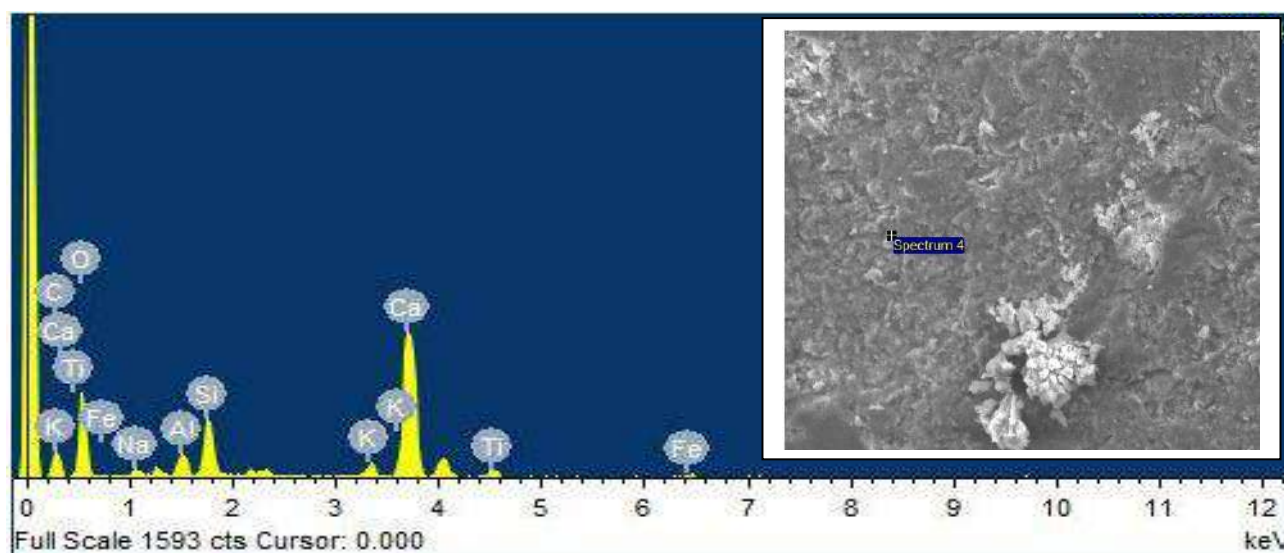


Figure 1: SEM-EDX analysis of TiO₂/ZXD nanopowder

Using adsorbent natural material for ammonium and ammonia removal

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The usage of natural sorbents in N recovery can be helpful in modification of the natural N cycle, to avoid further growth of anthropogenic reactive N environmental impact and its changes. Although natural minerals possess advantage such as good selectivity to NH_4^+ , good availability, and low cost, they have not been widely used on a commercial scale for wastewater treatment, probably because the exchanged minerals require further disposal, or because of the application of the regeneration process.

Natural material (NM), metal oxide material derived from the quartz sand enrichment process have been successfully utilized for their ammonia removal efficiency. A comparison of mathematical model applied to the adsorption of ammoniacal nitrogen was evaluated for the Langmuir and Freundlich adsorption models. We obtained much higher R^2 values (0.993) for the Freundlich model, compared to the Langmuir model for the ammonium removal by NM. Various kinetic models have been proposed and used to study and describe the mechanism of a solute uptake by an adsorbent from aqueous solution. In the present study two models are considered to describe the adsorption kinetics for the experimental data: the pseudo-first order kinetics model by Lagergren and the second-pseudo order kinetics model by Ho & McKay. The obtained data revealed that pseudo-second order equation provides the best correlation coefficient with high values (0.9988).

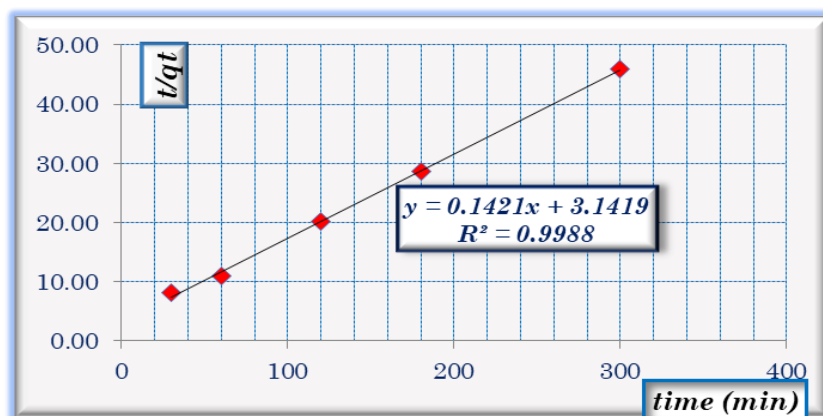


Figure 1: Pseudo-second order graph

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Catechol-based coatings and incorporation of AgNPs into nanofibrous and commercial membranes structure for antibacterial properties in water filtration

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Abstract

Nowadays it is very important to recycle and reuse raw materials. This allows for sustainable development, proper waste management and reduction of production costs. As the population grows and industry expands, the demand for water increases [1]. It is important to find a quick and efficient way to regenerate water. One of these ways is membrane filtration. However, the limiting factors for the speed and efficiency of filtration are the decrease of water flow over time, fouling and the growth of microorganisms on the membrane used [2]. To overcome these problems, a membrane with anti-fouling and antibacterial properties has to be designed. Our membranes were coated based on the reaction of catechol with hexamethylenediamine or (2-aminoethyl) amine. The reactions were optimized so that a coating rather than a thin film was formed on the membrane surface. For antibacterial properties, silver nanoparticles were attached after the coating reaction. The visual changes on the surface were observed, the size of the attached AgNPs was measured, changes in the water flux were checked, and antibacterial tests against *Escherichia coli* were performed.

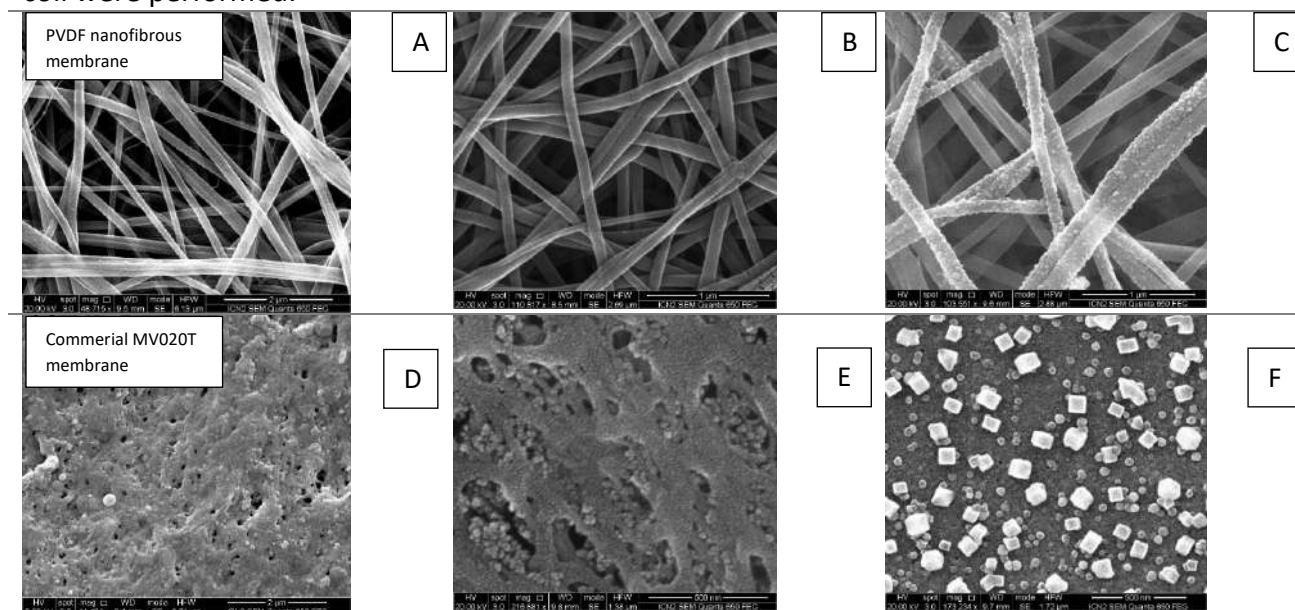


Figure 1: PVDF nanofibrous membrane and commercial available membrane Nadir MV020T A,D - pristine, B,E – CAT-TRIS coated, C,F – with Ag nanoparticles.

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Investigation of synthesized zeolite on the regeneration of used motoric oils.

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Zeolites are crystalline substances characterized by a three-dimensional, porous structure [1]. Their physic-chemical properties including ion-exchange capacity, sorption, or catalytic activity are attributed to their structure [2]. In this study, bentonite-embedded zeolites and activated mixtures are used to investigate their efficiency on used lubricating oil treatment and purification. Lubricating oils are used to reduce friction between car engine parts (UMO) [3]. The used oil for 15000-20000km was treated with zeolite and zeolite, activated carbon, and untreated or treated bentonite mixture. The physic-chemical parameters of the used motor oil (UMO) carried out before and after treatment are density, kinematics viscosity, viscosity index and pour points. It was observed that the values of treated oil compared to those of untreated oil were highly improved.

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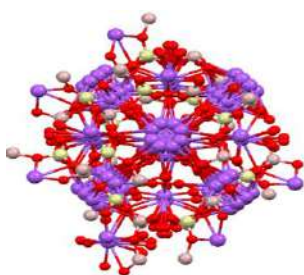


Figure 1. Crystalline structure of zeolite type X.

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Most properties of plasmonic nanostructures follow from the tunability of their optical response as a function of their shape and dimensions [1-3]. The accurate description of the optical properties of the nanoparticles is crucial for a theoretical understanding of the physical phenomena occurring at the plasmon resonance frequency [4]. In this context, we have recently presented an atomistic, yet classical, approach to predict the optical properties of nanostructures of complex shapes. The approach, which is called ω Fluctuating Charges Fluctuating Dipole (ω QF μ), is based on the Drude model for conduction in metals, classical electrostatics, quantum tunneling [5] and introduce an atomic polarizability to model interband effects [6]. The model is able to reproduce all typical “quantum” size effects arising in noble metal nanoparticles, such as the sign and the magnitude of the plasmon shift, the progressive loss of the plasmon resonance for gold, the atomistically detailed features in the induced electron density, and the non-local effects in the nanoparticle response. Moreover, the approach has shown a qualitative and quantitative agreement with full *ab initio* calculations [5]. The classical nature of ω QF μ allows for the treatment of systems composed by thousands of atoms [6-7]. However, in order to be applied to even more realistic cases (with size of tens/hundreds nm), its computational cost needs to be further decreased. In this contribution, we present a step forward in this direction by coupling ω QF μ with the well-known Boundary Element Method (BEM) [8-10], which models the nanostructure as a homogenous continuum through its dielectric function. In the resulting ω QF μ /BEM approach [11], the core of the nanoparticle is described at the BEM level, whereas the surface retains its atomistic nature. In this way, finite size and edge effects are preserved in a simple and affordable computational way. Here, the theoretical method is presented and applied to selected test cases, demonstrating the reliability of the approach.

This work has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 818064).

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Theoretical and experimental study of paracetamol adsorption by the aqueous model system through graphene oxide

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Abstract

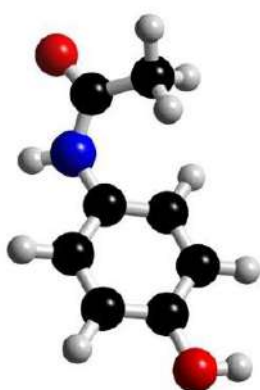
Graphene oxide (GO) is the aim in this investigation to test its adsorptive properties toward paracetamol (Acetaminophen). The GO synthesis was done using the Hummers process of chemical oxidation, which converts graphite particles into oxide-rich ones. FTIR and UV-Vis spectroscopy were used to analyze the produced GO adsorbent.

This material was used to absorb the paracetamol molecule in aqueous systems by tracking the pH value factor, adsorbent mass, and adsorption time. The concentration of molecule after the adsorption was determined using UV-VIS Spectrometry (UV-VIS).

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Figures



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Figure 1 : 3D view of the acetaminophen molecule

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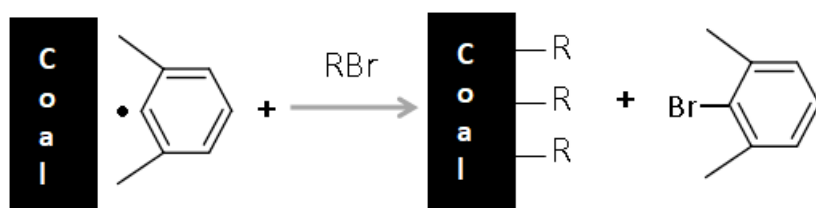
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Coal surface is chemically modified with alkyl moieties when it is immersed in the aqueous acid solution of alkyl bromide, in the presence of 2,6-dimethylbenzediazonium salt, (2,6-DMBD). 2,6-DMBD is synthesized in situ from 2,6-dimethylaniline when it reacted with the equivalent amount of sodium nitrite. Alkyl bromide serve as a source of alkyl radicals and they are generated when aryl radicals obtained during the chemical reduction of 2,6-DMBD remove the bromine atom of corresponding alkyl bromide. [1] This crossover reaction of aryl radicals is enabled due to the particular behaviour of 2,6-DMBD radicals, which because of steric hindrance don't react with the coal surface at the difference of other aryl radicals, Scheme 1. [2] This new approach enabled the modification of GC, Au and polymer surface with alkyl layers when aryl radicals were produced during the electrochemical reduction of 2,6-DMBD. [3,4] We have modified coal with hexyl carboxylic groups derived from 6-bromohexanoic acid and after rinsing in ethanol and acetone under sonication during 10 min, the sample is characterized with ATR IR and XPS techniques. ATR IR spectrum of modified coal presents a strong pic at 1715 cm^{-1} attributed to the absorption of C=O groups while XPS high resolution spectrum of C1s showed the presence of the pic at around 289 eV which is characteristic for the presence of COOH groups. This results confirm the attachment of hexylcarboxylic acid groups onto coal surface by diverting the reactivity of aryl radicals derived from 2,6-DMBD in the presence of 6-bromohexyl carboxylic acid.



Scheme 1: Grafting of coal surface with alkyl layers derived from alkyl bromide through C-Br activation with a sterically hindered aryl radical obtained by reduction of the 2,6-dimethylbenzen diazonium salt.

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EIS and theoretical investigation of the formation of oxygen on the surfaces of different materials. The effect of the electrolyte on the formation of the oxygen bubbles

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Solid surfaces can gather gas bubbles via processes such as direct immersion in water, temperature or pressure fluctuations, solvent exchange, microwaves, ultrasounds, cosmic rays, and (photo) (electro)chemical gas evolution reaction [1-3].

In this study, a pathway for ion transport between oxygen bubbles and (semi)conducting catalysts was found. To comprehend how bubbles affixed to catalysts affect crucial gas-evolving events in nature and technology, it is critically necessary to identify this portal. This urgency is heightened by the harmful effects that trapped gas bubbles play in catalysis, such as reaction inefficiency and overpotential. As a result, the dissemination of these discoveries to the broad audience of Nature Chemistry will aid continuing study in this fast advancing field of catalysis.

Here, we demonstrate that metal alkali ions restricted to the EDL area of the surfaces of oxygen bubbles may be transferred to and from the EDL of hematite surfaces. Controlling the amount and polarity of an externally applied electric potential traveling through hematite permits direct control of this gateway. Specifically, a negative electric potential enhances ion transport through hematite, whereas a positive electric potential inhibits it. In addition, we demonstrate that ion transport is inhibited when bubbles formed on a catalyst are transferred to an insulator, such as polytetrafluoroethylene.

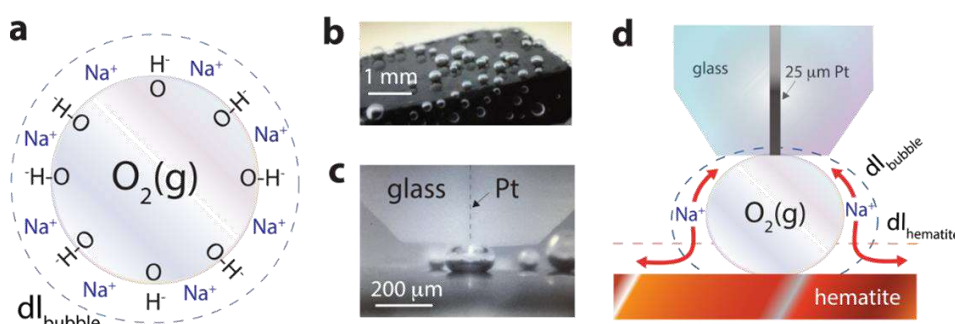


Figure 1. O₂ microbubbles produced and measured electrochemically.

In this investigation, the findings of theoretical MC and MD calculations for the experiments conducted in the study are reported. This is done to evaluate the effect of the electrolyte on the early stage of bubble formation, the adsorption of oxygen on the surface.

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Size-adsorption related studies of four Albanian natural clays toward pesticides

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Abstract

The use of natural soil components, such as clays has recently gained increasing interest for their promising properties as adsorbents and pesticide carriers. Four natural Albanian clays (Brari, Currila, Dardha, Prrenjasi) were characterized by granulometric analysis and powder X-ray diffraction. The granulometric analysis performed by Andreasen pipette and Torsion balance techniques were employed to categorize the samples based on their particle sizes and to correlate these parameters to their adsorption behavior toward selected pesticides. Currila and Dardha clays reveal finer textures, consisting mostly of particles with a mean diameter of 2.6 μm . Brari and Prrenjasi clays have a higher percentage of particles with mean diameters varying between 8 and 14 μm . Differential distribution charts show that Andreasen Pipette method reveals better distribution results (fig. 1), especially on the determination of the largest size of particles, which are clearly disregarded by Torsion balance method. The particle size distribution and their content strongly influence the adsorptive capacities of these clays towards selected pesticides.

The adsorption behavior and the adsorption capacity of each clay employed were studied for pesticide concentrations varying below their solubility limit in water. The overall adsorption process in each case is studied by the adsorption isotherm based on Freundlich, Langmuir, Temkin and Dubinin-Radushkevich models for a selected concentration and a variable time as well as for a selected time against variable pesticide concentrations. Aspects of the adsorption kinetics and intra-particle diffusion mechanisms are considered for the elucidation of the adsorption mechanisms.

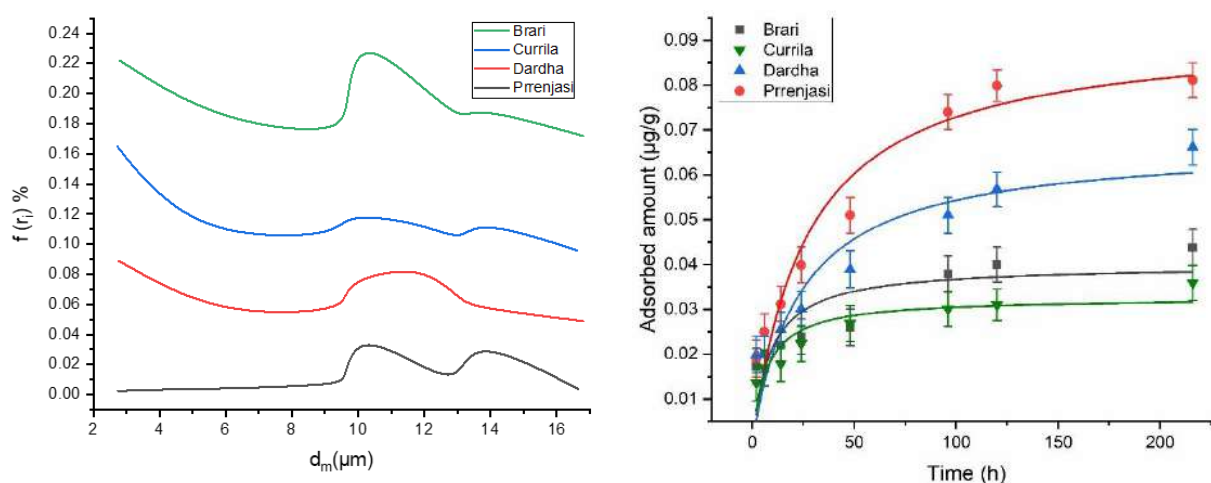


Figure 1: Differential distribution plots for four natural Albanian clays derived by Andreasen pipette analysis (left) and Langmuir adsorption isotherms of endrin (right).

Using the alternative (low-cost) adsorbent for environmental pollution control: a cadmium removal from aqueous solutions

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Abstract

Over the last few years, pollution of water is a high concern from natural and anthropogenic sources. Another apprehensive fact of pollution is the high presence of contaminants in the environment, especially those with toxic and hazardous properties. Since we are dealing with a high amount of contaminants, remediation of the environment has an enormous cost, and reducing pollution is critical. The big challenge currently is to find the most eco-friendly path that leads to the decontamination of the environment.

This study presents the use of environmentally low-cost waste adsorbents, such as potato and pumpkin peels, shells of peanut and sunflower seeds, chamomile tea residues, and coffee as a cadmium removal from an aqueous solution. The known concentration of this metal was measured before and after the peel treatment. For the cadmium ion concentration measurement, a Thermo Scientific Orion star A211 benchtop pH-meter with a cadmium ion-selective electrode was used and confirmed with inductively coupled plasma atomic emission spectroscopy. (ICP-AES). The adsorption properties of the peels and waste were studied with scanning electron microscope (SEM) infrared spectra (FTIR) and differential scanning calorimetry (DSC). Preliminary results of our research showed promising outcomes using these bio waste-derived bio sorbents for the removal of cadmium from an aqueous solution.

Keywords: cadmium, environmental pollution, ICP-AES technique, SEM.

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Nowadays the significance of developing analytical methods and sensors for enantioseparation is well recognized in chemical and pharmaceutical industries. Several methods, including electrochemical and optical sensors, high performances liquid chromatography, capillary electrochromatography, capillary electrophoresis, and supercritical fluid chromatography have been used for this purpose. In recent years, the process of developing and applying novel molecular imprinted polymers (MIP) in the field of chiral separation is extensively explained in the literature [1,2]. Omeprazole (OMP) is a racemic drug with both enantiomers entering the parietal cells where, in the presence of an acid, they are converted to an achiral sulphonamide that, in turn, inhibits the proton pumps therein. The pharmacological effects of omeprazole are, therefore, not stereoselective.

In this work, a novel molecularly imprinted polymer (MIP) electrochemical sensor was developed for the detection of the omeprazole enantiomers. The sensor was prepared using β -cyclodextrin, tetraethyl orthosilicate and cetyltrimethylammonium bromide in the presence of ammonium hydroxide on the glassy carbon electrode. Cyclic voltammetry and differential pulse voltammetry were applied to follow the changes in the MIP-layer related to rebinding and removal of the target omeprazole enantiomers by using the redox marker $[\text{Fe}(\text{CN})_6]^{3-/4-}$. The results of selectivity tests of the molecularly imprinted polymer (MIP) showed a high specificity towards OMP enantiomers compared to other similar molecules. Furthermore, the developed sensor was successfully applied to detect OMP enantiomers in tablets and biological samples with a good recovery percentage.

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Since about a decade, Textile and Fashion Department has worked on making possible the linkage between textiles and nanotechnology in their research. First on the smart textiles field, where the necessity and potential to further increase the functionality of textiles has been revealed, especially in the field of health care. Here an intense research efforts were put in the development of textile-based electrodes which can be integrated into garments [1-3]. The biosensors called "textile electrodes", in our research, consisted of two silver conductive inks screen-printed on eight different textile substrates. All printed textile biosensors showed to be promising for the use of screen-printed textile biosensors in health monitoring applications. Moreover was worked on the application of the electrospinning, first on Needleless Electrospinning of PAN Fibers, where was introduced another type of fibres production of PAN and casein. The casein was chosen as a biodegradable and eco-friendly material, which provides high comfort properties with a pH value close to the human skin in order to be applied in medical applications. The research was focused on the electrospinning and investigation of the PAN and casein fibres, in order to improve the properties of these fibres, where was observed that the fibres with concentration of 2 grams of casein showed better regularity of fibres in the nonwoven electrospinning membrane [4]. Furthermore, in the field of electrospinning, was contributed in several studies [5-6] and on the project ZEiNANOF, through preparation of the polymeric solution in different percentages, in order to study the polymer concentration influence on fiber diameter and shape, and preparation of the nano/microfibrous membranes with zeolites incorporated in the structure [7-8].

The focus of the research group at the Textile and Fashion Department in the near future is the screen printing with conductive nanoparticles ink on textile, 3D printing with conductive nanoparticles wire on textile & flexible materials and the investigation of halo-chromic at the Needleless Electrospinning for pH-sensors.

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Figure 1: Screen printed textile-based electrodes

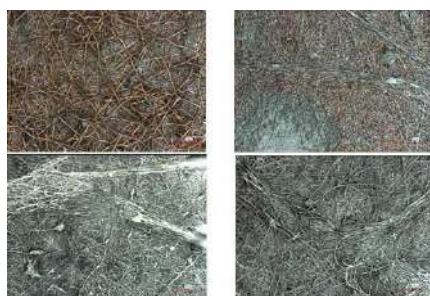


Figure 2: Microscope view of the electrospinning layer of 9.8 grams of PAN 16% and 2 grams of casein

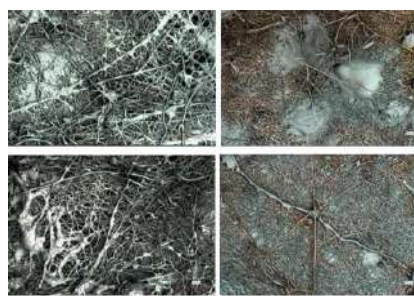


Figure 3: Microscope view of the electrospinning layer of 9.6 grams of PAN 16% and 4 grams of casein.

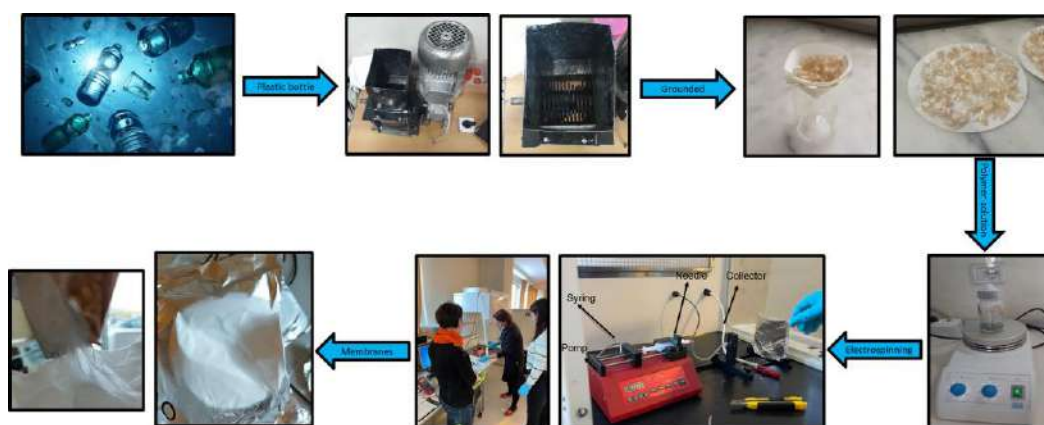


Figure 4: Recycling of plastic bottles into nano/microfibrous membranes

Evaluation of removal and adsorption of endrin on activated Albanian clays.

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Abstract

The fate of persistent organic pollutants (POP) in soils and sediments has been of great concern due to their toxicity, persistency and bioaccumulation. Sorption is an important process determining the fate of POPs on soils and sediments. It has been discovered previously that clay minerals may have a great potential on adsorbing pesticides.

This study aims to shed light on the utilization of the adsorbent properties of Albanian clays in their natural and activated form in the practice of cleaning surface and ground waters contaminated with different pesticides. Initially, the adsorption process of endrin, a nonionic persistent organochlorine pesticide, to Prrenjasi (region in Albania) clay was investigated. In addition, trying to improve clay adsorptive properties, a comparison was made using different solutions as activators. CH₃COOH (20%) and HNO₃ (20%) were used as a traditional form of activating clays and NaCl (0.5M) as well leading to the aim on finding new activation solutions based on the physical and chemical properties of the contaminants. Meanwhile an important aspect of these processes is the contact time, which varies from 2 – 672 hours.

The obtained results reveal that Prrenjasi clay activated with NaCl shows the highest adsorption towards endrin, followed by HNO₃, CH₃COOH activated clays and finally natural clay. Within the first 2 hours of contact time endrin desorbs up to 77% of the initial amount contained in the clay. Meanwhile during the whole process up to 95.5 % of endrin is desorbed from the clay. NaCl activated clay samples used on this study for the removal of endrin from aqueous solutions turn out to be an effective, low-cost and environmentally friendly method on the treatment of contaminated waters.

Development of ferritin electrochemical immunosensor based on modified GCE platform

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Ferritin is a clinically important biomarker which reflects the state of iron in the human body. In this study has been proposed an electrochemical immunosensor for the determination of ferritin in serum of human blood. The glassy carbon electrode was used as platform for immunosensor construction. The immobilization of ferritin antibody (FeAb) can be effectively improved by using a thin film of surfactant, trimethyl-tetradecylammonium chloride (TTDC), onto the GCE platform. The modification procedure of the immunosensor is optimized and characterized by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The quantitative determination of ferritin is based on the change in DPV response before and after antibody-antigen reaction. All measurements are done in pH = 7 phosphate buffer saline (PBS) at room temperature. The optimal antibody immobilization was found to be obtained using 0.1 g/L FeAb incubation solution. Calibration method of the immunosensor was based on the reduction of the DPV peak (%) in relation to the ferritin concentration. The thin layer of surfactant (TTDC), improves the process of antiferritin immobilization, which affects the increase of sensitivity and improve the analytical performance of the immunosensor (sensitivity 107.01 L/mg, R² 0.9992, LOD 0.011 mg/L).

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Thermoplasmonic ITO nanoparticles' Ink for IR-enabled applications

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Counterfeiting of goods is a rapidly expanding issue in our society. To date, the most common anti-counterfeiting technologies use tags that can be easily cloned, making it necessary to constantly search for novel methods that are simple to fabricate but complex to replicate. Notably, anti-counterfeiting strategies could make use of nanoparticles: compared to molecular technologies, these approaches are more complex to counterfeit since they cannot be easily reverse-engineered. In this work we propose a thermoplasmonic transparent ink made of a colloidal dispersion of tin-doped indium-tin-oxide nanoparticles (ITO-NPs) able to generate heat by absorption of NIR radiation.

The synthesized undoped ITO-NPs (ITO-0) and 10% tin-doped ITO NPs (ITO-10) have a spherical shape and, notably, ITO-10 shows a smaller average diameter: this aspect contributes to decrease scattering and, therefore, to the increase in absorption, which is the main contribution to the conversion of photons into heat. Moreover, we observed how it is possible to tune the absorption peak by finely controlling the dopant concentration.

The functional ink made of ITO-10 can be directly printed on transparent substrates in order to obtain arbitrary patterns with fine features (in the order of 75 microns) and high thermal resolution (of about 250 microns). We printed several figures in order to characterize the printing process and the temperature dynamics. Among these, we built a demonstrator comprising a QR Code invisible to the naked eye which became visible in thermal images under NIR radiation. The high transparency of the printed ink (transmittance >99%) and the fast thermal read-out (figures appear/disappear in less than 1s) allow an effective fabrication and decryption of security labels against counterfeiting, offering a solution for low-cost, scalable production of photothermally active invisible labels. Noteworthy, tin doped adjustable functional ink can be of great practical interest toward specific and tailored sensing applications in the NIR range.

Figures

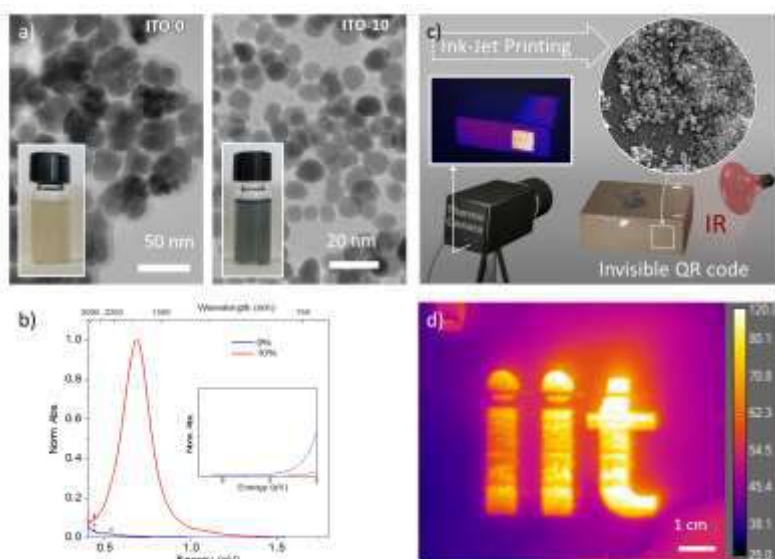


Figure 1: a) TEM pictures of tin-doped (red) and undoped (blue) ITO nanoparticles and b) their absorption spectrum; c) demonstrator of a real application for the custom ink; d) thermal image of one of the printed figures while irradiated with a NIR lamp.

Corrosion inhibition performance of the Nystatin Drug toward the Mild Steel in Acidic Media – An Experimental and Theoretical Study

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The corrosion behaviour of mild steel in 0.5 M aqueous hydrochloric acid medium in the presence and absence of nystatin drugs was investigated using potentiodynamic polarization measurements, quantum chemical calculations, and molecular dynamic simulations [1]. Potentiodynamic measurements indicate that as a result of its adsorption on the mild steel surface, this molecule operates as a mix inhibitor. The objective of this study was to use theoretical calculations to acquire a better understanding of how inhibition works.

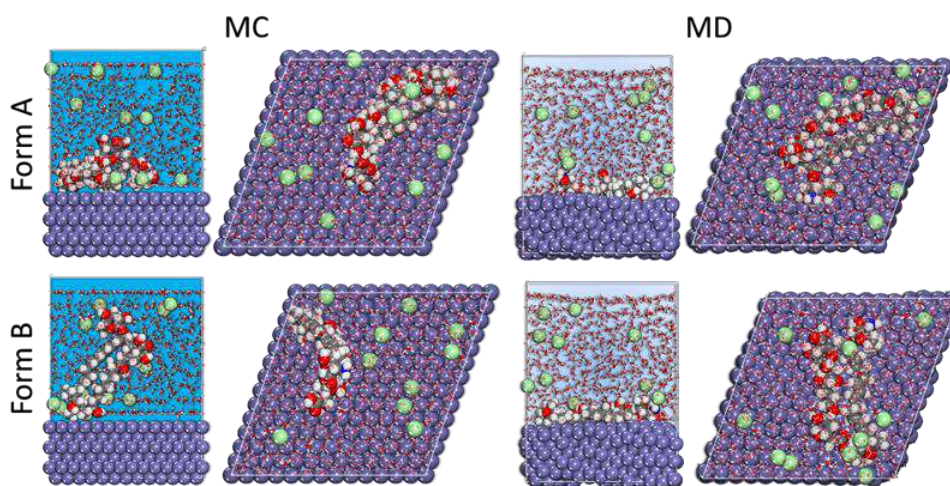


Figure 1: A. MC and B.MD obtained from the adsorption configurations of the Nystatin inhibitor in the simulated corrosion media on the Fe surface.

The adsorption behaviour of the examined compound on the Fe (1 1 0) surface was evaluated using Monte Carlo simulation. Furthermore, the molecule was studied using Density Functional Theory (DFT), to determine the relationship between the molecular structure and its corrosion inhibition behaviour. Adsorption energies between Nystatin and mild steel were calculated more precisely using Molecular Dynamics under Periodic Boundary Conditions (PBC). The predicted theoretical parameters were found to be in agreement with the experimental data, which was a considerable help in understanding the corrosion inhibition mechanism displayed by this inhibitor.

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Evaluation of different electrochemical sensors for heavy metals detection and removal

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Heavy metals (lead, cadmium, mercury, arsenic, copper, etc.), which pose the risk to the environment and the human body, are ubiquitous in natural waters due to their high solubility and can accumulate in different matrices, causing issues with respect to their removal. Their accumulation in human body may cause potent toxicity such as irritation, acute or chronic intoxication, carcinogenicity, etc. For example, copper and its compounds are also well-known to be used in agriculture as fertilizer and pesticide, but its accumulation can cause problems in the environment, and diseases in humans such as the Wilson disease. The detection of heavy metals, combined with new low-cost and green approaches to remove them from different matrices, is a very important topic. Although standard methods such as atomic absorption spectroscopy (AAS) and inductively coupled plasma mass spectrometry (ICP-MS) offer accurate detection, the requirement of time-consuming procedures, skilled personnel and expensive equipment often limit on-site application. As such, portable and user-friendly devices, which can operate on-site intervention are highly demanded, and electrochemical methods have been widely used for sensing heavy metals to fulfill this need. Two commonly used platforms of metallic sensing electrodes are: 1) bismuth-electrodes for sensing cadmium and lead and 2) gold-electrodes for sensing copper and arsenic; both are chosen for their high conductivity and limited toxicity. The electrochemical techniques used for heavy metals detection is the anodic stripping voltammetry (ASV) including linear sweep voltammetry (LSV), differential pulse voltammetry (DPV), and square wave voltammetry (SWV). Particularly, screen-printed electrodes are harnessed to operate the electrochemical detection. Herein, we will evaluate three different screen-printed heavy metal sensors in the literature [1-3] and compare the influence on their sensing performance from two aspects: the different substrates with different levels of porosity (i.e., plastic and paper), the sensing nanomaterials and the simplicity of their application for non-specialized users.

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Birnessite synthesis and their application as adsorbents of heavy metals

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Abstract

Birnessite is the most abundant manganese mineral on planet's surface, occurring as fine-grained, poorly crystallized aggregates in soils, sediments, grain, and rock coatings. This non-stoichiometric compound contains MnO₂ layers and a water intermediate layer in which there are usually alkaline cations. Birnessite is well known for its ability to adsorb heavy metals by exchanging Na⁺ cations within the intermediate layer. In the research work that is represented by this poster, birnessite is synthesized by a very simple method using MnSO₄·H₂O and H₂O₂. An extremely fine crystalline material with dark color is obtained. A possible use of this material as environmental cleaning agent, is considered by examining its adsorptive properties towards heavy metals (Cd, Pb, Cu). The synthesized Birnessite was put in contact with heavy metal solutions for different time intervals and the adsorbed amount was measured using AAS (atomic absorption spectroscopy). During the exchange process of heavy metal ions with Na⁺ cations, the birnessite intermediate layer outgrows 70 nm. Considering the adsorption graphs the highest adsorbed amount of Cu and Cd was observed at respectively after 12h at 5.8 mg/L and after 10 h at 1.25 mg/L. The adsorption of Pb was very low at the first 10 hours but after that the adsorbed amount increases significantly with much higher amounts compared to others.

The adsorptive removal of curcumin derivative from acetonitrile solution using GrapheneOxide(GOx)

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Curcumin is a bright yellow chemical produced by plants of the *Curcuma longa* species[1] and its derivatives give colored solutions in acetonitrile as solvent, which makes it a good specimen to be analyzed using UV-VIS spectrometry analyzing method. The adsorptive agent is Graphene Oxide (GOx) (synthesized using modified Hummers method)[2]. In further analysis we can come to conclusions of GOx capacity to remove (2E,5E)-2,5-bis(2-methoxybenzylidene)cyclopentanone from the solution. This experiment is backed up with theoretical calculations.

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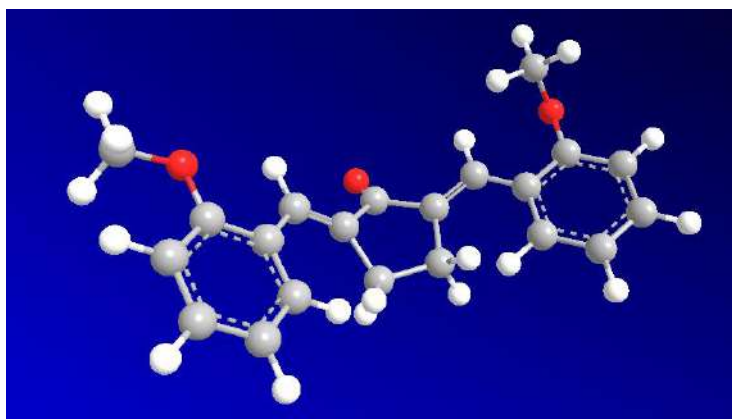


Figure 1. Structure of (2E,5E)-2,5-bis(2-methoxybenzylidene)cyclopentanone

Nanostructured DNA-based sensors for detection of the prostate cancer biomarker miR-21 – a feasibility study

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Prostate cancer (PCa) is a common tumour disease in western countries and a leading cause of cancer-driven mortality in men. The miR-21 is overexpressed in PCa patients when compared with healthy patients. Due to the statistically relevant of these data, it is promising the use of miR-21 for non-invasive and specific detection of PCa [1]

In the present feasibility study, we are investigating the use of electrochemical detection based on screen printed electrodes and DNA-based hybridization recognition of the miRNA strand of interest. The results of the present work will be the basis for an evaluation of the present technology for the development of a non-invasive, simple to use, cost-effective and rapid point of need diagnostic system.

This preliminary study is based on a DNA probe, designed analogously as similar literature reported probes used for the detection of nucleic acids of similar length (e.g. [2]). miR-21 was spiked in buffer solutions of different concentrations of NaCl, mimicking the range found in urine.

The selective binding of miR-21 to the DNA probe induces its conformational change, which displaces the electrochemical marker methylene blue. The signal is detected by square wave voltammetry. At a frequency of 15 Hz the sensors displays signal-on behaviour with a maximum signal gain of 96.0% \pm 5.7% and an estimated dissociation constant (K_D) of 137.7 \pm 4.4 nM (n=4). The useful dynamic range (defined as the range from 10 to 90% of the maximum signal change) is from 55 nM to 343 nM with a limit of detection (LOD) of 31 nM (n=4).

This preliminary study will be followed by an extensive study aimed at the test and optimization of further parameters related to the target application in view, such as pH sensitivity, shelf life, stability of the biomarker in solution, etc. The analytical optimization will be followed by evaluating performance in real matrix, i.e. urine

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The adsorption of (2E, 5E)-2,5 Bis [(4-dimethylamino) benzylidene] cyclopentanone onto graphene oxide, a combined experimental and theoretical study

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Abstract

Graphene oxide (GO) represents a nanomaterial of immense interest for the adsorption of different chemical species ranging from small ions to relatively huge molecules such as peptides and even proteins. For the adsorption from solutions GO is material of choice as it possess huge surface. For the evaluation of its adsorption properties (both experimentally and theoretically) "(2E, 5E)-2,5 Bis [(4-dimethylamino) benzylidene] cyclopentanone" is selected in this study. The experimental results based on the UV-Vis spectrophotometry technique are quite satisfactory and promising. Both adsorbent (GO) and adsorbate (pre-synthesized) are characterized by some powerful spectroscopic techniques. The data generated through theoretical techniques are consistent with the experimental results!

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Figures

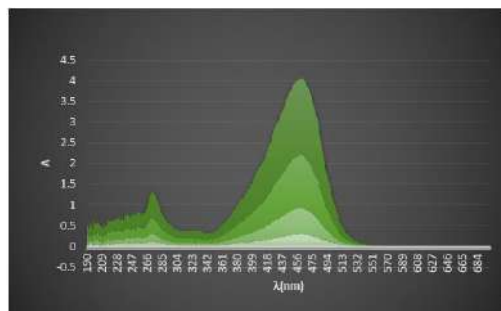


Figure 1: UV-VIS spectrum of (2E, 5E) -2,5 Bis [(4-dimethylamino) benzylidene] cyclopentanone in acetonitrile solution

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One of the main challenges in nanobiotechnology is to artificially re-create sensing and transduction mechanisms that occur in biological systems by making use of artificial lipid vesicles. Quatsomes are synthetic unilamellar nanovesicles constituted by surfactants and sterols in defined molar ratios, that present an excellent morphological stability over years and superior brightness in comparison to conventional liposomes. Nucleic acid-responsive Förster resonance energy transfer (FRET)-active nanovesicles can be easily obtained by anchoring fluorescent amphiphilic nucleic acid-probes to dye-loaded quatsome nanovesicles.¹ Here we envisage potential applications of responsive DNA-grafted quatsome nanovesicles for biosensing applications.

Acknowledgments

This work was in part supported by the Marie Skłodowska-Curie grant agreement (“SERENA” project no. 101029884 to M.R.), by the Marie Skłodowska-Curie grant agreement “Nano-Oligo Med” (No 778133 to A.P., E.P. and N.V), Furthermore, ICMA-B-CSIC acknowledges support from the MINECO through the Severo Ochoa Programme for Centers of Excellence in R&D (SEV-2015-0496 and CEX2019-000917-S). Quatsome production and their physicochemical characterization has been performed by the Biomaterial Processing and Nanostructuring Unit (U6) of the ICTS “NANBIOSIS”, a unit of the CIBER network in Bioengineering, Biomaterials & Nanomedicine (CIBER-BBN) located at the Institute of Materials Science of Barcelona (ICMA-B-CSIC).....

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Complement inhibition, an important tool in the treatment of human diseases

In the perspective of nanomedicine

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Abstract

Complement system is part of our innate immune system and it is composed of more than 50 plasma proteins, circulating in their inactive forms as zymogens or proenzymes. Proteins of the complement cascade together form a key innate immune sensor that mediates immunosurveillance and tissue homeostasis by interacting with each other in a cascade like manner. The complement system is actually a very fine modulator of a lot of functions and biological processes that happen not only at the interface of innate and adaptive immunity, but it interacts with a lot of other biological pathways including the coagulation system, tissue remodelling and regeneration as well as other biological processes. It is observed that C3 and C5 proteins are specifically expressed in the regenerating zones of different organisms, starting from different species of low vertebrates (amphibians) to mammals.

There is a wide range of diseases caused by abnormal complement activation, including kidney disease like Paroxysmal Nocturnal Hemoglobinuria (PNH), Age-related Macular Degeneration (AMD), Systemic Lupus Erythematosus (SLE), etc. Convertase enzymes play a central role in complement activation by cleaving C3 and C5 and mediate nearly all complement effector functions, being so ideal targets for therapeutic complement inhibition. Targeting the complement system has been established for rare clinical disorders such as paroxysmal nocturnal haemoglobinuria and atypical haemolytic uraemic syndrome and is a very promising solution to a wide group of diseases, including orphan diseases. The peptide Compstatin and the new analogs of this complement C3 inhibitor, inhibits all complement pathways. In the field of dental medicine, there is shown a very promising potential of these therapeutics to periodontal diseases and gingival inflammation. During the last years, several studies present the important role of these inhibitors in the treatment of covid-19 infection too.

Comstatin has a very good solubility profile and an exquisite plasma half-life which is quite long for peptide therapeutics and exceeds over 50 hours in plasma with favourable toxicology and safety profile. These facts and all the data from clinical studies to date in non-human primates and in first human studies on complement therapeutics are opening new perspectives for clinical application in various clinical conditions.

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New methods of bentonite activation and their efficiency in the regeneration of used lubricating oils.

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Bentonite is well known for its adsorbent properties, low cost, and high exchange capacity [1]. To improve these physic-chemical parameters, in this study, bentonite has undergone acid and basic treatment combining with microwave curing [2,3]. A comparison of the structure of the bentonite before and after activation was made to see and evaluate the changes in bentonite structure. The bentonite was tested for its regeneration efficiency on used motor oils, UMO (used for 15000-20000km). Some of the main parameters measured for evaluating the quality of lubricating oils are: density, sulfur content, viscosity, viscosity index, pour point, etc. Purification of UMO by activated bentonite gives higher results and is more economical and ecological than other methods used before.

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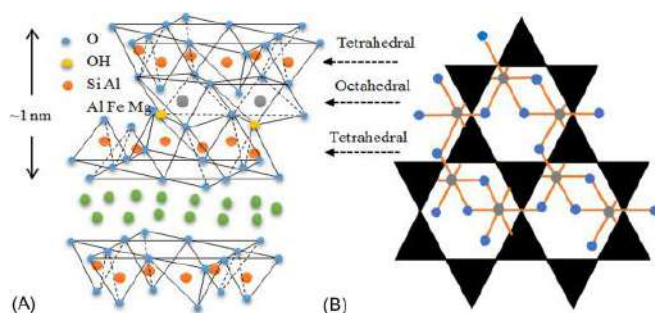


Figure 1: Structure of montmorillonite.

Characterisation of Natural Clay and Application to the Adsorption of Erythromycin from Water Media

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Abstract

Erythromycin (ERY) is an antibiotic that is suggested to be classified as one of the prior drinking water contaminants at latest European Union Water Framework Directive (EU – WFD). Since most antibiotic residues can hardly be removed from wastewater using conventional treatments, alternative methods such as adsorption receive great attention considering one of the most efficient and cost-effective treatment methods for antibiotics. Among the adsorbents, clay minerals have garnered increasing attention due to their unique properties including availability, high specific surface area, low cost and cation exchange capacity. In this work natural clay was characterized and applied for the removal of erythromycin from water solution. The clay was dug up in the form of soft stones, it was dried and ground in a mortar, then washed with distilled water. The separated clay was studied by X Ray Diffraction analysis which revealed its chemical composition as 55.2% $\text{KAl}_2(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$, 23.6% SiO_2 , 21.2% Li_2CO_3 . Surface area was determined by N_2 adsorption/desorption isotherms and the BET equation, it appeared to be 79.33 m^2/g . Erythromycin solution 50 μM after being treated for 24 hours was centrifuged and its concentration was monitored by electrochemical methods such as cyclic voltammetry. The voltamogram was recorded in a three electrodes electrochemical cell, using a screen printed carbon electrode as working electrode (SPCE). The electrochemical signal measured after the adsorption process was almost invisible compared to a 14 μA peak observed for the initial concentration, which means Erythromycin was almost completely removed from the solution. The application of these natural materials in real samples purification, their reuse, economic analysis and life cycle assessment are other issues that should be considered.

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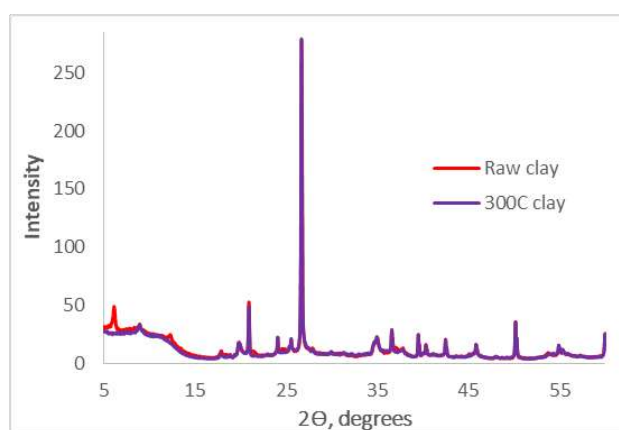


Figure 1: XRD spectrum of the studied clay. Cu $\text{K}\alpha$ at 40 kV and 40 mA, $2\theta=5-60^\circ$, 2684 steps, time per step 0.764 s.

A theoretical and experimental study of adsorbent dye removal from (2E, 5E) -2,5-Bis (4-methoxybenzylidene) cyclopentanone using diatomaceous earth as an adsorbent

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This study is focused on the adsorption of (2E,5E)-2,5-Bis (4-methoxybenzylidene) cyclopentanone using diatomaceous earth. First, the monocarbonyl compound was synthesized, then crystallized and characterized was done with IR, NMR, etc. The theoretical calculations based on Density Functional Theory (DFT) and Monte Carlo (MC) calculations were used to explore the preferable adsorption site, interaction type, and adsorption energy of the (2E,5E)-2,5-Bis(4-methoxybenzylidene) cyclopentanone onto diatomaceous earth.

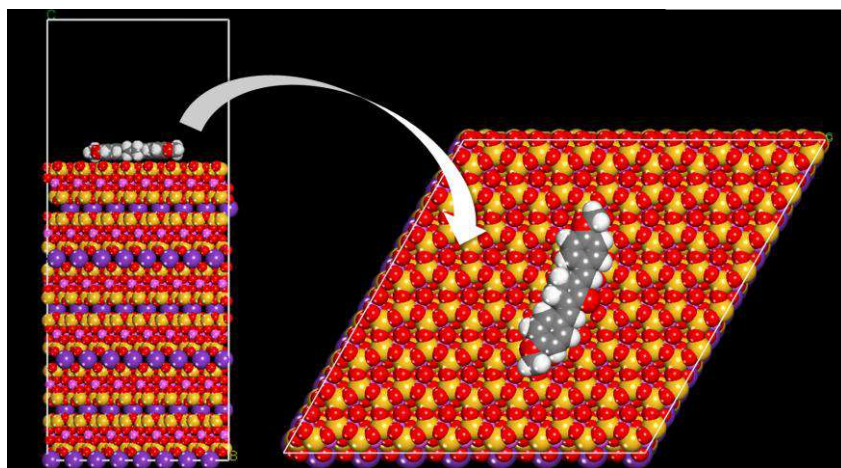


Figure 1: Monte Carlo lowest energy geometry obtained during the adsorption of the adsorption of the 2E, 5E)-2,5-Bis (4-methoxybenzylidene) cyclopentanone using diatomaceous earth modelled using Muscovite structure (Amcsd 0000854).

Diatomaceous earth soil is cleaned, homogenized and characterized by various spectroscopic methods and is used as an adsorbent. The adsorptive ability of the diatomaceous earth toward the (2E, 5E)-2,5-Bis(4-methoxybenzylidene)cyclopentanone was evaluated using UV-Vis measurements.

Keywords: MACs; adsorbent; theoretical calculation; NMR; synthesis.

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Abstract

Point of care testing (POCT) represents important part of the diagnostics and subsequent treatment of patients. Diagnostic tests performed from the comfort of the patient's home with a smartphone readout enable diagnosis without the laboratory equipment and the presence of a specialized laboratory trained personnel. The tests are designed to be simple and thus allow the patient to do them themselves. They also have the potential for testing in medical facilities due to their small dimensions and lower economic demands than other classical diagnostic methods based on the PCR reaction. The importance of POC approaches increases during the pandemics, like in case of SARS-CoV-2.

In the present work, a microfluidic device, which uses RNA isolated by magnetic nanoparticles with a specifically modified surface, is developed. Magnetic nanoparticles represent a fast tool for obtaining the RNA of high quality, compatibility with other downstream RNA detection platforms and the possibility of miniaturizing into a chip. For RNA analysis, we have developed a sensitive reverse-transcription loop-mediated isothermal amplification (RT-LAMP) assay, which utilizes a fluorescence readout with sensitivity and specificity comparable to the RT-qPCR. Its advantage lies primarily in the isothermal profile of the reaction and a shorter time of the whole analysis. The fluorescent detector could be replaced by an electrochemical sensor, which could provide even higher sensitivity of the detection. The difference between both types of detection has been preliminary studied in this work.

This approach could be utilized as a universal tool for the detection of various pathogens in human and veterinary medicine. The biggest challenge is the diagnosis of neonatal sepsis due to the low weight of the birth child, small blood volume and insufficiently developed immune system. This approach could provide accelerate an accurate diagnosis, just right on the place of need and therefore treatment targeting within 40 minutes from a drop of the patient's blood.

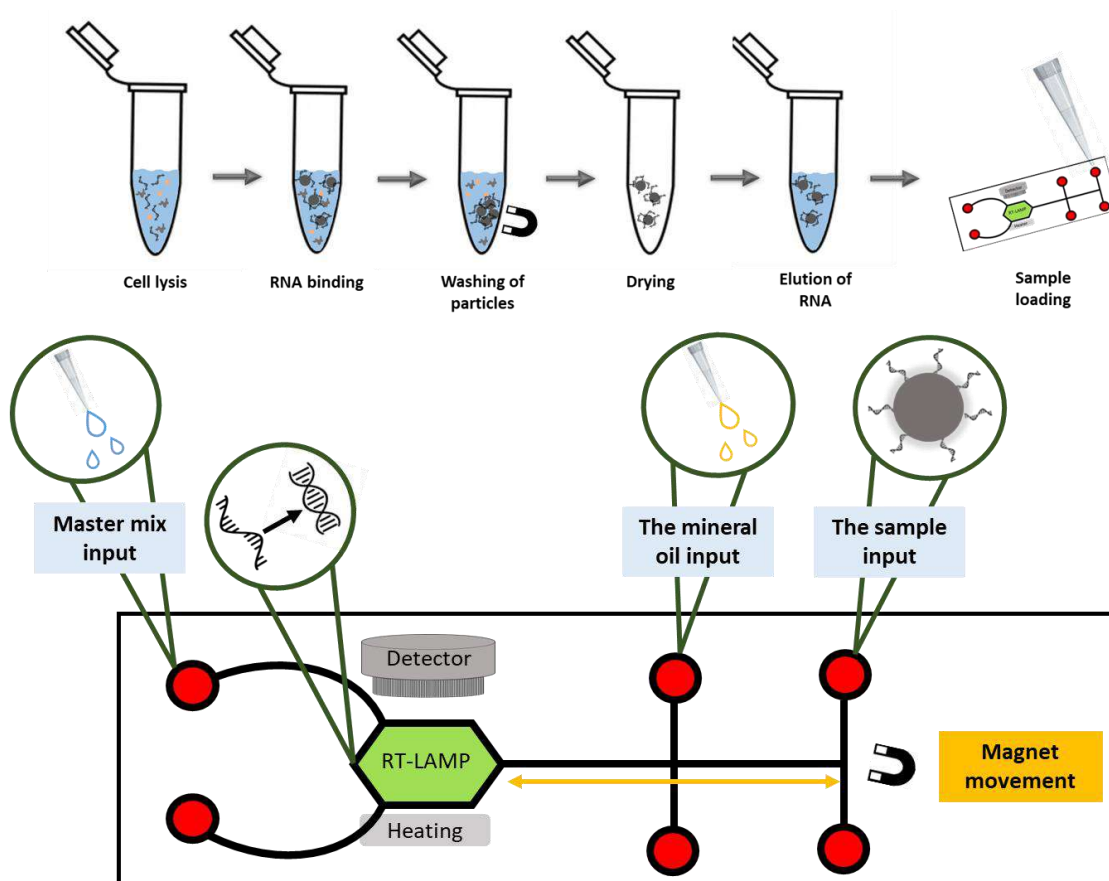


Figure 1: Scheme of the reaction

Metal-free Cysteamine Functionalized Graphene Alleviates Mutual Interferences in Heavy Metals Electrochemical Detection

Presenting Author (Qiuyue Yang and David Panáček)

Co-Authors (Qiuyue Yang, Emily P. Nguyen, David Panáček, Veronika Šedajová, Vítězslav Hrubý, Giulio Rosati, Cecilia de Carvalho Castro Silva, Aristides Bakandritsos, Michal Otyepka, Arben Merkoçi*)

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Abstract:

The detection of heavy metal pollutants is of great concern in environmental monitoring due to the potent toxicity. Electrochemical detection, one of the foremost sensing techniques, is hindered by the mutual interference between target heavy metal ions. In particular, the sensitivity to Cd^{2+} (one of the most toxic heavy metals) is often overshadowed by other heavy metals (e.g., Pb^{2+} and Cu^{2+}) when using carbon electrodes. ^[1,2] Strategies are frequently required using additional metallic particles embedded in the electrode, which faces recycling and reusability issues. In this study, a metal-free cysteamine covalently functionalized graphene (GSH), is employed to tackle this issue by selectively enhancing a 6-fold boost in Cd^{2+} sensitivity of screen-printed carbon sensors (SPCE), while the sensitivities to Pb^{2+} and Cu^{2+} not being influenced in the simultaneous detection. The selective enhancement is attributed to grafted thiols on GSH, which have good affinity to Cd^{2+} based on Pearson's hard and soft acid and base principle. Moreover, GSH-SPCE features high reusable times (23 times) due to the covalent functionalization of thiols, surpassing the state-of-art SPCEs modified by non-covalently functionalized graphene derivatives. Finally, GSH-SPCE was validated in tap water.

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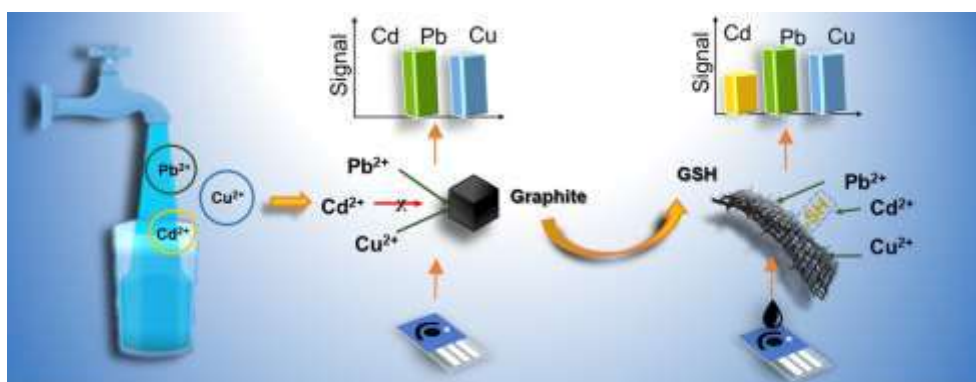


Figure 1: Schematic illustration of the significant effect of GSH relieving the mutual interference in simultaneous multiple heavy metals detection.

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Unique properties of ZnO and the ease of the growth of its nanostructures make this material extremely attractive for a variety of optoelectronic applications. To fully exploit the potential of ZnO, there is one essential problem, which must be solved: the preparation of a high-quality rectifying junction. The lack of p-type electrical conductivity in ZnO emphasizes the importance of the study of hybrid heterojunctions. One of the key issues in these heterojunctions is to understand the charge transport mechanism.

In this work, we focus on a systematic analysis of charge transport mechanisms in the hybrid heterojunctions formed between single or arrays of ZnO nanorods with other p-type materials (CuO; GaN; PEDOT:PSS) [1-4] or 2D graphene [5]. These nanostructured heterojunctions showed potential in different applications, such as highly sensitive UV photodetectors, or hydrogen sensors operated at room temperature.

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Figures

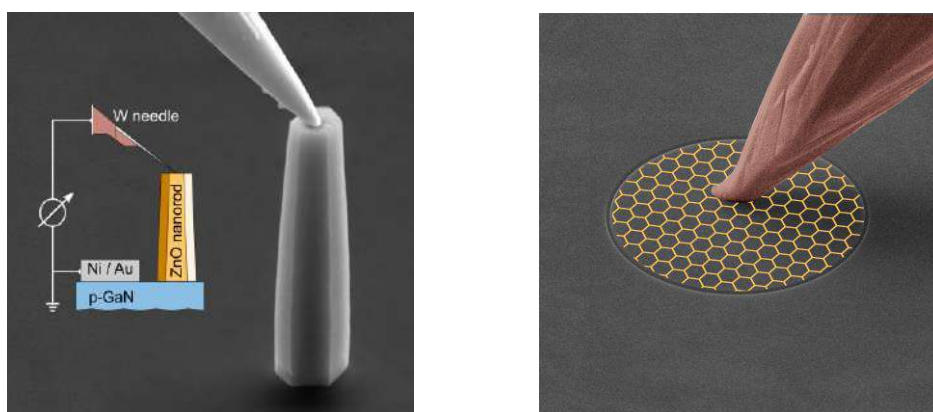


Figure 1: SEM image of the ZnO nanorod/GaN heterojunctions (left) and FIB-patterned graphene/ZnO structure (right) contacted by the tungsten nanoprobe for the SEM in-situ electrical measurements.

The adsorptive removal of Pb(II) and Cr(VI) ions from aqueous solution by graphene oxide

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Graphene oxide (GO) is the aim in this investigation to test its adsorptive properties toward chromium and lead ions. The GO synthesis was done using the Hummers process of chemical oxidation, which converts graphite particles into oxide-rich ones. FTIR and UV-Vis spectroscopy were used to analyze the produced GO adsorbent.

This material was utilized to adsorb Cr(VI) and Pb(II) ions. The concentration of these ions after the adsorption was determined using Atomic Absorption Spectrometry (AAS). To study the best adsorption location, adsorption type, and adsorption energy of GO toward Pb(II) and Cr(VI) ions, the DFT and Monte Carlo calculations were used.

Finally, to determine noncovalent interactions, adsorption sites that are the most stable were selected.

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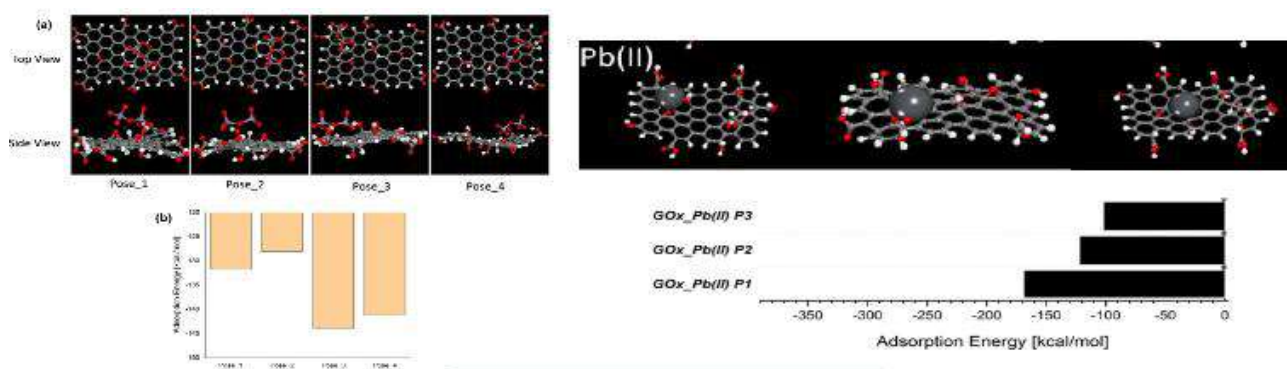


Figure 1:

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Although antibiotics have improved in a significantly way our life, the residues in food and the environment have negative effects on human health. Therefore, this study aims to develop a carbon paste electrode (CPE), modified with multi wall carbon nanotubes (MWCNT) for the determination of azithromycin. Azithromycin detection was accomplished via cyclic voltammetry (CV) and square wave voltammetry (SWV). Firstly, modified sensor (CPE/MWCNT) was tested for electroactive properties of the surface in the electrolytic cell in the presence of the redox couple $\text{Fe}^{3+}/\text{Fe}^{2+}$. The experimental parameters, such as pH, the indifferent electrolyte, the amplitude and the frequency were optimized and in these conditions analytical parameters were specified. Afterwards, it is tested in real sample of milk, which eventually resulted contaminated with azithromycin. It was found that the sensitivity of sensor was $56 \mu\text{A}/\mu\text{M}$, the limit detection $0.047 \mu\text{M}$, $R^2=0.9900$ and the relative standard deviation 3.75%. Based on the results, this sensor can be used for the determination of azithromycin in milk samples.

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Figures

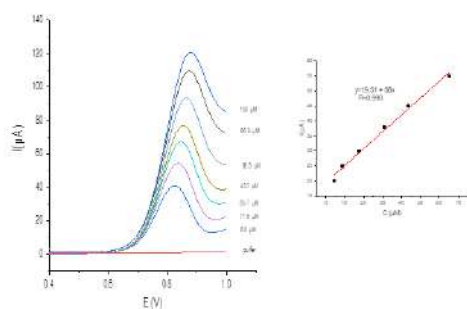


Figure 1: SWVs of azithromycin obtained using CPE modified with MWCNT in PBS pH 8.5

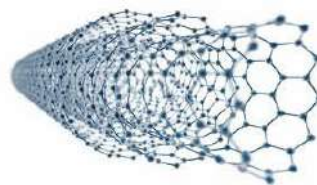


Figure 2: Modifier of CPE- MWCNT

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