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

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

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

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

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

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

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

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

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

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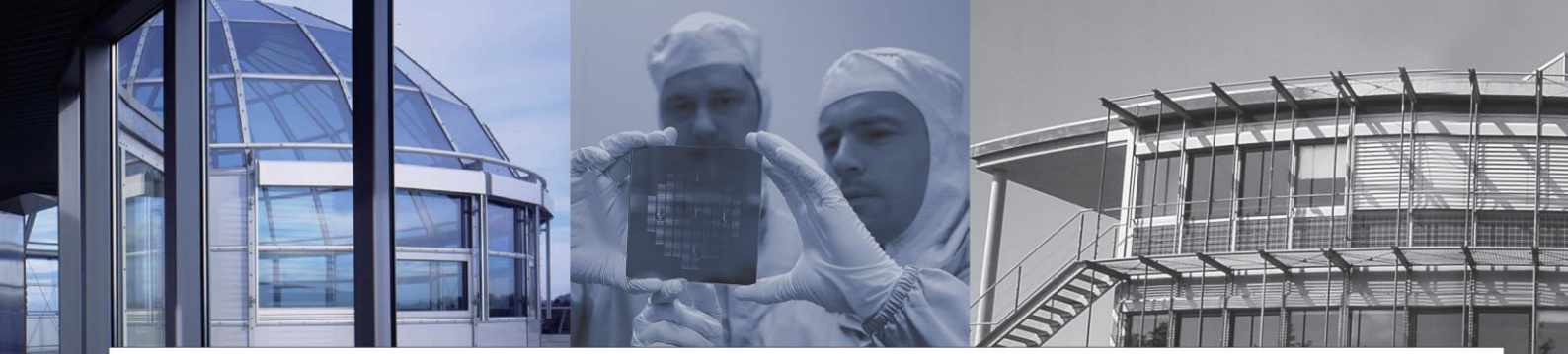

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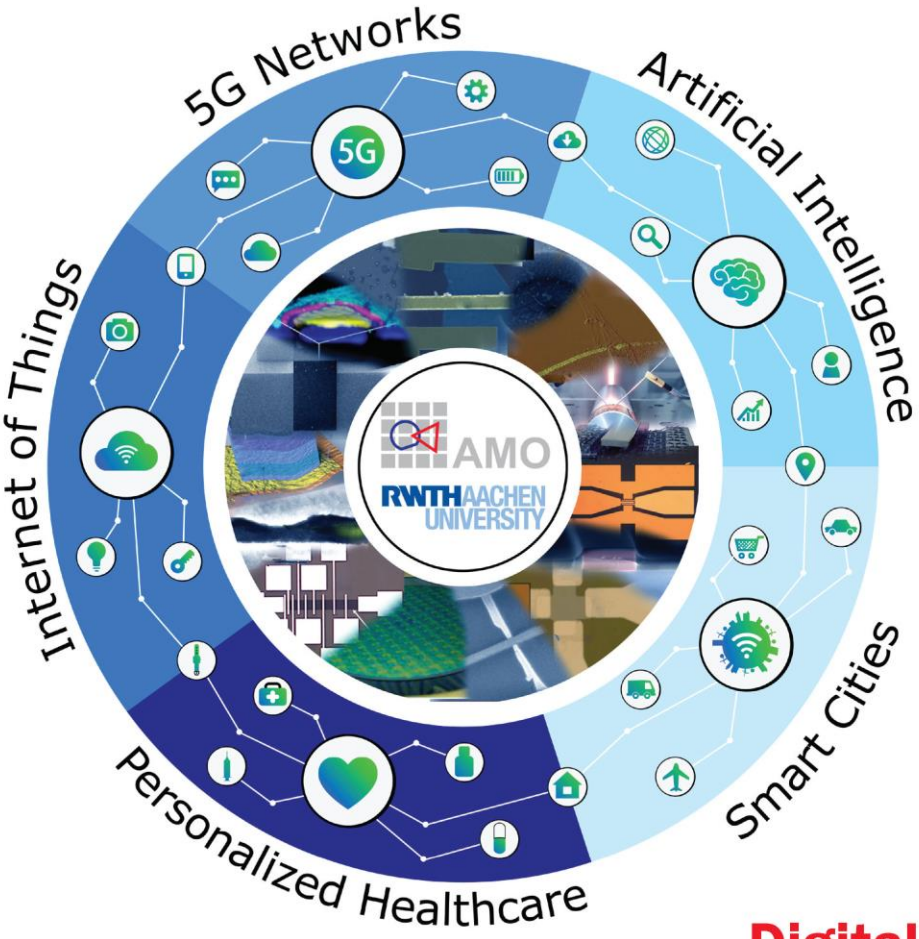

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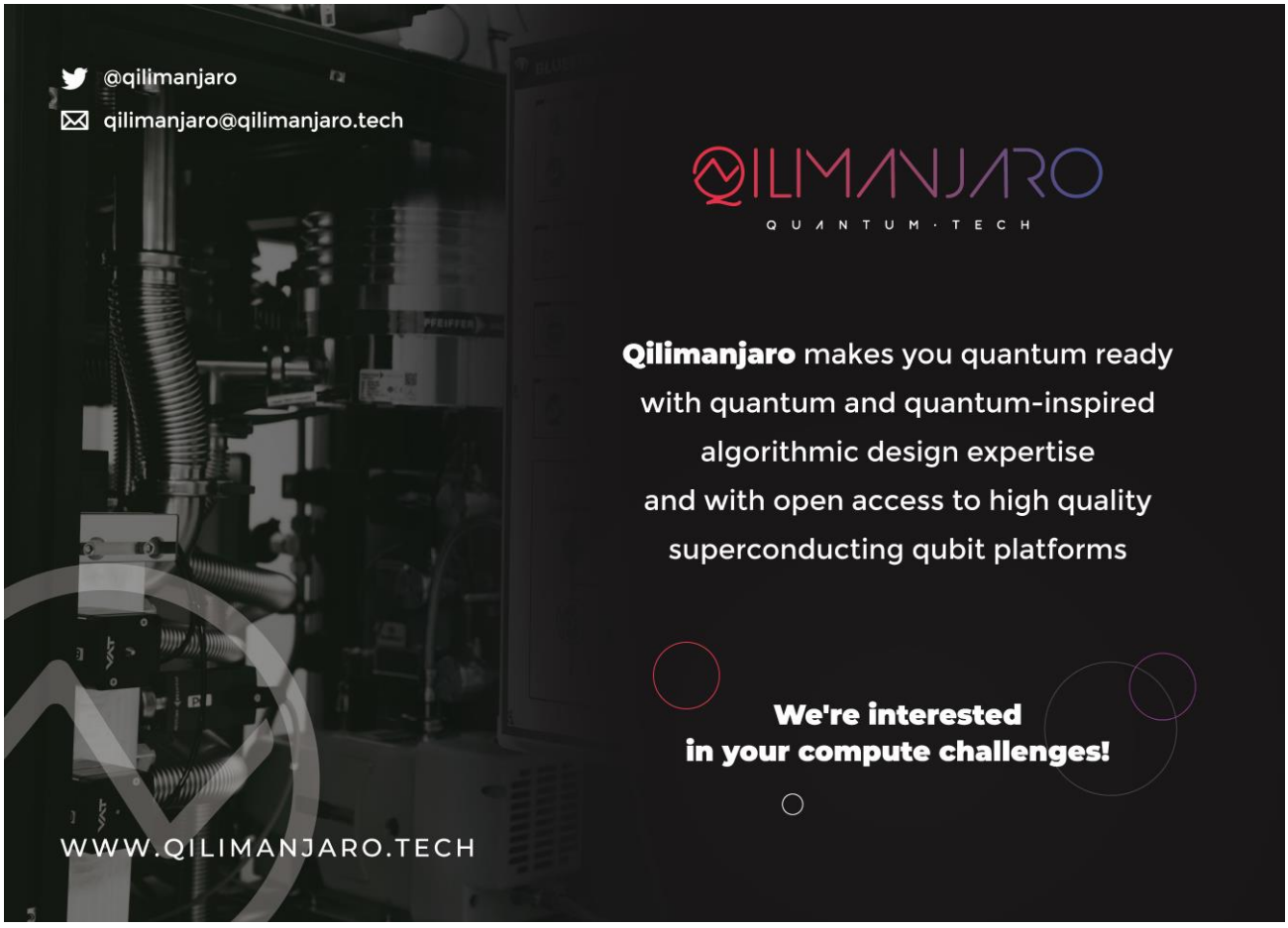

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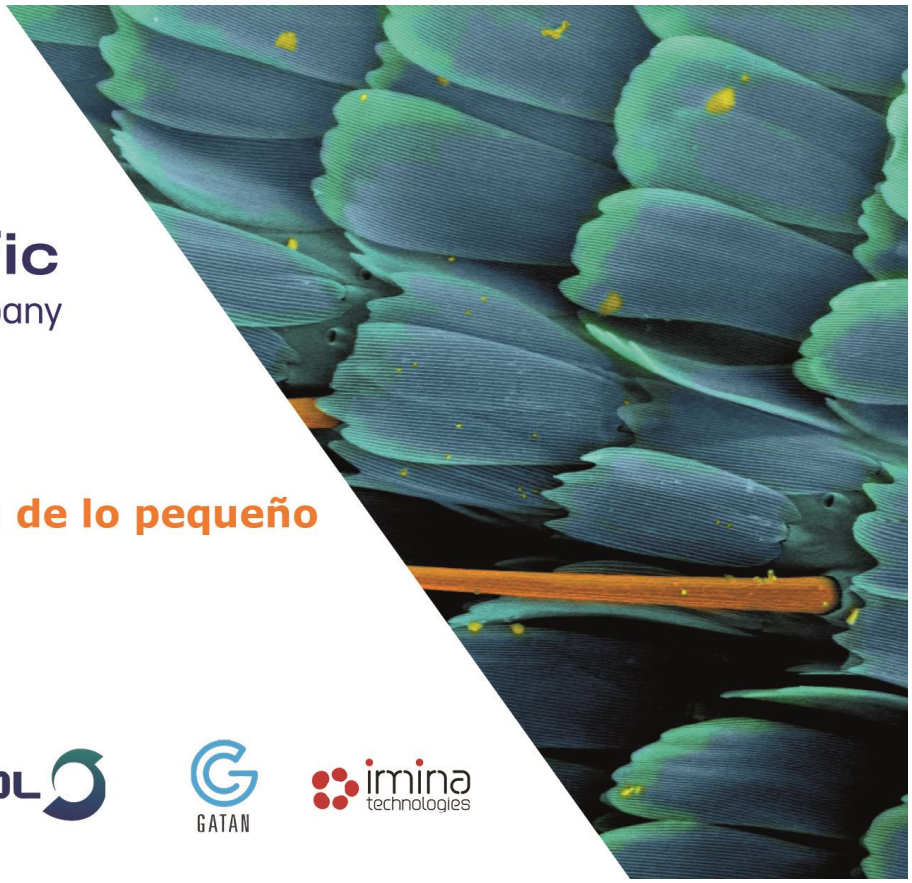

Spin-orbit proximity in van der Waals heterostructures

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Two-dimensional materials are an exciting new material family that has the capability to advance toward the implementation of novel spin-based devices. For these atomically-thin layers, the proximity effect is especially important and opens ways to transfer properties from one material into another. In van der Waals heterostructures, transition metal dichalcogenides (TMD) can be used to enhance the spin-orbit coupling of graphene, leading to new spin transport channels with unprecedented spin textures [1]. We have optimized bilayer graphene/ TMD heterostructures to achieve magnetic-field-free spin precession. Remarkably, we observe in graphene/WSe_2 devices that the sign of the precessing spin polarization can be tuned electrically by a back gate voltage and by a drift current [2]. Our result is the first realization of a spin field-effect transistor at room temperature in a diffusive system, a long-awaited goal of spintronics that could be a cornerstone for the implementation of energy efficient spin-based logic.

Another notable consequence of the spin-orbit proximity in graphene/TMD van der Waals heterostructures is the occurrence of spin-to-charge conversion (SCC) due to the spin Hall effect (SHE), which was first observed by our group using MoS_2 as the TMD [3]. To quantify the SCC, the significant figure of merit is the SCC length which can be calculated by the product of spin Hall angle, θ_{SH}, and the spin diffusion length, λ_s. The combination of long-distance spin transport and SHE in the same material gives rise to an unprecedented SCC length of up to 41 nm solely due to the SHE in graphene proximitized with WSe_2. Furthermore, a gate-tunable SCC is observed [4]. Such highly efficient and gate-tunable SCC up to room temperature will play a crucial role for the future integration of spintronic devices into existing electronic infrastructure.

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[4] F. Herling, C. K. Safeer, J. Ingla-Aynés, N. Ontoso, L. E. Hueso, and F. Casanova, APL Mater. 8 (2020) 071103.

Figures

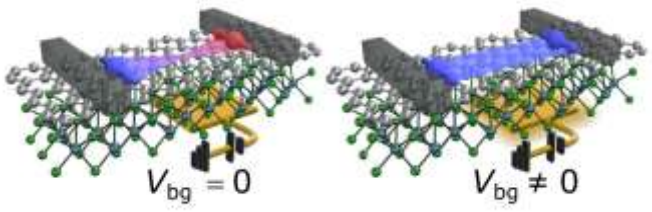

Figure 1: Sketch of a spin field-effect transistor operating at the strong spin-orbit coupling regime, where the valley-Zeeman induced spin precession is tuned by a back gate voltage to control the sign reversal.

2D magnetic molecular materials

Eugenio Coronado

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Abstract

Graphene and other 2D materials are almost exclusively based on inorganic lattices. Except for the chemical functionalization of the surface of the 2D material, molecules have been scarcely considered in this area. Here I will illustrate the role of functional molecular materials in this area by selecting some relevant examples:

1) Molecular 2D magnets. I will focus on the design of molecular 2D magnets that, in contrast to what happens with the inorganic 2D magnets, are chemically stable in open air, keeping their magnetic properties preserved upon functionalizing their surface with different organic molecules [1].

2) Smart molecular/2D heterostructures. I propose to create hybrid heterostructures by interfacing stimuli-responsive molecular systems with graphene and semiconducting transition metal dichalcogenides (MoS_2 and WSe_2). The aim is that of tuning the properties of the "all surface" 2D material *via* an active control of the hybrid interface. This concept will provide an entire new class of smart molecular/2D heterostructures, which may be at the origin of a novel generation of hybrid materials and devices of direct application in highly topical fields like electronics, spintronics and straintronics. As smart-molecular systems I will choose magnetic spin-crossover materials able to switch between two spin states upon the application of an external stimulus (temperature, light or pressure) [2]. This spin transition is always accompanied by a significant change of volume in the material (by ca. 10%), so it can generate strain in its surrounding. I will show that in these heterostructures the electronic properties of graphene and the optical photoluminescence of monolayers of semiconducting metal dichalcogenides can be switched by light or by varying the temperature due to the strain concomitant to the spin transition [3,4]

References

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"Slide-Tronics"

Moshe Ben Shalom
M. Vizner Stern, Y. Wais, W. Cao, I, Nevo, E Sela, M Urbakh, O Hod, M Ben Shalom
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A new ferroelectric system, only two-atoms-thick is presented [1]. Stacking two layers of hexagonal boron nitride (hBN) atop each other, with a parallel crystal orientation, results in a permanent electric polarization pointing out of the plane. Furthermore, applying an opposite external electric field switches the vertical polarization by a horizontal sliding between the layers of a full atomic spacing distance. I will describe our atomic force experiment, DFT calculations, and a simplistic cohesion model, allowing us to explore the interfacial-ferroelectricity and its unique Slide-Tronics switching mechanism.
If time allows, I will further discuss our efforts to induce intrinsic electric and magnetic gauge-fields in graphene by particular strain-engineering schemes [2].

References

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https://www.tau.ac.il/~moshebs

Figures

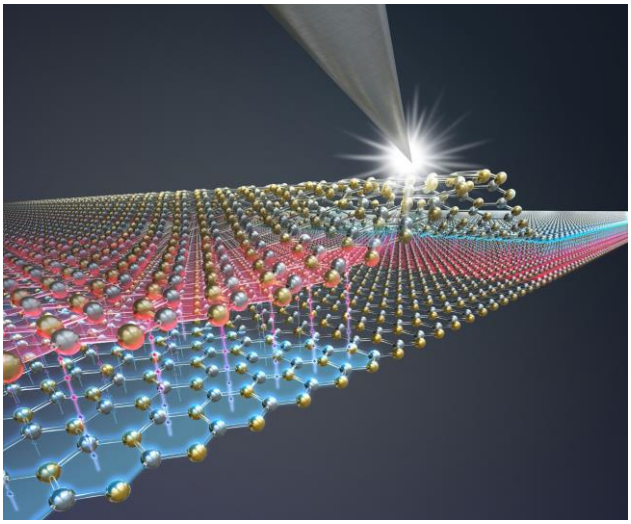

Figure 1: Interfacial ferroelectricity by Sliding

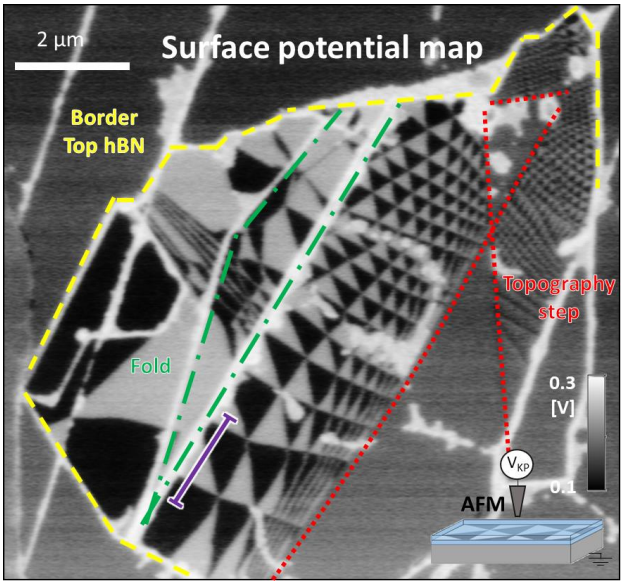

Figure 2: Surface potential map of ferroelectric domains in 3R-like hBN

Innovative 2D Nanomaterials for Electronics and Energy Storage

Adelina Braun

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Abstract

Innovative and high-quality nanomaterials are critical in accelerating 2D research for energy and electronics applications. Through academic collaborations and internal R&D, we have developed graphene oxides, graphene derivatives, and 2D nanomaterials including germanane and black phosphorus. In collaboration, these 2D nanomaterials were formulated into well characterized, ready-to-use inks containing few-layered graphene, exfoliated hexagonal boron nitride, or transition metal dichalcogenides. Our cutting-edge inks enable device fabrication through scalable additive printing methods such as aerosol, inkjet, gravure, screen, and 3D printing. These materials have been used in a variety of applications including printed electronics, printed micro-supercapacitors, next generation lithium-ion batteries, and photodetectors. We will highlight a few examples using these 2D nanomaterials for high-temperature lithium-ion battery separators, electrodes, solid-state electrolytes, as well as barrier materials in printed electronic devices and bioactive 3D printable scaffolds.

Figures

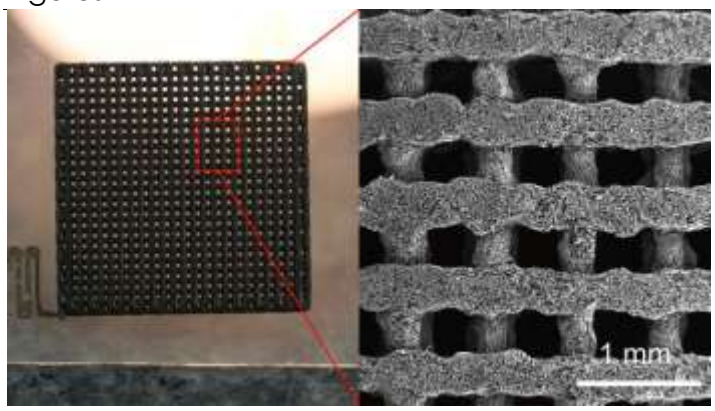

Figure 1: 3D printable Graphene Oxide ink; Direct extrusion printable Graphene Oxide ink, Catalog Nr 916579

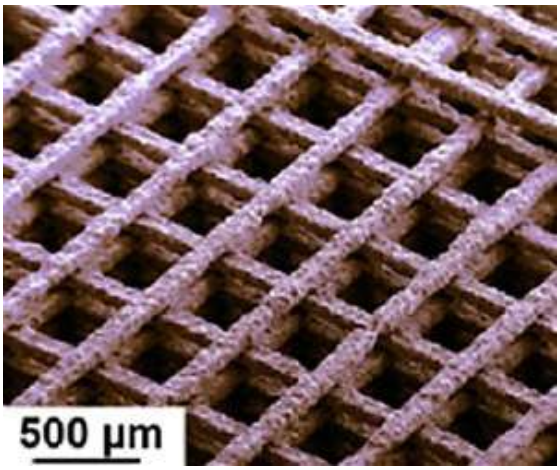

Figure 2: 3D printing Graphene ink, Catalog Nr 808156

Graphene-based materials in next generation electrochemical capacitors

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The rapid development of portable electronic devices, such as tablets and cell phones which incorporate complex applications and functionalities, requires new compact energy storage devices with improved energy and power densities.[1]

In this talk I will summarize and discuss some of our most recent research on the integration of graphene in the electrodes used in different electrochemical capacitors.

First, a novel strategy for the preparation of graphene-based self-standing electrodes for EDLC is presented. Wafers obtained by the hydrothermal heating of an aqueous suspension of graphene oxide in the presence of small amounts of either carbon nanotubes, which leads to monolithic hydrogels that can be finally compacted under pressure. These as-obtained highly-packed composite wafers can be directly tested as binder-free electrodes for supercapacitors using 6M KOH aqueous solution as electrolyte. The results show that in the presence of just a 2 wt.% of carbon nanotubes into the graphene-based wafer produces a significant enhancement of the capacitance retention at high current densities when compared to its counterpart without carbon nanotubes.

This improvement, was especially relevant in those systems using electrodes with large mass loadings. Thus, volumetric capacitance values of 255 F/cm^3 at 1 A/g and very good rate capability (185 F/cm at 10 A/g) were achieved even using electrodes with a mass loading as high as 13 mg/cm^2.[2]

The impact of the incorporation of graphene in electrodes for dual carbon lithium-ion hybrid supercapacitors (LICs) will be also discussed. An easy, eco-friendly and cheap synthetic approach for the preparation of carbon composites from the pyrolysis and activation of coffee waste and graphene oxide is presented. [3]

The effect of some important parameters such as particle size, electronic conductivity or mass loading is investigated for the battery-type electrode; whereas the optimum combination of specific surface area and pore size distribution is evaluated for the capacitive-type electrode. Optimization stages carried out in both electrodes leads to a significant improvement mainly in terms of power density of the full cell. Assembled LICs reach values of 100 Wh/kg at 9000 W/kg and retain above 80% of the initial capacitance after 3000 cycles, which can be enhanced to 15,000 cycles by decreasing the voltage window. [3]

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Broken symmetries in heterostructures based on 2D materials

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Two-dimensional (2D) crystals are particularly well suited for studying the interplay between symmetry and nonlinearity due to their high level of ordering. Remarkably, electronic states in these systems display quantum effects that give rise to novel and intriguing nonlinear effects simplifying further symmetry analysis.

In addition to the spin degeneracy, charge carriers in graphene have an additional degree of freedom called valley pseudospin. At the corners of the Brillouin zone (K and K' points), the electronic states on the two sublattices in pristine graphene are decoupled and have the same energy, giving rise to the so-called valley degeneracy. This degeneracy can be lifted, as for example, by stacking graphene with hexagonal boron nitride (hBN) and twisting properly the layers of the heterostructure leading to the appearance of an angle-dependent Moiré pattern. Such effect can break several symmetries and enhances collective interactions, providing the appearance of a plethora of exotic states of matter.1-8

We have fabricated several hBN / graphene / hBN heterostructures where the relative rotation angle between the flakes has been controlled and released on a graphite back gate placed over standard SiO2 / Si substrates. We will present detailed local and non-local magneto-transport measurements at low-temperatures demonstrating the occurrence of exotic quantum edge states due to the angle-dependent Moiré pattern. We will also present preliminary measurements as evidence of unconventional photoresponse in other 2D heterostructures with broken symmetries..

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Actual and future industrial applications of graphene and other 2D materials

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Abstract (Century Gothic 11)

The application bulk graphene materials in different markets start to arrive in high-volume orders [1]. Most of the actual aplications are in polymers or composites . However, there are several bottles neck for the use by end user of the graphene & 2D materials, such as:

- The low apparent density that extremely penalize the cost of transport,
- Graphene material is a "fluffy" and there is the risk of release
- Manipulation by end user is not easy and need adaptation of the process.
- Final properties are extremely sensible to dispersion

Adecuate processing of Graphene and related material can solve these problems. Allowing to introduce them in conventional production techniques and finally in large and massive markets paving the Way for business success in the graphene & 2D materials Supply Chains.

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Figures

Figure 1: GRM application in rubber

Graphene GO-ing Green

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Graphene oxide (GO) is a highly defective chemically modified form of graphene containing many different types of oxygen functional groups [1-3]. Their presence imparts hydrophilicity allowing for the development of water dispersions and inks. This enables unique opportunities for the synthesis of water soluble advanced hybrid materials and the fabrication of functional interface structures in macroscopic device platforms using "green" solution processing technologies. In this presentation we will discuss our latest findings on the use of GO as unique inter-face layers. We show that GO dispersions, when processed in a controllable way into films can be effectively used to block charges or to facilitate charge transport across layered interface structures. This opens important pathways for improved thin film optoelectronic of photoelectrochemical device structures of relevance in sustainable energy and catalytic applications [4-10].

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Figures

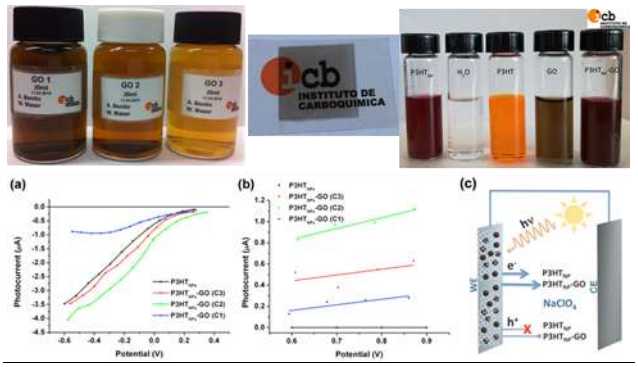

Figure 1: Aqueous dispersions of GO, a processed GO film, GO-P3HT aqueous dispersions, photocathodic and photoanodic currents of GO-P3HT thin films operating in a photoelectrochemical device.

Distorsion and electronic structures in two-dimensional magnetic ilmenenes systems

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Ilmenene is a new 2D material that recently has been exfoliated from ilmenite ($FeTiO_3$)[1]. With the synthesis of this 2D material, the door is open to design other similar ilmenene systems. In this work, using density functional theory, we performance calculations of the structural, electronic and magnetic properties of the ilmenenes $TMTiO_3$, TM ended (with TM running from V to Zn). The ground state of magnetic states is antiferromagnetic, except for Zn with a spin compensated solution. The difference with the ferromagnetic system is around 0.01 eV/TM-atom, although for Cr and Cu ilmenenes differences are considerably larger. We established a simple electronic filling model for all materials, except for Cr and Cu, for which we find a Jahn-Teller type distortion, breaking the degeneracy of the dxz and dyz orbitals. Magnetism in two-dimensional materials is promising for spintronics, and the synthesis of these materials would confirm the presence of structural distortions as well as the antiferromagnetic coupling.

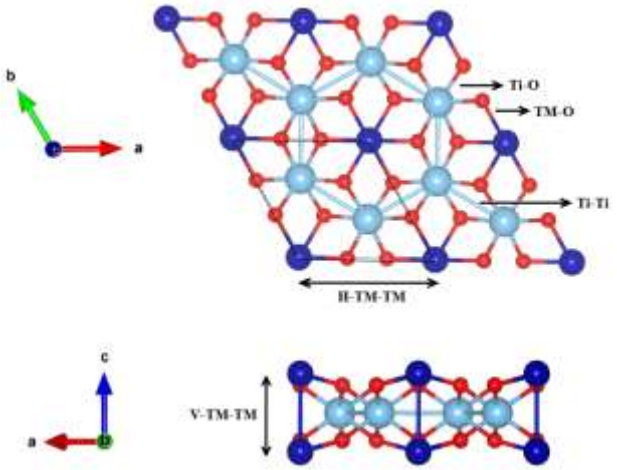

Figure 1: Top and side view of ilmenenes $TMTiO_3$, TM ended, where TM = V – Zn.

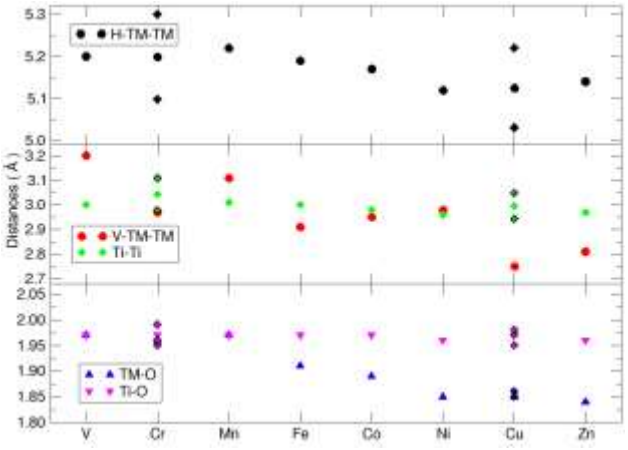

Figure 2: Interatomic distances (Following notation in Figure 1). The rhombus symbols denote distortions in the geometries due to the Jahn-Teller effect.

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Figures

Fundamentals of thermal properties of amorphous sp2 carbon monolayers

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In a recent experiment breakthrough, the synthesis of wafer-scale two-dimensional amorphous carbon monolayers have been reported. This new material seems to present unprecedented properties when integrated as coating of metals, semiconductors or magnetic materials, hence opening a new dimension for atomic layer deposition and ultracompact technologies. Here, we propose a structural characterization of the structural degree of amorphousness of such carbon membranes which could be controlled during the growth phase. We identify how energy is dissipated in such system by a systematic analysis of emerging vibrational modes whose localization increases with the loss of spatial symmetries, resulting in tunable thermal conductivity varying by more than one order of magnitude. Our simulations provide some recipe to design most suitable “amorphous graphene” (am-G) based on the target applications such as ultrathin heat spreaders, energy harvesters or insulating thermal barriers.
Specifically, using MD we design large scale models of disordered sp2 carbon monolayers with a varying degree of amorphousness. We characterize the degree of disorder in real space and k-space and follow how vibrational properties evolve with increasing the loss of crystallinity. We identify the class of phonon modes emerging in such structures, and connect their emergence with the resulting thermal properties of those membranes. Compared to the pristine graphene value, by tuning the crystalline order, the thermal conductivity is found to vary by more than one order of magnitude, although remaining quite high compared to other forms of amorphous materials.

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Figures

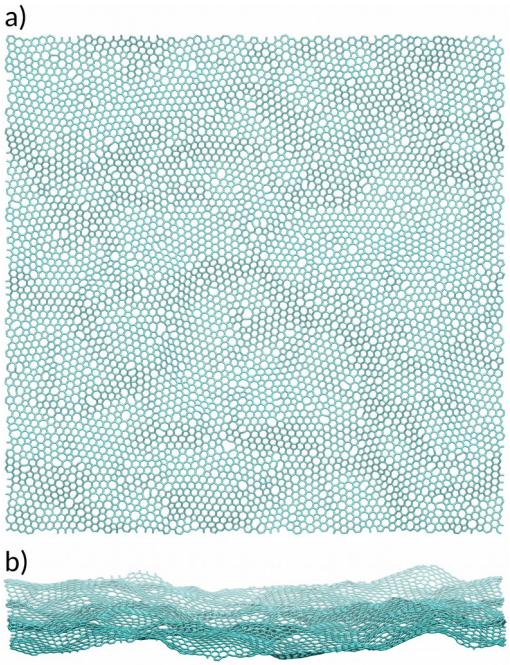

Figure 1: Am-G sample.

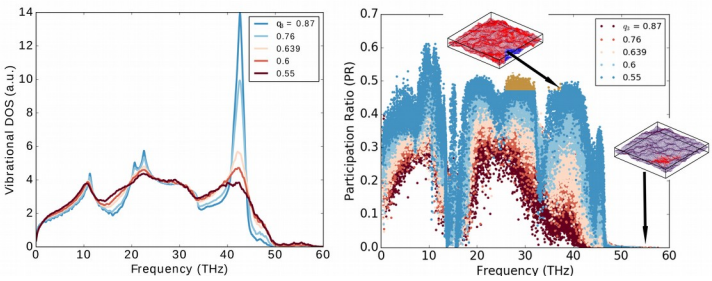

Figure 2: (Left) Vibrational DOS of Am-G for different degrees of amorphousness. (Right) Participation Ratio of the samples and atomic displacements (insets).

Relative Stability of Bernal and Rhombohedral Stackings in Trilayer Graphene under Distortions

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Stackings in graphene have a pivotal role in properties to be discussed in the future, as seen in the recently found superconductivity of twisted bilayer graphene[1]. Beyond bilayer graphene, the stacking order of multilayer graphene can be rhombohedral, which shows flat bands near the Fermi level that are associated with interesting phenomena, such as tunable conducting surface states[2] expected to exhibit spontaneous quantum Hall effect[3], surface superconductivity[4], and even topological order[5]. However, the difficulty in exploring rhombohedral graphenes is that in experiments, the alternative, hexagonal stacking is the most commonly found geometry and has been considered the most stable configuration for many years. Here we reexamine this stability issue in line with current ongoing studies in various laboratories. We conducted a detailed investigation of the relative stability of trilayer graphene stackings and showed how delicate this subject is. These few-layer graphenes appear to have two basic stackings with similar energies. The rhombohedral and Bernal stackings are selected using not only compressions but anisotropic in-plane distortions. Furthermore, switching between stable stackings is more clearly induced by deformations such as shear and breaking of the symmetries between graphene sublattices, which can be accessed during selective synthesis approaches. We seek a guide on how to better control – by preserving and changing - the stackings in multilayer graphene samples [6].

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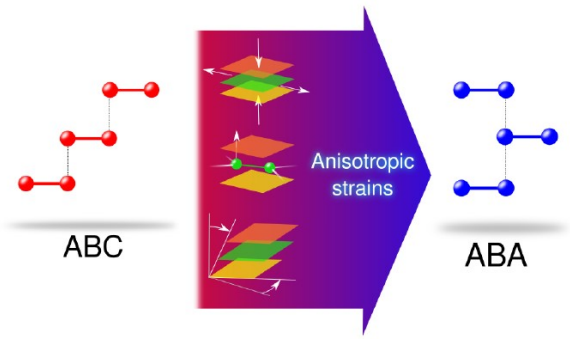

Figure 1: Graphene stacking changes from rhombohedral to Bernal due to small lattice deformations.

MoS_2 as the Sensing Platform for the Non-Enzymatic Detection of Cortisol: A First-Principles Study

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Atomically thin two-dimensional (2D) materials have been —and are still currently being— extensively studied due to their unique mechanical, electrical, and optical properties, which, together with their ultra-thin size, enable the development of compact devices and innovative technologies. Within the vast chemical space of transition metal dichalcogenides (TMDs), single-layer molybdenum disulphide (MoS_2) is with no doubt one of the most studied material due to its stability and its direct optical band gap of 1.8 eV, which make it the ideal candidate to be used in a wide range of nanoelectronic devices, going beyond conventional CMOS technology. [1] Here we look at MoS_2 in the context of biosensing, and we study such material as the core component of field-effect biosensors (Bio-FETs) for the detection of cortisol. Ultimately, the aim of this study is to design and integrate such biosensors in wearable health monitoring devices. [2] We want to bridge the gap between materials' properties and device physics and to do so, we carry out first-principles atomistic computer simulations in the framework of density functional theory (DFT). Our study constitutes the first step of a wider multi-scale modelling approach in which the goal is to construct a full atomistic-to-device level model.

Recently, MoS_2 has been studied as a sensing platform for detecting mainly gas and small biological molecules, such as glucose. [3] Enzymatic biosensing is the most common approach, however, non-enzymatic sensing can provide higher sensor stability and prompt response, at the expense of chemical selectivity. Here, we are interested in the non-enzymatic detection of cortisol in human sweat as a mean to monitor the risk of cardiovascular diseases. However, the mechanisms that govern the interaction between the analyte and MoS_2 at the molecular level are far from being understood. Thus, we thoroughly explore the MoS_2/cortisol interaction in terms of both structural, electronic, and charge transfer properties to assess viable sensing mechanisms. We study the impact of some of the most used metal dopants employed in lab-scale experiments, such as Ni, Pt, Pd, in order to modulate the sensing platform with respect to bare MoS_2. In addition to single-atom doping, we also explore the use of metal nanocluster (e.g., Pt and Au) to decorate the MoS_2 layer as yet another mean to detect cortisol.

Overall, our work ultimately aims to obtain a deep understanding of the properties of MoS_2 when used as a sensor to drive the design of devices towards better performance.

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Non- Hydrostatic Pressure dependence of Raman modes in Monolayer Graphene

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Abstract

Raman spectroscopy studies performed in graphene under hydrostatic pressure with diamond anvil cell have shown a great dispersion of the G and 2D pressure coefficients modes [1,2] . Moreover, the information related to the D–band is not accessible due to the presence of the first-order Raman mode (T_{2g}) of diamond in the pressure cell. This dispersion can be attributed to: 1) the different types of substrates used in the experiments; 2) the distinct pressure transmitting media inducing different charge–transfer mechanisms, and 3) the existence of a non–homogeneous distribution of the number of graphene layers in the sample to be analyzed.

Raman spectroscopy experiments on monolayer graphene films subjected to non-hydrostatic conditions have been carried out on anvil pressure cells up to 7 GPa to studying the effect of the pressure/stress on the D, G, D´ and 2D grapheme bands. In this work we have used single-layer graphene films grown by CVD on copper foil substrate prepared by Graphenea (Spain). Raman images constructed from the spatial distribution of the G and 2D band frequencies and the I_{2D}/I_G intensity ratio have been used to verify the homogeneous distribution of monolayers. Diamond anvils have been substituted by sapphire ones to allow the observation of the D–band and the second-order Raman scattering without signal overlaps [3]. In this experiment the sample is placed directly between the sapphire anvils without optical pressure sensor (figure 1). The pressure/stress is estimated from the axial (σ_z) and radial (σ_R) stress coefficients, which are calculated from the phonon A_{1g} (417 cm^{-1}) of sapphire. From the results we can obtain the coefficients of axial stress $d\omega/d\sigma_z$ of the different bands of monolayer graphene and have evidences of the formation of nano-domains in the recovered samples at ambient pressure after a cycle of extreme pressure/stress.

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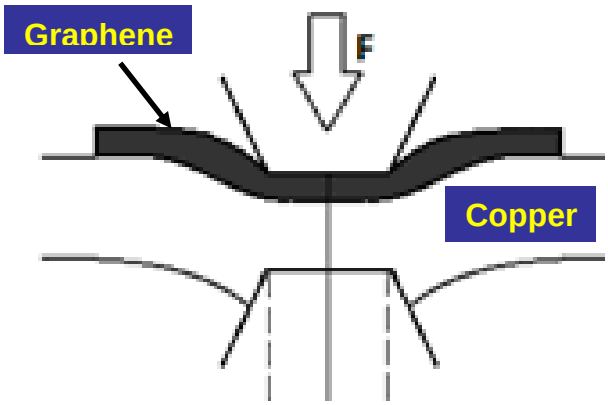

Figure 1: Monolayer Graphene on copper substrate between the sapphire anvils

Spin-momentum Locking in Defect Line Array Bilayer Graphene under Gate Voltage and n-doping

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Abstract

Graphene few-layer structures still presenting exciting phenomena to discover. For instance, recent studies on twisted bilayer graphene show superconductivity [1], a fact that has expanded research on the stacking of few-layer graphenes [2]. Patterning with domain walls in gated bilayer graphene produces a change between AB to BA stacking and presents topological states in the gap [3-4]. In fact, the domain walls can be due to defect lines with pentagons and octagons (8-55), see Fig. 1, that in layer graphene are inducing localized states [5,6]. In this work using density functional theory calculations, we investigate an array of these defect lines in bilayer graphene. We found that the band structure shows a magnetic phase in which the spin is locked to the momentum, as in topological insulators. We also follow the topological states that appear even without a gate because of the array of defect lines. We lastly study the differences in spin bands and identified topological states when engineering by doping and/or electric field. All these results are summing to the new interesting data of the correlated behavior of electrons with the stacking in two-dimensional materials.

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Figures

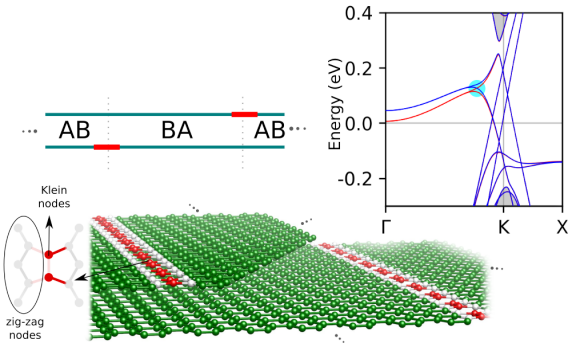

Figure 1: Scheme of the defect line array and band structure of the unperturbed defect line system. Note in the band structure the crossing with spin-momentum locking, as shown in the cyan circular region.

Hybrid graphene quantum dot-manganese oxide nanoparticles for photodynamic therapy

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Photodynamic therapy (PDT) is a novel approach in cancer treatment owing to its reduced side effects and improved selectivity [1]. Nontoxic photosensitizers absorb near infrared light at specific wavelength and damage cancer cells by generating reactive oxygen species (2). The photosensitizers are excited by light exposure resulting in fluorescence emission, which acts as both therapeutic and imaging agents [3,4]. We synthesized core manganese oxide (Mn3O4) nanoparticles and functionalized with highly reduced graphene oxide (HRG). The synthesized nanocomposites were found to be stable and therefore suitable for storage and biomedical applications. The cellular uptake of nanoparticles was evaluated in lung cancer cell line (A549) following exposure of nanoparticles solutions (25, 50, and 100 µg/ mL) and incubation for 4 h. The cells were then washed before quantification of intracellular Mn. Cellular uptake of nanoparticles was directly proportional to their concentration. More than 95% of cells survived even after the exposure of a high concentration of nanomaterials (100 µg/mL), indicating that these nanoparticles are nontoxic and biocompatible. We performed fluorescence microscopy for live/dead cellular analysis. A549 cells were incubated with nanoparticles for 24 h and stained with fluorescein diacetate (green emission for live cells) and propidium iodide (red emission for dead cells) to visualize live and dead cells, respectively. Almost 100% cells were viable when treated with phosphate buffered saline or Mn3O4 while only few dead cells were detected after exposure of HRG-Mn3O4 nanoparticles. However, laser irradiation resulted in massive cellular damage by HRG-Mn3O4 nanoparticles. These findings suggest the imaging and therapeutic potential of these nanoparticles for photodynamic therapy. (Supported by National Plan for Science, Technology and Innovation, KACST, Saudi Arabia, No. 14-NAN-862-02)

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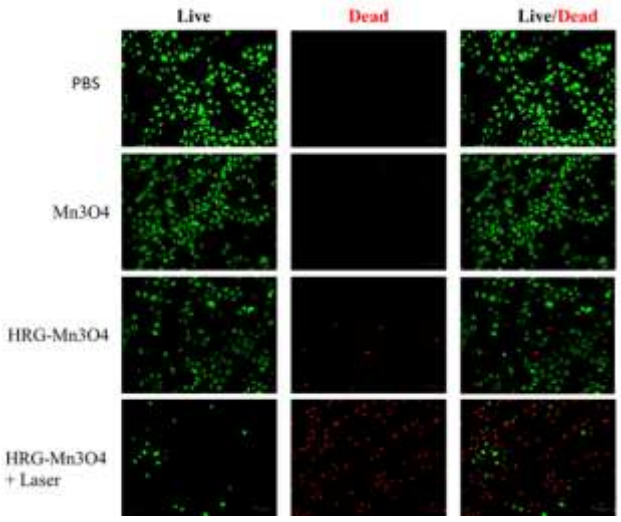

Figure 1: Fluorescence microscopy images of A549 cells co-stained with fluorescein diacetate and propidium iodide after exposure of nanoparticles with/without laser irradiation (670 nm, 0.1W/cm2) for 5 min.

New method for nanographene oxide high yield production and its biomedical applications

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Graphene is increasingly attracting interest from the scientific and business community, due to its great potential for the development of new high-value technologies in the scientific and industrial environment. Current methods for graphene oxide (GO) production, like mechanical exfoliation, chemical exfoliation, chemical vapor deposition, and others, are not capable of producing nanosized GO with high yield and concentrations, having water stability, and being biocompatible. Therefore, improvement of the methods is necessary to achieve higher yield and higher concentrations of materials that meet the quality specifications demanded for different industrial applications, especially in areas related to biomedicine. Among the limitations in the production of graphene from current production methods are high cost, low efficiency and low reproducibility on a high scale. [1,2] Herein, single layer nano-sized graphene oxide (GOn) was produced through the modified Hummers method, followed by ultrasonication using a custom-built industrial grade system with technical specifications that allowed to achieve materials with the desired characteristics, for biomedical applications, in very high concentrations with a simple process.

Particle size was determined by transmission electron microscopy (TEM) and dynamic light scattering (DLS). Surface charge was measured using a zeta potential analyser. Oxidation degree was characterized by X-ray photoelectron spectroscopy (XPS) and Fourier-transform infrared spectroscopy (FTIR). Thermal stability of the samples was determined by thermogravimetric analysis (TGA; 30-1000 °C, 10 °C min^{-1}, under N_2 flow). Biocompatibility was evaluated using human foreskin fibroblasts (HFF-1) and by ssessing cell viability through resazurin assay. Single layer GOn was obtained with mean lateral dimensions of 99 ±43 nm (52 % <100 nm, 99 % <200 nm). Original GO size was of 1178 nm ± 479 nm. GOn dispersion showed colloidal stability with zeta potential values around -39.4 ± 1.8 mV, at neutral pH and a concentration of 8 mg mL^{-1}. After 6 months no decrease in particle stability was observed. XPS analysis revealed that GOn oxygen atomic percentage (at.%) was of 30% and that its carbon at.% was of 70%, also a typical FTIR spectra was obtained, confirming that a material with the desired chemical functionalities was produced. TGA analysis revealed that a first step of 25% weight loss occurred between 141 ˚C and 200 ˚C, due to the degradation of thermolabile oxygen-containing functional groups. Also, a second step of 5% weight loss occurred between 200 ˚C and 548 ˚C, corresponding to the combustion of the carbon skeleton. The material revealed to be biocompatible at concentrations (100 – 250 µg mL^{-1}) above the usual amount used for biomedical applications or that can be release in vivo by implants containing those. At our team it has been characterized for biomedical applications in skin disease and cancer phototherapy, as produced, modified or incorporated in pharmaceutical formulations. This work will also be presented. In sum, a biocompatible single layer nanosized material was obtained with high yield and at high concentrations, which presented stability for at least 6 months kept at room conditions. Currently, materials with such characteristics are not available commercially. Therefore, we are seeking translation to industry and exploring their applications in the biomedical field and other areas.

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Acknowledgements
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Ionic Glass Gated 2D Material Based Field Effect Transistor and Phototransistor: $MoSe_2$ over LaF_3 as case study.

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Abstract : Modulating the carrier density of two dimensional ('2D') materials is pivotal to tailor their electrical properties, with novel physical phenomena expected to occur at higher doping level. Here, the use of ionic glass as a high capacitance gate is explored to develop 2D material based phototransistor operated for the first time with higher carrier concentration up to $5x10^{13}$ cm^{-2}, using $MoSe_2$ over LaF_3 as archetypal system [1]. Ion glass gating allows low operating biases, then circumventing the possible electrical breakdown of conventional dielectric gating, while preserving low temperature operation which is not possible using electrolytes gating. It reveals to be a powerful technique combining the high carrier density of electrolyte gating methods while enabling direct optical addressability impeded with usual electrolyte technology. The $LaF_3/MoSe_2$ phototransistors demonstrate I_{ON}/I_{OFF} ratio exceeding 5 decades and photoresponse times down to 200 µs, up to two decades faster than $MoSe_2$ phototransistors reported so far. Careful phototransport analysis unveils that ionic glass gating of 2D materials allows tuning the nature of the carrier recombination processes, while annihilating completely the traps contribution in electron injection regime. This remarkable property results in photoresponse that can be modulated electrostatically by more than two orders of magnitude, while at the same time increasing the gain bandwidth product. This study demonstrates the potential of ionic glass gating to explore novel photoconduction processes and alternative architectures of devices. Finally, this approach reveals to be a promising technology to develop 0D based phototransistor for IR detection. [2].

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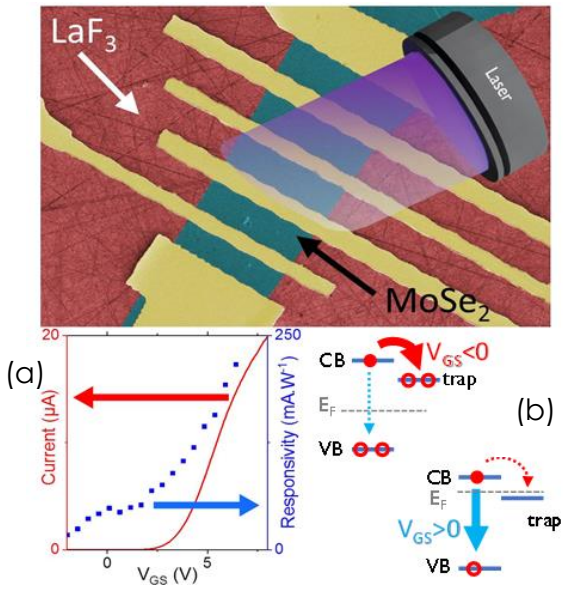

Figure: (a) Transfer curve in red and responsivity gate dependent in blue; (b) Schemes illustrate relaxation mechanisms for negative biases (top) and for positive biases (bottom

Boron Substitution in Graphene Nanoribbons: One-dimensional Spin Chains with Tuneable Interactions

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Graphene nanoribbons (GNRs), low-dimensional platforms for carbon-based electronics, show the promising perspective to also incorporate spin polarization in their conjugated electron system. However, these magnetic moments are usually localized around zigzag edges, difficult to fabricate and very reactive. This combined theoretical and experimental study demonstrates that magnetism can also be induced away from physical edges through atomically precise engineering of topological defects in its interior. A pair of substitutional boron atoms inserted in the carbon backbone of the 7-armchairGNR breaks the conjugation of its topological bands and builds two spin-polarized boundary states around them. Therefore, a spin moment of 2 Bohr magnetons localizes around each pair of B atoms in the structure (see Figure 1).

First indications of the presence of magnetism were given by the appearance of characteristic Kondo peaks in electrical transport experiments performed at nanoGUNE. Transport was measured through boron-substituted GNRs suspended between the tip and the sample of a scanning tunneling microscope (STM). These observations were rationalized in terms of the theory and first-principles simulations performed at CFM and DIPC, which predicted for each isolated boron pair a S=1 spin state as well as a strong dependence on the spacing between pairs. The interaction between two of such topological defects was further explored, outlining a route to engineer topological spin chains, with the promising tunability of their magnetism by modifying their spacing [1].

Therefore, the present results demonstrate a route to embed spin chains in graphene nanoribbons, turning them into basic elements of spintronic devices. We are currently examining the effect of B substitution for other GNRs.

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Figures

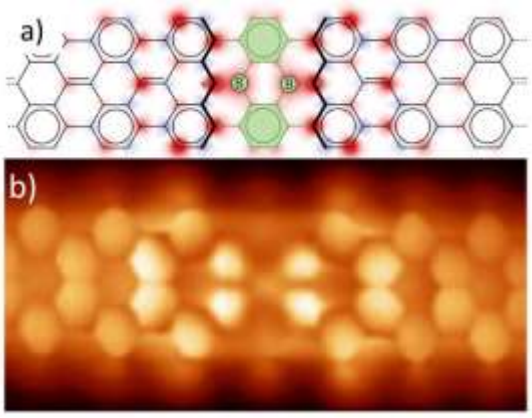

Figure 1: a) Structure of the 2B-7AGNR defect together with the computed spin density map. b) Constant height STM scan (V=2 mV) using a CO-functionalized tip of a 2B-7AGNR defect.

PECVD of Graphene on sapphire substrates: A Design of Experiments (DoE) approach

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The use of graphene in the semiconductor industry is not yet widespread because controlling the properties of material and reproducibility of the process is still challenging. In addition, the catalyst-free growth of graphene directly on technologically relevant substrates (such as sapphire) at low temperatures is highly desirable for back end of line integration [1]. By using the plasma enhanced chemical vapour deposition (PECVD) technique, the temperature of the synthesis of graphene on sapphire can be reduced significantly, since the plasma provides the energy to break the molecules from the precursor [2]. Thus, providing a controllable synthesis procedure of catalyst-free graphene on such dielectric substrate will boost the use of graphene in the industry [3].

In this work, the optimization of the PECVD growth of graphene on c-plane sapphire is carried out by means of the statistical Design of Experiments (DoE) method. The quality and defects of the synthesized graphene layers are characterized by means of Raman spectroscopy. Factorial DoE with one central point is performed to evaluate the effect of the growth parameters and the extent of their interactions on the quality of the graphene layers. We found that the main factors affecting the ratio I_{2D}/I_G are the flow of methane and pressure. In addition, we found that a transition from graphene to amorphous carbon can be controlled by tunning the flow of methane, the pressure, and plasma power. Finally, the graphene layers were functionalized using 1-pyrenebutyric acid N-hydroxysuccinimide ester (PBASE), as a molecule that binds to both graphene and to antibodies, demonstrating its potential for future applications in biosensing.

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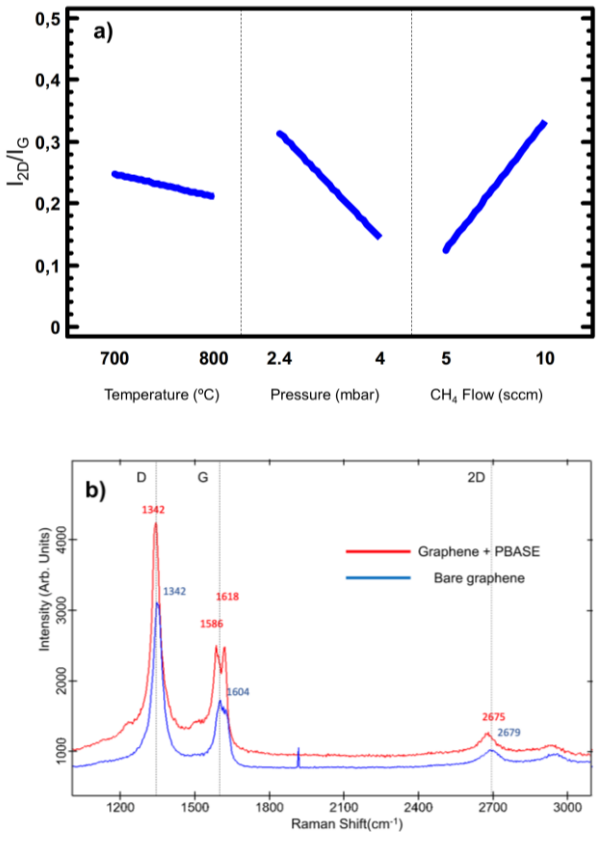

Figure 1: a) Main effect plots of the factors temperature, pressure and CH_4 flow for the response I_{2D}/I_G; b) Raman spectra of graphene before and after functionalization with PBASE molecule.

Interfacial Ferroelectricity by van der Waals Sliding

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Co-Authors (Century Gothic 10)

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Abstract

Despite their partial ionic nature, many layered diatomic crystals avoid internal electric polarization by forming a centrosymmetric lattice at their optimal van-der-Waals stacking. In my talk, I will present a stable ferroelectric order emerging at the interface between two naturally-grown flakes of hexagonal-boron-nitride, which are stacked together in a metastable non-centrosymmetric parallel orientation. We observe alternating domains of inverted normal polarization, caused by a lateral shift of one lattice site between the domains. Reversible polarization switching coupled to lateral sliding is achieved by scanning a biased tip above the surface. Our calculations trace the origin of the phenomenon to a subtle interplay between charge redistribution and ionic displacement, and our minimal cohesion model predicts further venues to explore the unique "slidetronics" switching.

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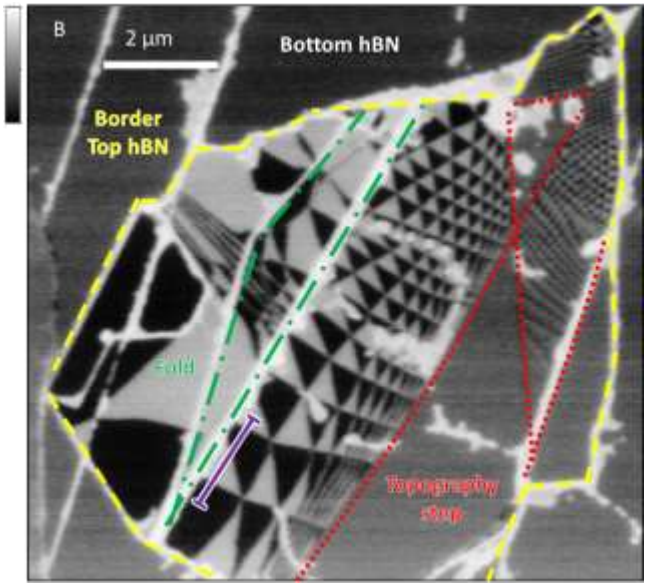

Figure 1: Surface potential map showing oppositely-polarized domains (black & white)

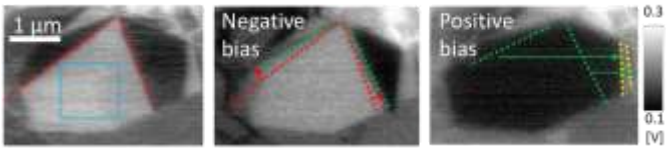

Figure 2: Dynamic flipping of polarization orientation by domain-wall sliding.

Cross Plane Heat Transport Across the 2D/3D Material Interfaces

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Abstract

Understanding the heat transport in two-dimensional (2D) materials is necessary for the reliable operation and performance of the devices made from these materials. When the device sizes decrease, the interfaces between the 2D materials and their substrates contribute more to the thermal transport mechanisms. As a result, thermal boundary conductance (TBC) that defines the thermal transport rate at the interfaces becomes a key parameter for the thermal characterization and design of 2D devices. In this study, we perform approach – to – equilibrium molecular dynamics simulations to evaluate the TBC of interfaces between popular 2D materials (h-BN, MoS_2, WS_2, WSe_2) and substrates (GaN and SiO_2) Simulation results are used to calculate the lattice vibration (i.e. phonon) properties of the materials using a new approach based on the fluctuation-dissipation theorem and atomistic Green's functions. Our results suggest that the TBC of the interfaces mostly depend on the similarities and the differences between the lattice vibrational properties of the materials making the interface. Moreover, the number of 2D material layers and the lattice match between the 2D and substrate materials also affect the TBC. The results of the simulations are used to generate a correlation to calculate the TBC of the interfaces based on a function, *I*, that depends on the materials' phonon dispersions, temperature, mass ratio of atoms, and number of 2D material layers. These findings are also compatible with the existing TBC data in the literature [1-3]. We believe the correlation obtained in this study will be a good guide for the selection of the thermally superior substrates for 2D-based applications.

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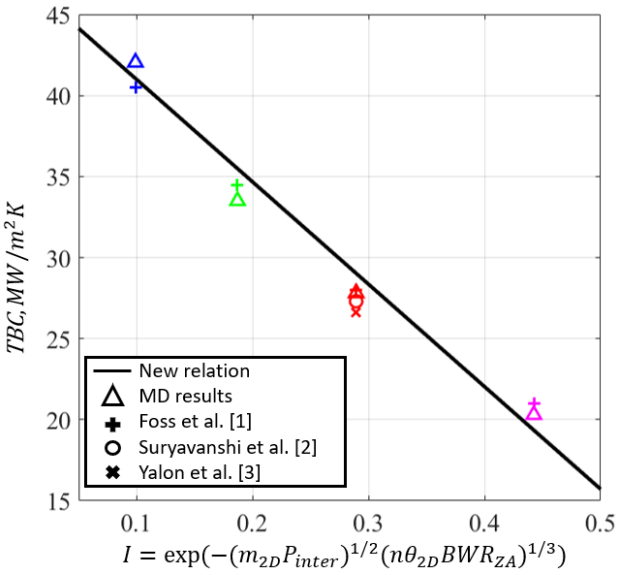

Figure 1: Comparison of the proposed model, MD results of this study, and the results from the literature [1-3].

Graphene functionalization with SARS-CoV-2 antibodies

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Current situation of COVID-19 demands a rapid, reliable, cost-effective, facile detection strategy to break the transmission chain and biosensors have emerged as a feasible solution for this purpose. Among the existing variety of biosensors, photonic biosensors allow real-time detection of infinitesimal quantities (even isolated molecules) of a great variety of biochemical substances, since they measure instantaneous changes in the optical properties of matter. Generally, photonic biosensors are composed by two parts: the photonic part, which is responsible for transducing a biochemical change into a change in the optical response; and the chemical part, a molecular recognition element that ensures that only the targeted analyte adheres to the biosensor and provokes the optical change. In this context, Graphene has demonstrated its potential in the rapid detection of SARS-CoV-2 by its integration in a FET-based biosensor [1].
In this work we have developed a faster, less toxic, and a cost-effective functionalization of graphene with PBASE (- 1-pyrenebutyric acid N-hydroxysuccinimide ester), which is a key molecule to immobilize SARS-CoV-2 spike antibodies onto graphene surfaces (Figure 1a). The PBASE functionalization as well as the SARS-CoV-2 antibody immobilization has been probed in Graphene layers and flakes prepared by means of plasma enhanced chemical vapour deposition and the scotch-tape method. Atomic force microscopy together with Raman spectroscopy confirm all the functionalization steps (Figure 1b).
This demonstration would mean the viability of the chemical part of a graphene-based photonic biosensor for ultra-rapid detection of minimal amounts of the SARS-CoV-2 virus in nano-pharyngeal fluid through the integration of functionalized graphene in a low-cost plasmonic metamaterial photonic biosensor that can be manufactured on a large scale.

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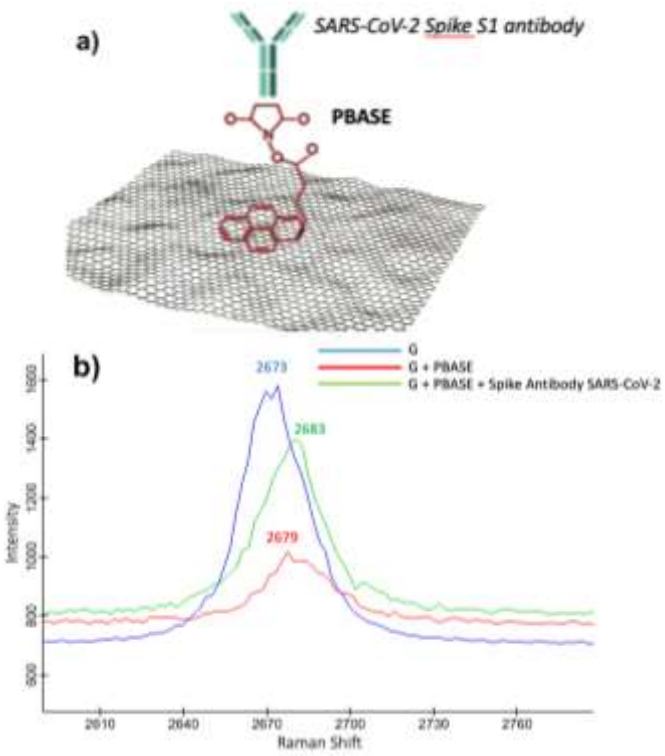

Figure 1: a) Schematic representation of the graphene sheet functionalized with PBASE and SARS-CoV-2 spike antibodies; b) Raman spectra of bare graphene, functionalized with PBASE and with PBASE and SARS-CoV-2 spike antibodies.

Multi-gate quantum dots from armchair graphene nanoribbons

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Atomically precise graphene nanoribbons (GNRs) have attracted much interest from researchers worldwide, as they constitute an emerging class of quantum-designed materials, all tailored by controlling their width and edge structure during the chemical synthesis.[1-3] The major challenges toward their exploitation in electronic applications include reliable contacting, complicated by their small size (<50 nm), and the preservation of their physical properties upon device integration. In recent years, the exploitation of GNR properties for electronic devices has focused on their integration into field-effect-transistor (FET) geometry.[4] However, such FET devices, due to the presence of a single gate, have limited electrostatic tunability. Here, we report on the device integration of armchair GNRs into a multi-gate FET geometry and a one-dimensional contact geometry as well. With the above geometries, we measured the quantum dot behavior at low-temperature. By demonstrating the preservation of the armchair GNRs' molecular levels upon device integration, as demonstrated by transport spectroscopy, our study provides a critical step forward in the realization of more exotic GNR-based quantum devices.

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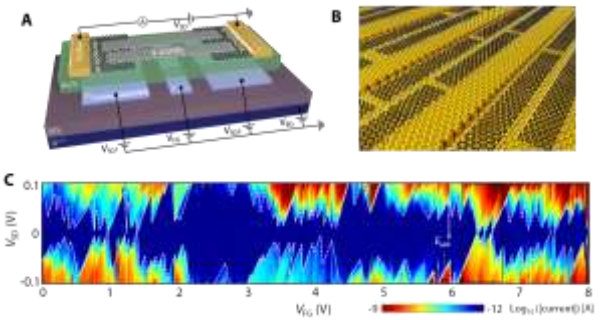

Figure 1: GNR device and the transport measurement. (A) Artistic illustration of a multi-gate 9-AGNR quantum dot device. (B) A sketch of the GNRs grown parallel to the Au(788) terraces. (C) Coulomb diamonds in a multi-gate 9-AGNRs device at low temperature.

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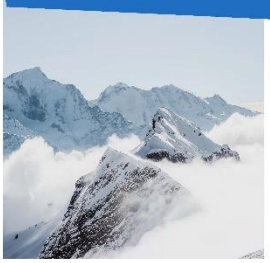
1 What it is



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

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

2 Its objectives

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

3 Flagship Areas

- Neurobiosciences
- Quantum Technologies (QT)
- NeutriOnics

High Performance Computing & Artificial Intelligence (HPC-AI)

4 Expected impact

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

5 Governance

- ikerbasque Basque Foundation for Science — Recruitment and attraction of research personnel
- Management of IKUR funds
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- Fundación Biofísica Bizkaia / Biofisika Bizkaia Fundazioa — Neurobiosciences
- DIPC — QT + HPC-AI
- MPC Materials Physics Center — NeutrIOnics
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Scientific Direction of IKUR's Flagship Areas