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## TNT2023 Foreword

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On behalf of the Organising Committees, we take great pleasure in welcoming you to Lyon (France) for the “Trends in NanoTechnology” International Conference (TNT2023).

TNT2023 is being held in large part due to the success of earlier TNT Nanotechnology Conferences and will feature again a high-level scientific program addressing key factors for the future of the Nanoscience and Nanotechnology community in Europe. TNT events have demonstrated over the past 22 years that they are particularly effective in transmitting information and promoting interaction and new contacts among workers in this field.

We are indebted to the following Scientific Institutions and Government Agencies for their financial support: Université de Lyon/Ecole Doctorale de Chimie, The Research & Innovation Center for Graphene and 2D Materials (RIC-2D)/ Khalifa University of Science and Technology, Faculté des Sciences et Technologies/UCBL, GDR-HOWDI, CNRS, LMI-UMR5615, Institut des Nanotechnologies de Lyon (INL), C’Nano, Institut de Chimie de Lyon, Institut Lumière Matière (ILM) and Université Grenoble Alpes (UGA).

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

Hope to see you again in the next edition of the “Trends in NanoTechnology” International Conference (TNT2024).

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# Functionalized Graphene Oxide Enabled Hybrid UF Membranes for Water Treatment

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Water scarcity challenges have been intensified by the ever-deteriorating freshwater resources worldwide. The demand of freshwater is mounting and, hence, it is anticipated that five billion people worldwide would suffer from water stress in 2050. This drives water treatment technologies, including membrane-based filtration processes [1-3]. A major challenge in membrane filtration is fouling which reduces the process performance. Fouling mostly happens due to the adhesion of foulants on the surfaces or within the pores of the membranes [3,4]. Thus, high performance membranes with superior fouling resistance are in demand to overcome the fouling problem encountered in surface water treatment. To achieve this goal, hybrid ultrafiltration membranes were manufactured using functionalized graphene oxide: sulfonated poly (ether ether ketone) polymer chains grafted graphene oxide (SPK-g-GO) or polydopamine-coated graphene oxide (PDGO), commercial poly(ether sulfone) and sulfonated poly (ether sulfone; SPES)) via the non-solvent induced phase separation (NIPS) method. All the membranes demonstrated typical asymmetric porous structures with a compact skin layer and porous sublayer with finger-like structure. These finger-like pores were elongated towards the bottom surface upon the integration of different wt.% functionalized GO. Hydrophilic and charge tunable hybrid UF membranes were finally produced. The rate of water penetration into the membranes matrix was tunable with the progressive addition of functionalized GO into the matrix of PES or SPES membranes. The hybrid membranes were tested in UF of humic acid and synthetic natural organic matter (NOM) solutions at 1.0 bar feed pressure. The membranes were competent in rejecting NOM in the feed solution. A remarkable improvement in fouling resistance efficacy of the hybrid membranes was observed during the cyclic filtration of NOM solution. Both reversible and irreversible fouling efficiency were significantly reduced with the loading amount of functionalized GO into the matrix of hybrid membranes. The synergic combinations of functionalized GO, PES or SPES were credited for the production of high-performance membranes with the stable fouling resistant. Tailor-made hybrid UF membranes can be easily produced via phase-inversion using this approach for efficient organics removal from contaminated surface water.

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# The Nanowire (R)evolution viewed at atomic scale: from VLS vertical systems to planar quantum networks

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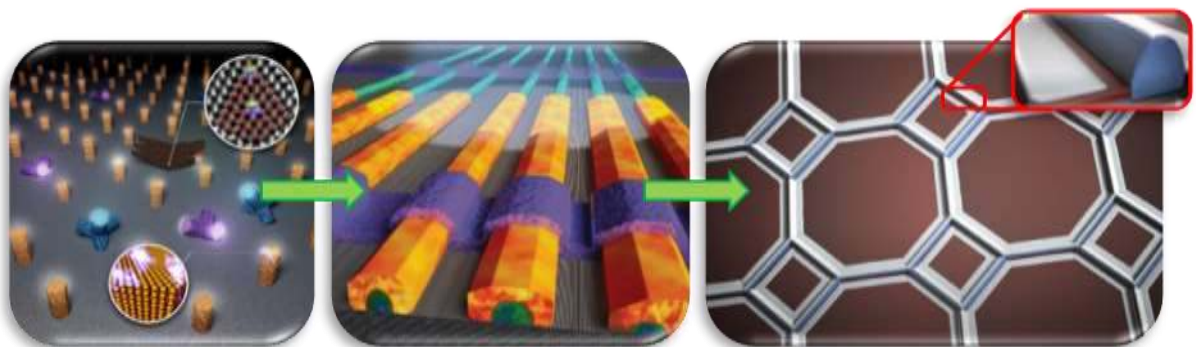
## Abstract

Hybrid superconductor/semiconductor-based quantum devices (e.g.: for quantum computing applications) are mainly based on 3 different technologies: vapour-liquid-solid (VLS) grown vertical nanowires, selected area growth (SAG) nanowire networks and 2-dimensional electron gases (2DEG). By using AC STEM and 3D modelling, we will study the influence of polarity on the development and properties of these complex NW-like hybrid heterostructures vertically grown by VLS.[1-6] In a second part, we will show the natural evolution of this vertical technology to the flat SAG growth of NW networks on III-V substrates. In these complex core@shell or confined multilayer nanostructure configurations, strain relaxation mechanisms during the epitaxial growth play a key role in determining their final morphology, crystal structure and physical properties. To analyze these mechanisms, atomic-scale AC STEM studies are performed on horizontal arrays of nanowires. Monochromated Valence Electron Energy Loss Spectroscopy will be employed to spatially map the heterostructure's bandgap with sub-nanometer resolution and certify the influence of the high mismatch induced strain on the topological electronic properties at the interface of the core-shell region.[7-12] Finally, we will address the newly developed 2DEG heterostructures based on SiGe, fully compatible with CMOS technology, where the strain and composition at the Ge quantum wells will determine their final quantum properties [13].

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## Figures



**Figure 1:** Semiconductor nanowires (r)evolution: from vapour liquid solid to guided growth and selected area growth.

# Swinging Crystal Edges of Growing Carbon Nanotubes

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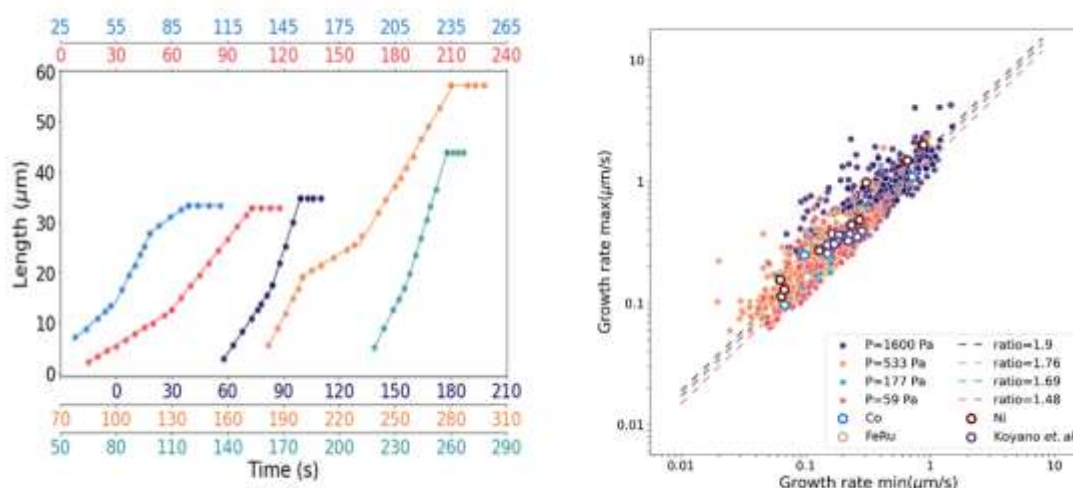
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Recent measurements of the growth kinetics of individual carbon nanotubes revealed abrupt changes in the growth rate of nanotubes maintaining the same crystal structure [1]. A simple model, derived from our previous analysis of the role of the configurational entropy of the nanotube edge [2] and supported by Kinetic Monte Carlo [3] and Molecular Dynamics simulations [4], shows that these switches are caused by tilts of the growing nanotube edge between two main orientations, close-armchair or close-zigzag, inducing different growth mechanisms. Beyond providing new insights on nanotube growth, these results point to ways to control the dynamics of nanotube edges, a key requirement for producing arrays of long structurally-selected nanotubes. More generally, the thermodynamics and kinetics of carbon nanotube growth are discussed.

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## Figures



**Figure 1** Left: Experimental growth rates showing sharp changes for tubes maintaining the same chirality. Right: Strikingly, the ratio of fast over slow growth rates is almost constant, around 1.7, for all pressure (and temperature) conditions and catalysts [1, 3].



# Molecular systems in complex environments: an embedded many-body perspective

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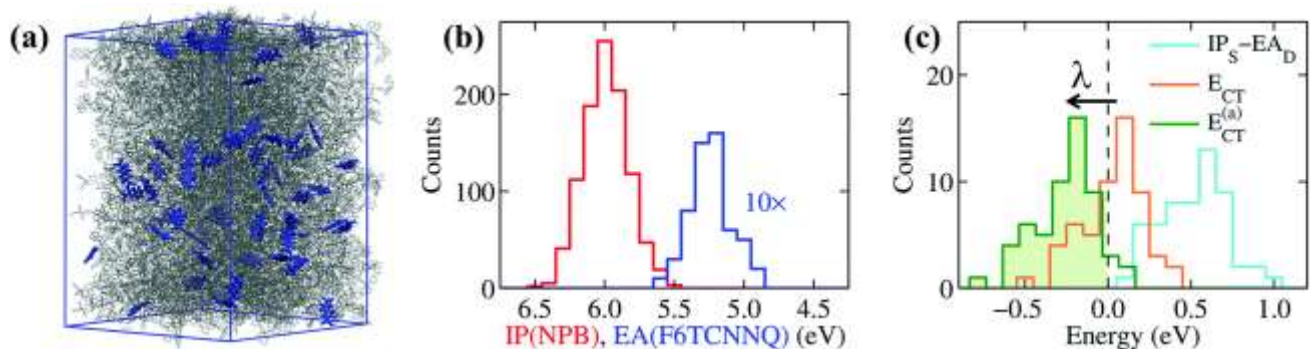
[xavier.blase@neel.cnrs.fr](mailto:xavier.blase@neel.cnrs.fr)

Molecules between two metallic electrodes, at a donor/acceptor interface, in a solvent or a biological environment, are few examples of systems associated with different properties and applications. They share however a common characteristic, namely they are active subsystems immersed in a complex and large, often disordered, environment that strongly renormalizes their electronic properties (energy levels, optical spectra, conductance, etc.) We will present a specific family of *ab initio* techniques, namely embedded many-body perturbation theories [1,2] allowing to study the electronic and optical excitations of active subsystems immersed in very large scale electrostatic and dielectric media. The case of molecular dopants [3] and defects in stacked 2D materials [4] will be given as important examples of the usefulness of such theoretical approaches. Work done in collaboration with G. D'Avino, J. Li, D. Amblard, M. Comin, S. Fratini (Institut Néel, Grenoble), I. Duchemin (CEA, Grenoble), D. Beljonne (Mons, Belgium) and D. Jacquemin (Univ. Nantes).

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## Figures



**Figure 1:** (a) Doped amorphous organic semiconductor with dopants (acceptors) in blue. In (b) Distribution of host highest occupied (red) and dopant acceptor (blue) levels within accurate embedded many-body GW calculations. c) Histogram of charge-transfer excitation energies from dopants to host with polaronic contribution ( $\lambda$ ). From Li *et al.* *Mater. Horizons*, **6** (2019) 107.

# Water and ion flows in 1D and 2D nanochannels, from carbon memories to quantum friction

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The emerging field of nanofluidics explores the molecular mechanics of fluids. This world of infinitesimal fluidics is the frontier where the continuum of fluid dynamics meets the atomic nature of matter, or even its quantum nature. Nature fully exploits the fluidic oddities at the nanoscale and it is capable of breath-taking technological feats using a fluidic circuitry made of multiple biological channels, such as ionic pumps, proton engines, ultra-selective pores, stimuable channels, ... A major challenge at stake is to harness the strange properties of fluid transport at nanoscale to reproduce or mimick some of these functionalities.

In this talk, I will discuss various experimental and theoretical results that we obtained recently on the transport of water and ions in ultra-confinement, both in 1D nanotubes and 2D channels obtained by van der Waals assembly. I will in particular discuss the water-carbon couple, which highlights a variety of exotic transport properties. I will focus on two such phenomena: the emergence of memory in quasi-two-dimensional water channels and the development of elementary ion-based computing, with basic forms of Hebbian learning [1,2]; and the nearly frictionless flows of carbon nanotubes and its quantum roots [3,4,5].

I will conclude by briefly discussing how such nanoscale emerging phenomena can be exploited to develop technological innovations for water and energy.

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# Local Electrical Excitation of Excitons in 2D Semiconductors and of Surface Plasmons in Metallic Structures

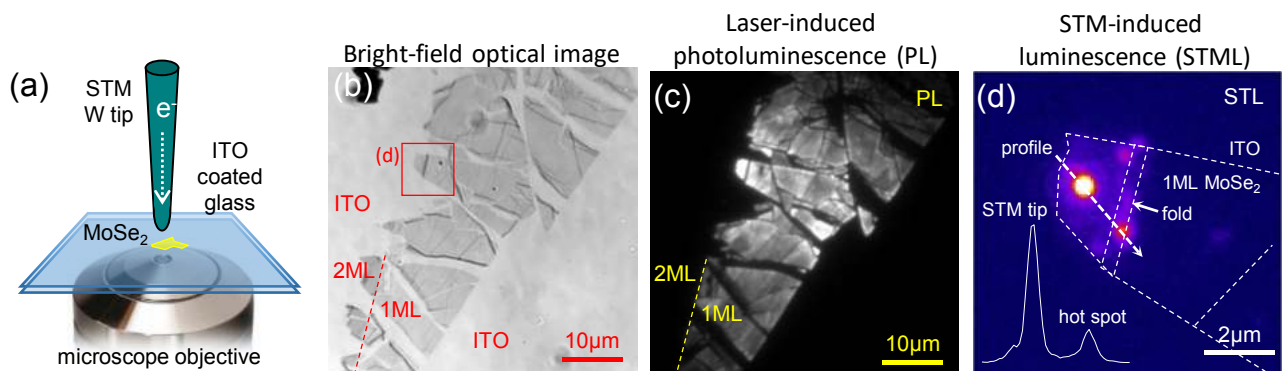
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We use a biased tunnelling junction to locally and electrically excite surface plasmons and excitons. The tunnelling junction used may be between the tip of a scanning tunnelling microscope (STM) and a conducting plasmonic sample[1], between an Au nanoantenna and a gold film[2], or between an STM tip and a conducting substrate on which has been deposited a monolayer of a transition metal dichalcogenide (TMD) material[3-5]. Our setup combines ambient scanning probe microscopy (STM/AFM) with an inverted optical microscope, leading to wide-field imaging capabilities. More precisely, thanks to *real plane* imaging, we can determine from where on the sample the collected light is emitted, while through *Fourier plane* analysis the emission angle of the light is known, thus providing a powerful tool for the interpretation of the physical phenomena at play. In plasmonics we have used this technique to produce a directional nanosource of light[6], and a cylindrical vector beam[7]. In the area of exciton physics, thanks to this technique we have studied exciton diffusion, the orientation of the transition dipole moments, and the controlled quenching of luminescence [3-5].

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**Figure 1:** STM-induced generation of excitons in 2D semiconductors. a) Experiment: tunnelling current flows between the tungsten STM tip and the biased sample, which is a mechanically exfoliated MoSe<sub>2</sub> flake on ITO on glass. b) Monolayer and bilayer regions are identified with difficulty using transmission optical microscopy. c) Monolayer and bilayer regions are easily identified using laser-induced photoluminescence. d) STM luminescence is induced locally; the bright spot in the image at the tip location demonstrates that most of the created excitons recombine close to the excitation position. Note that others diffuse in the flake and recombine at a "hot spot".

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In this presentation we will provide an overview of the strategy of BeDimensional S.p.A. in the development of industrial-scale, reliable, inexpensive production processes of graphene and related two-dimensional materials (GRMs).<sup>[1-3]</sup> This is a key requirement for their widespread use in several application areas,<sup>[1-8]</sup> providing a balance between ease of fabrication and final product quality. In this context, we will show the effectiveness of the production of GRMs by wet-jet milling<sup>[3]</sup> and the route towards future Industrial scale up, maintaining the high-quality production ruled by the ISO standard.

Afterward, we will provide a brief overview on some key applications of the as-produced GRMs, with particular focus on the energy sector. In this context, the production of GRMs in liquid phase by wet-jet milling<sup>[3]</sup> represents a simple and cost-effective pathway towards the development of GRMs-based energy devices, presenting huge integration flexibility compared to other production methods. We will provide an insight into some application areas such as anticorrosion coatings and energy conversion and storage devices.<sup>[4-10]</sup>

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## Abstract

Disordered materials structured on scales ranging from tens of nanometers to micrometers scatter light, which is at first sight a disadvantage. However, scattering is also an effective way of modulating light-matter interaction. In particular, being able to control the level of disorder offers a powerful degree of freedom to tune the level of absorption [1], create structural coloration or transparency [2,3], to cite a few examples.

In fact, the possibility of engineering disorder, by creating materials halfway between amorphous systems and photonic crystals, is a subject of growing interest, as will be illustrated in the talk [4].

Another interesting feature is that strongly scattering non-linear materials (powders) can exhibit an efficient response, for example in terms of generation of harmonics. We will analyze the mechanism for preserving the efficiency in the case of second harmonic generation [5].

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# Structural and electronic properties of low-angle twisted bilayer graphene

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Around a specific magic twist angle, twisted bilayer graphene exhibits correlated insulating phases and superconductivity, thus boosting the new field of "twistronics" where strong electron-electron interactions play a dominant role on its electronic properties.

In this work, atomistic calculations using the Green's function techniques are developed to solve the tight-binding Hamiltonian for low-angle multilayer graphene, whose atomic structures have been previously optimized [1].

Below a threshold twist angle  $\theta_c \sim 1.1^\circ$ , the twisted bilayer graphene superlattice undergoes lattice reconstruction (Figure 1), leading to a periodic Moiré structure which exhibits a slight-corrugation that is found to strongly modify both its electronic structure [2] and its vibrational properties [1,3]. The electron-phonon coupling [4] is also found to be affected by the atomic structure reconstruction at the magic angle.

In twisted multilayer graphene [5], the dependence of the local electronic properties on the twist angle and on the stacking configuration are also investigated in order to fully taking into account atomic reconstruction effects.

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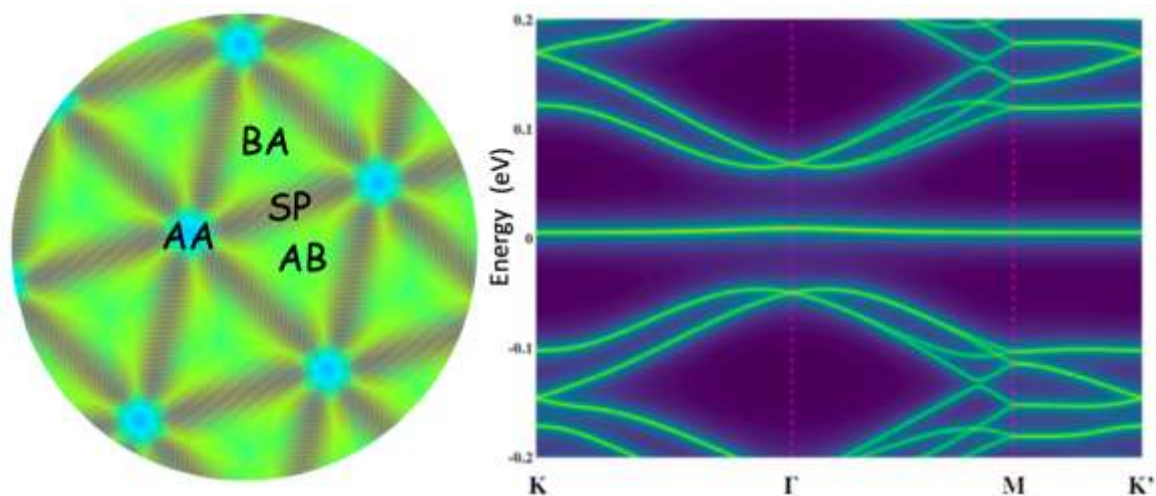
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## Figures

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**Figure 1:** Atomic reconstruction (left) and electronic properties (right) of twisted bilayer graphene at the  $1.1^\circ$  magic angle.

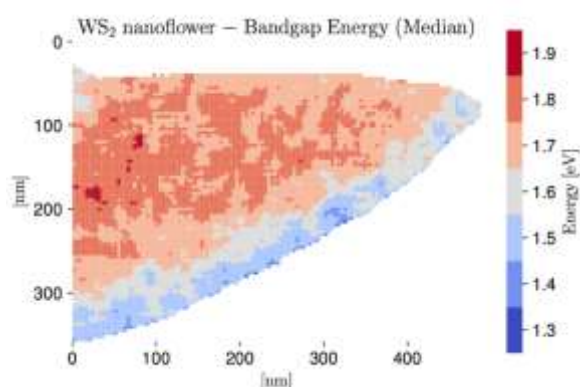
# Tunable van der Waals Materials as Building Blocks for Quantum Nanoptoelectronics

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The understanding of the properties of two-dimensional (2D) van der Waals (vdW) materials has posed significant challenges to researchers in the field of quantum nanoptoelectronics. These materials, with their unique nanoscale crystalline structure and resulting physical properties, hold immense potential as versatile building blocks for various applications, such as nanophotonics and quantum computing. However, effectively harnessing these properties requires in-depth characterization, made possible through recent advancements in fabrication methods and characterization techniques such as transmission electron microscopy combined with artificial intelligence algorithms. In this talk, I will present recent findings focused on unravelling the core properties of vdW materials for nanotechnology applications. One key aspect of my research is the development of a novel strategy for fabricating position-controlled Mo/MoS<sub>2</sub> core-shell nanopillars, enabling significant nonlinear optical processes driven by the MoS<sub>2</sub> shell [1]. This breakthrough allows for the precise localization of nonlinear signals, which is a critical requirement for nanophotonics. Additionally, I will delve into the quantification of the interplay between strain fields, thickness, and bandgap energy in twisted WS<sub>2</sub> nanostructures. By utilizing advanced techniques [3], we gain insights into how local strain influences the bandgap energy, providing valuable knowledge for designing functional devices such as quantum emitters. Lastly, I will explore local collective excitations in one-dimensional (1D) MoS<sub>2</sub>, showcasing how this configuration provides a new platform to tune excitonic/plasmonic resonances and bandgap energy, distinct from planar configurations. Through these investigations, we aim to enhance our understanding of the fundamental properties of vdW materials, opening new avenues for their application in nanotechnology.



**Figure 1:** Spatially resolved determination of the bandgap of WS<sub>2</sub> nanostructures.

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The controlled assembly of 2D materials in van der Waals heterostructures provides the opportunity to design unconventional materials with novel properties. Here I will illustrate this concept through two examples:

1) A twisted 2D heterostructure formed by two ferromagnetic monolayers of CrSBr rotated by an angle of  $90^\circ$  [1]. Magneto-transport measurements in this new material show a multistep spin switching with the opening of hysteresis, which is absent in the pristine bilayer case (angle of  $0^\circ$ ) [2], as a consequence of the competition between the inter-layer exchange interactions (which favor an antiparallel orientation of both spin layers) and the local spin anisotropy and an external magnetic field applied along the easy magnetic axis  $b$  (which tend to orient the spins along this easy axis).

2) A molecular/2D heterostructure obtained by interfacing a stimuli-responsive spin-crossover molecular system with CrSBr layers. We observe that in this hybrid heterostructure the properties of the 2D magnet changes when the molecular spin transition of this molecular component —induced by temperature or light— occurs. This is a consequence of the significant change generated in the volume of the spin crossover material (by ca. 10%) upon the spin transition [3, 4]. We will show that in this heterostructure the optical properties of CrSBr can be switched by varying the temperature, due to the strain concomitant to the spin transition.

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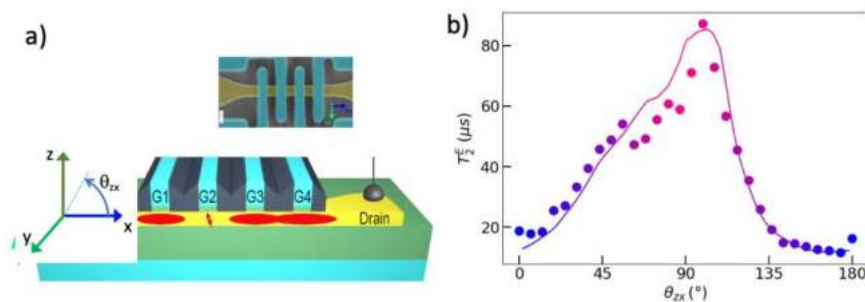
## Abstract

Hole spins in semiconductor quantum dots are emerging as a promising candidate for the realization of scalable spin-qubit architectures. Following an introduction to the field, I shall present recent advances in the development of hole-spin qubits based on foundry-compatible Si-MOS devices: the discovery of operational sweet spots maximizing hole-spin coherence<sup>1</sup> and the first demonstration of a strong-coupling between a hole-spin and a microwave photon in a superconducting resonator<sup>1</sup>. I shall conclude with an outlook on hole devices made from Ge/SiGe heterostructures, an emerging platform offering a unique combination of attractive properties<sup>3</sup>.

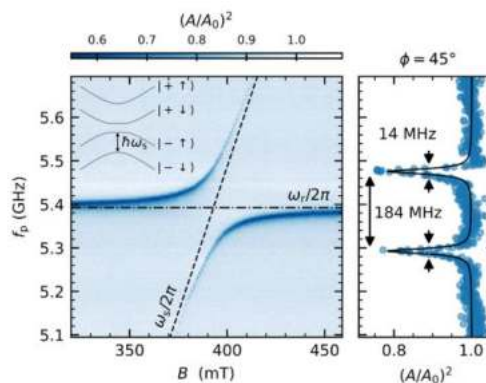
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## Figures



**Figure 1:** a) Four-gate Si-MOS device confining a single-hole spin qubit. b) Hahn-echo hole-spin coherence as a function of magnetic field angle. A sweet spot is obtained by aligning the field to the z axis.



**Figure 2:** Vacuum Rabi splitting indicating strong quantum mechanical coupling between a microwave photon in a superconducting coplanar resonator and a hole spin confined in a device similar to the one in Fig. 1a.

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## Abstract

We recently depicted the “Nano-immunity-by-design” where the characterization of 2D materials is not solely based on their physical-chemical parameters but also on their immuneprofiling. [1] The immune-profiling can be revealed on its complexity by unique, informative ways: high dimensional approaches. [2,3] We exploited high-dimensional approaches, such as single-cell mass cytometry and imaging mass cytometry on graphene and other novel two dimensional materials, such as transition metal carbides/carbonitrides (MXenes). [4-6] We revealed that the amino-functionalization of graphene oxide increased its immunocompatibility. [4] Moreover, we combined graphene with AgInS<sub>2</sub> nanocrystals, enabling its detection by single-cell mass cytometry on a large variety of primary immune cells. [5] Recently, we reported the immune modulation of specific MXenes, and their label-free detection by single-cell mass cytometry and other high dimensional approaches. [6-7] Together with our published works, I will present unpublished results on a wider variety of novel 2D materials, Mxenes, MoS<sub>2</sub>, WS<sub>2</sub>, and bismuthene. Our results conceptualize that chemical and immunological designs of 2D materials offer new strategies for their safe exploitation in biomedicine.

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# Engineering Tamm Plasmons Resonances in Nanoporous Anodic Alumina Photonic Crystals

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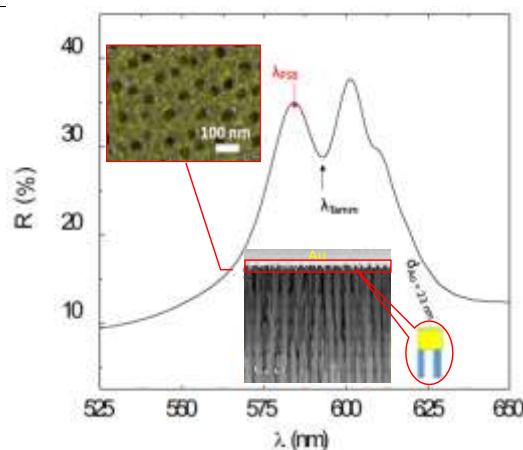
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Photonic structures based on nanoporous anodic alumina (NAA) can be fabricated using periodic anodization conditions. The optical properties of NAA structures rely intrinsically upon its nanoporous architecture, and on the geometry and distribution of its nanopores, which can be precisely engineered during the anodization process [1, 2, 3]. This work demonstrates how a sinusoidal or Gaussian pulse-like anodization approach can be used to generate nanoporous photonic crystals with highly tunable and controllable optical properties across the visible–NIR spectrum. By modifying the anodization conditions and parameters of the period function (Gaussian or sinusoidal) in the input profile, we can adjust the photonic stop bands (PSB) [4-5]. The outstanding set of properties of NAA photonic crystal (NAA-PC) demonstrate its versatility and potential for developing new photonic structures. The combination of a porous gold coating layer on top of a NAA-PCs creates a hybrid metal–dielectric structure with a narrow photonic stop band and Tamm plasmon resonances [6]. Tamm plasmon resonances are a class of surface plasmons in which incident light is confined at the interface of a hybrid structure consisting of a thin metallic coating layer and a dielectric mirror (i.e. PSB) [7]. Our analysis focuses on the design of Tamm plasmonic structures by adjusting the geometric characteristics of the plasmonic and photonic components of these hybrid optical structures. The results offer exciting new opportunities to integrate these unique photonic structures into photonic sensors and other platform materials for light-based technologies.

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## Figures



**Figure 1:** Reflection spectrum of Au-coated NAA-PC reveal an apparent dip within the PSB (Tamm resonance). Insert SEM images of the top view and cross section of Au-coated NAA.

# AlGaN/AlN Quantum Dots and Dots-in-a-Wire for UVC Emission

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## Abstract

The demand for germicidal UVC lamps has significantly risen during the COVID-19 pandemic, as they are widely used for disinfection purposes. Initially, low-pressure mercury lamps were the primary choice, but they are now being replaced by AlGaN LEDs due to their enhanced safety and sustainability benefits. However, AlGaN LEDs emitting at 270 nm still face challenges in terms of efficiency and cost per Watt compared to mercury lamps, primarily due to issues related to efficient electrical injection. Additionally, the 270 nm wavelength poses health risks such as carcinogenic and cataractogenic effects, which has spurred research into radiation sources with shorter penetration depth, particularly around 230 nm. To tackle this challenge, electron-pumped UVC lamps using AlGaN nanostructures as active material have emerged as a promising solution to provide high radiant power [1]. These lamps consist of a vacuum tube with a semiconductor dice onto which electrons are pumped using a cold cathode, typically made of carbon nanotubes or microfibers.

Our research focuses on investigating the growth and performance of dots-in-a-wire structures and AlGaN/AlN Stranski-Krastanov (SK) quantum dot (QD) superlattices using molecular beam epitaxy. The aim is to develop efficient anodes for electron-pumped UVC emitters [2]. In the case of nanowires, we adjust precisely the growth parameters to achieve uniform active superlattices spanning over 400 nm in length, matching the penetration depth of the electron beam. Regarding SK-QDs, we optimize the incorporation of Al, metal/N ratio, and deposition time to attain efficient emission in the 270 nm to 230 nm range [3]. Both types of nanostructures exhibit high internal quantum efficiencies, averaging around 50% at room temperature, attributed to the effective three-dimensional carrier confinement within the quantum dots. Moreover, these efficiencies remain stable as a function of the pumping power, even up to 500 kW/cm<sup>2</sup>.

In the UVC range, planar SK-QDs achieve a power conversion efficiency of 0.5-1% under electron beam pumping, without requiring any surface treatment to enhance light extraction. We will also discuss the impact of the QD geometry and the presence of extended defects on the broadening of the emission line.

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# DFT simulations of nanoconfined water between electrified gold surfaces using Non-Equilibrium Green's Functions

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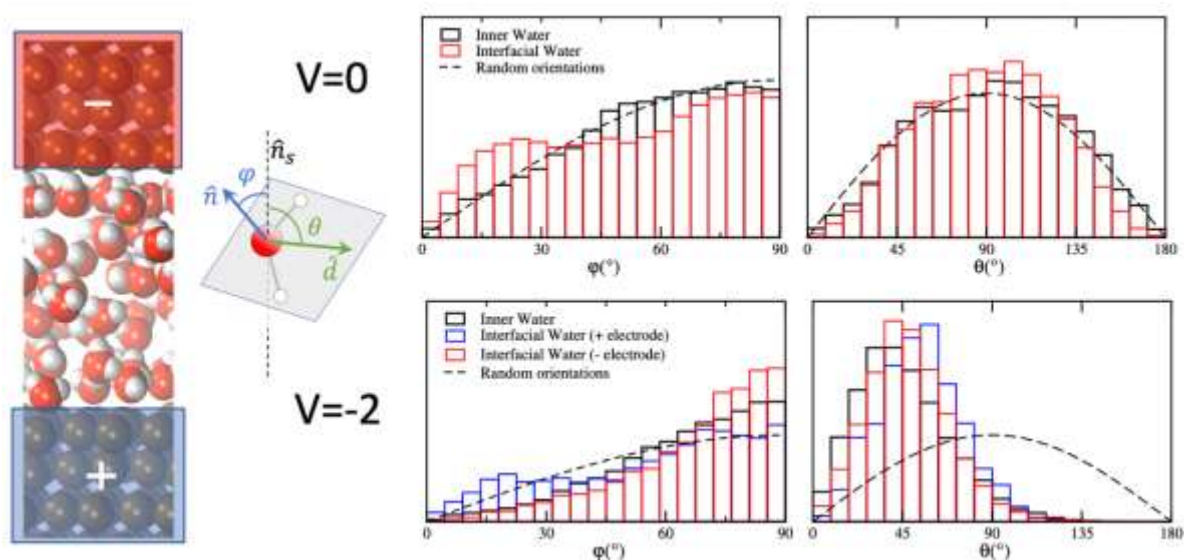
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Albeit water is the most common and best studied solvent, understanding its structure and properties at the surface of materials is still an open problem. Besides, important modifications of its structure and dynamics occur when the surfaces are electrified (as in electrochemical environments), and when the confinement space is nanometric. Density Functional Theory (DFT) simulations can deal with these issues, although imposing the external voltage in the simulation has proven difficult. Non-Equilibrium Greens functions (NEGF) techniques [1,2] as implemented in the SIESTA DFT package [3,4] are used here to address this problem, allowing first-principles molecular dynamics simulations of nanoconfined water in the presence of a finite voltage between the two confining surfaces. We will present proof of concept calculations of water between gold electrodes, showing the potential of our approach. Efforts for the massive parallelization of the simulations in large HPC infrastructure will be discussed, as well as the scaling of the CPU time with the system size. We also show how to increase the size of systems (in terms of number of atoms) and the simulation time which can be addressed by these simulations by using a quantum mechanics/molecular mechanics (QM/MM) approach coupled to the NEGF method, which will be the topic of the next oral presentation of this session, by Dr. Ernane Freitas.

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## Figures



**Figure 1:** Distribution of angles for the H<sub>2</sub>O molecules (both interfacial and inner) for water nanoconfined between Au electrodes, as shown on the representation on the left. The top graphs show the results when there is no voltage imposed between the electrodes, while ones in the bottom are for a voltage of V=2 Volt. We use two angles to characterize the molecular orientations, as shown in the second scheme on the left.

# Amino-acids functionalization of graphene oxide to achieve controlled adsorption of organic molecules in sensors and water filters

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New, dangerous emerging contaminants like pesticides, antibiotics, or fluorinated molecules have been detected in our water, defying current purification techniques and worsening the problems of water scarcity in Europe as well as in other continents.

Graphene oxide (GO) nanosheets are a robust, versatile and cheap nanotechnological platform that can be tailored to remove specific molecules. GO can be included at low cost and large scale in conventional water filters.

Here, we present a summary of diverse recent publications where we functionalize GO with different molecules, in particular amino-acids, to enhance its interaction with specific contaminants like perfluoroalkyl substances (PFAS), glyphosate or antibiotics.

The nano-composites are studied using absorption experiments, spectroscopic characterization and molecular simulations. The good interactions can also be used to sense such molecules using amperometric sensing.

Thanks to such tailored interaction, we demonstrate that these GO-based composites can remove the target contaminants with high efficiency.

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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 early detection of cancer, pathogens, emergency medicine as well as for pandemics like the COVID-19.

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# Marrying Spintronics with Topological Physics in low dimensional quantum materials

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## Abstract

We will present theoretical spin transport features in  $\text{MoTe}_2$  and  $\text{WTe}_2$ -based materials which are particularly interesting Quantum Materials [1]. By focusing on the monolayer limit, using DFT-derived tight-binding models, and using both efficient bulk and multi-terminal formalisms and techniques [2,3], I will first discuss the emergence of new forms of intrinsic spin Hall effect (SHE) that produce large and robust in-plane spin polarizations. Quantum transport calculations on realistic device geometries with disorder demonstrate large charge-to-spin interconversion efficiency with gate tunable spin Hall angle as large as  $\theta_{xy} \approx 80\%$ , and SHE figure of merit  $\lambda_s \theta_{xy} \sim 8\text{-}10$  nm, largely superior to any known SHE material [4]. We will show our theoretical prediction of an unconventional canted quantum spin Hall phase in the monolayer Td- $\text{WTe}_2$ , which exhibits hitherto unknown features in other topological materials [5]. The low symmetry of the structure induces a canted spin texture in the yz plane, dictating the spin polarization of topologically protected boundary states. Additionally, the spin Hall conductivity gets quantized ( $2e^2/h$ ) with a spin quantization axis parallel to the canting direction. We also predict the control of the canted QSHE by electric field [6]. We will finally discuss the emerging spin-orbit torque components at interface of van der Waals heterostructures [7]

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Acknowledgment. We acknowledge the European Union Seventh Framework Program under Grant Agreement No. 881603 Graphene Flagship, and Samsung Advanced Institute of Technology. We acknowledge "Proyecto PCI2021-122092-2" financiado por MCIN/AEI /10.13039/501100011033 y por la Unión Europea NextGenerationEU/PRTR"



# Liquid Phase Exfoliation of GRMs & Their Applications in Space and Beyond

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Two-dimensional (2D) materials flakes offer a range of exploitable electrical, thermal, and mechanical properties that make them attractive as performance enhancing additives, especially in energy storage, composites, inks, and coatings among others [1-4]. Thus far, the most promising method for affordable, industrial scale 2D flake production is liquid phase exfoliation (LPE). However, the state-of-the-art LPE techniques have challenges including but not limited to purification processes, large solvent volumes due to lower concentrations, unexfoliated material waste due to lower yield, lower flake sizes (typically hundreds of nanometres) and inadequate bulk characterization techniques, which lead to the widespread unreliability of 2D materials product specifications, increased costs, and limited process-property control [5].

Here I will talk about the production of 2D materials inks and suspensions via High Pressure Homogenization (HPH) based techniques [6] with a capability of producing flakes at higher concentrations (> 500 g/L) with no post-processing or purification and with semi-controllable properties. Through post solvent exchange 2D materials inks and suspensions can be produced nearly in any solvent. 2D materials such as graphene, hexagonal boron nitride and molybdenum disulphide are produced in water, ethanol, isopropanol, and for the first time in unconventional solvents such as hydrofluoroether (HFE) without fluorine functionalization. HFE is chosen due to its safety features in Space applications [7]. The use of these 2D materials inks suspended uniformly in HFE in microgravity conditions is demonstrated aboard sounding rockets (MASER14, and MASER15) [8, 9].

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# Out-of-equilibrium Raman spectroscopy of graphene and related 2D heterostructures

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At the Femtoscopy labs, we work at the development of time-resolved Raman microspectroscopies aiming at the enhancement of spectral and temporal resolutions, to address ultrafast dynamics in biomaterials and condensed matter. Here I will present recent results on the out of equilibrium interaction of lattice vibrations with charge carriers in 2D materials. Specifically, the way ultrafast photoexcitation transiently enhances the electron-phonon interaction in Gr by smearing the Dirac cone [1] and how it induces interlayer energy transfer in TMD-Gr heterostructures on the picosecond timescale [2], revealing an intermediate process with respect to the generation of a net charge underlying the slower electric signals detected in optoelectronic applications.

*This work has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement 881603*

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## References

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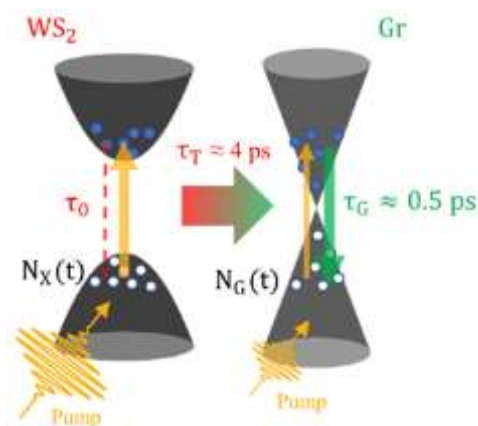
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## Figures

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**Figure 1:** Modeling energy transfer in a WS<sub>2</sub>-Gr heterostructure. The pump pulse can generate an exciton population in WS<sub>2</sub> or populate the electronic states of Gr with e-h pairs. These latter decay with a timescale  $\tau_G$ . In contrast, the excitons in bare WS<sub>2</sub> have a long lifetime  $\tau_0$ . Exciton decay is strongly accelerated in WS<sub>2</sub>-Gr due to energy transfer to Gr with a characteristic time  $\tau$

# Hexagonal and Amorphous Boron Nitride Thin Films

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Hexagonal boron nitride (hBN) is a promising two-dimensional (2D) material owing to its unique optical properties in the deep-UV region, mechanical robustness, thermal stability, and chemical inertness. hBN thin films have gained significant attention for various applications, including nanoelectronics, photonics, single photon emission, anti-corrosion, and membranes. Thus, wafer-scale growth of hBN films is crucial to enable their industrial-scale applications. In this regard, chemical vapor deposition (CVD) is a promising method for scalable high-quality films. To date, considerable efforts have been made to develop continuous hBN thin films with high crystallinity, from those with large grains to single-crystal ones, and to realize thickness control of hBN films by CVD. However, the growth of wafer-scale high crystalline hBN films with precise thickness control has not been reported yet. The hBN growth is significantly affected by substrate, in particular the type of metals, because the intrinsic solubilities of boron and nitrogen depend on the type of metal. In this talk, state-of-the-art strategies adopted for growing wafer-scale, highly crystalline hBN are summarized, followed by the proposed mechanisms of hBN growth on catalytic substrates [1]. Furthermore, various applications of the hBN thin films are demonstrated, including a dielectric layer, an encapsulation layer, a wrapping layer of gold nanoparticles for surface enhanced Raman scattering, a proton-exchange membrane, a template for growth of other 2D materials or nanomaterials, and a platform of fabricating in-plane heterostructures. In addition, amorphous BN (aBN) as a counterpart of crystalline hBN is introduced [2]. Detailed structural characterisation indicates that a-BN is  $sp^2$ -hybridised, with no measurable crystallinity, and mechanically robust, with excellent diffusion-barrier characteristics. The aBN thin film shows ultra-low dielectric constant ( $< 2.5$ ), indicating great potential for its applications in Cu interconnects of integrated circuits.

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# Broad-band single-photon sources based on carbon nano-emitters boosted by Cavity Quantum Electrodynamics

**Christophe Voisin**

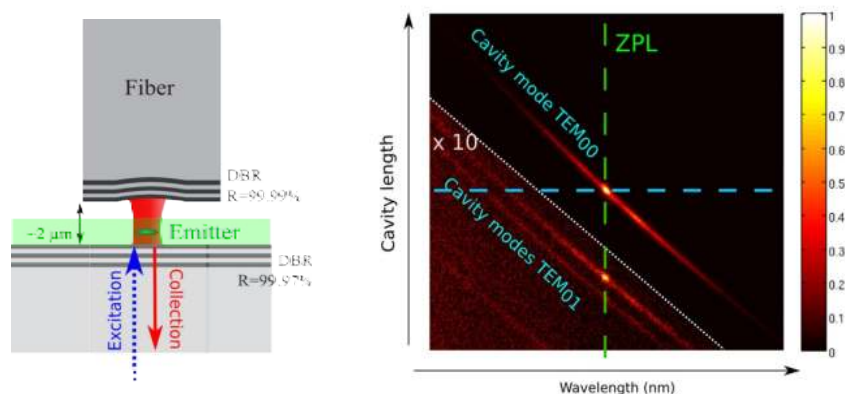
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Individual semi-conducting nano-structures are ideal candidates for solid-state sources of single-photons for future quantum secured telecommunications and other quantum technology applications. In particular carbon based nano-structures including single-wall carbon nanotubes, graphene quantum dots or ribbons are especially attractive since their emission wavelength is fully tunable through quantum confinement due to the gapless nature of their parent material – graphene. They are among the very few candidates for telecom band (1,3-1,5 $\mu$ m) single-photon operation, which are sought for long range telecommunication using the fiber network infra-structure. Nevertheless, these nano-emitters suffer from their inhomogeneity essentially because of the inevitable and poorly controlled interaction of the nano-structure with its local environment, resulting in wavelength and linewidth dispersion and possibly spectral diffusion. Hence, coupling of such nano-emitters to resonant photonic devices is challenging, especially for low temperature applications where the resonance conditions are more stringent. Here, we propose an original geometry where an open Fabry-Perot micro-cavity is engineered at the apex of an optical fiber, which makes it possible to deterministically match the cavity to the emitter position and wavelength by tuning the lateral and longitudinal position of the fiber. When resonance is met, we observe a strong enhancement of the emission properties through cavity quantum electrodynamics effects, including Purcell effect, resulting in the brightening of the emitter by more than an order of magnitude, a narrowing of its angular emission diagram and funneling of photons into the fiber mode. We further exploit the phonon side-bands to achieve a broad band tunable single-photon source.

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## Figures



**Figure 1:** (left) Sketch of an open-geometry Fiber Fabry Perot with high Q to tailor light-matter interaction with individual quantum emitters. (Right) Photoluminescence intensity as a function of cavity/emitter detuning showing a strong boost of emission at resonance.

# in-situ electron microscopy observation during CVD growth of Graphene and controlled stacking of graphene

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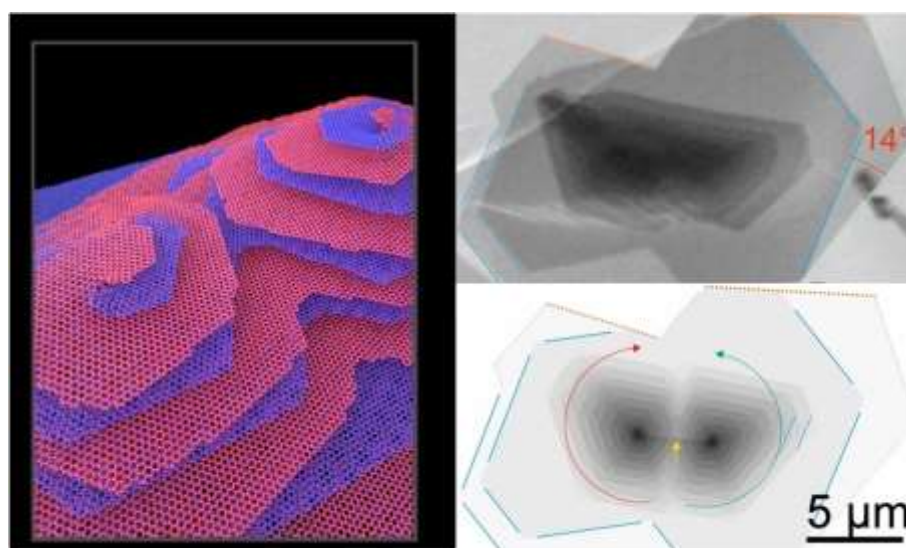
## Abstract

The properties of two-dimensional (2D) van der Waals (vdW) materials can be tuned through nanostructuring or by controlled stacking and modification of the electronic coupling between layers. Depending on the sacking angle, interlayer hybridization can induce exotic electronic states and transport phenomena. In my talk I will describe a viable mechanism for assisted self-assembly of twisted layer graphene. The process, which can be implemented in standard chemical vapour deposition (CVD) growth, is best described using the analogy to Origami and Kirigami of paper [1]. It involves controlled induction of wrinkle formation in single-layer graphene and subsequent wrinkle folding, tearing, and adlayer-growth. Inherent to the process is the formation of intertwined graphene spirals and conversion of the chiral angle of one-dimensional (1D) wrinkles into a 2D twist angle between layers in a three-dimensional (3D) superlattice. Seeded growth and substrate engineering can be used for tailored formation of layer stacks with pre-defined twist angles. The underlying principle is universal and can be extended to other foldable 2D materials and facilitates the production of miniaturized electronic components, including capacitors, resistors, inductors, and superconductors. The mechanistic insights were obtained through direct observation of CVD growth inside the chamber of a modified environmental scanning electron microscope [2-4].

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## Figures



**Figure 1:** Spirals of twisted layer graphene with pre-defined twist-angle. Comparison between simulation and in-situ observation during CVD growth.



# Towards the molecular-scale van der Waals capillaries and their applications in nanofluidics

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Isolated two-dimensional (2D) crystals can be assembled into designer structures layer-by-layer in a precisely chosen sequence – van der Waals (vdW) technology. Using this method, we have demonstrated the creation of two-dimensional capillaries by assembling 2D crystals. It can be viewed as if individual atomic planes were pulled out of a bulk crystal leaving an atomically thin void behind. This technology offers the smallest possible empty spaces that can vary from just a few angstroms in height up to many nanometers on demand. On this basis, we investigated mass transport process, including ions transport and the peculiar properties of water under such strong confinement. I will talk about our latest progress on capillary condensation at the atomic scale, and nanoconfinement effects study based on such capillaries.

## Anne-Laure Biance

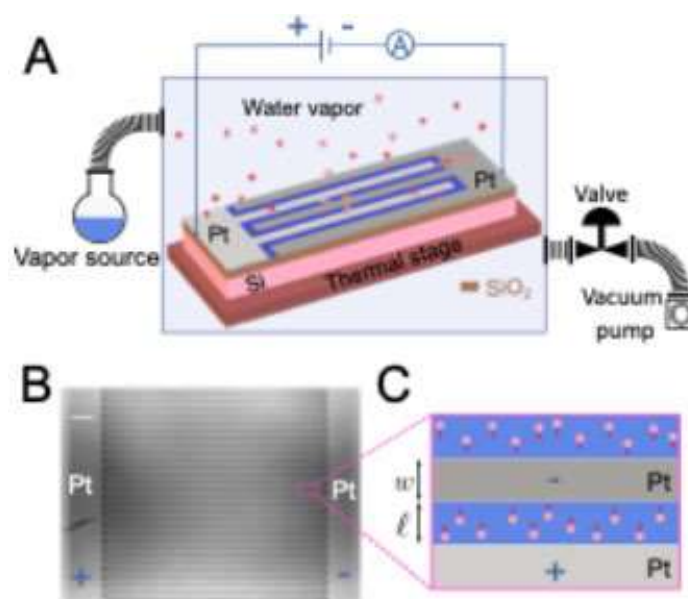
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Liquid and ionic transport through nanometric structures is central to many phenomena, ranging from cellular exchanges to water resource management or green energy conversion. While pushing down towards molecular scales progressively unveils novel transport behaviors, reaching ultimate confinement in controlled systems remains challenging and has often involved 2D Van der Waals materials. Here, we propose an alternative route, which circumvents demanding nanofabrication steps, partially releases material constraints, and offers continuously tunable molecular confinement. This soft-matter-inspired approach is based on the spontaneous formation of a molecularly thin liquid film onto fully wettable substrates in contact with the vapor phase of the liquid. Using silicon dioxide substrates, water films ranging from angstrom to nanometric thicknesses are formed in this manner, and ionic transport within the film can then be measured. Performing conductance measurements as a function of confinement in these ultimate regimes reveals a one-molecule thick layer of fully hindered transport nearby the silica, above which continuum, bulk-like approaches account for experimental results. Overall, this work paves the way for future investigations of molecular scale nanofluidics and provides novel insights into ionic transport nearby high surface energy materials such as natural rocks and clays, building concretes, or nanoscale silica membranes used for separation and filtering.

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## Figures



**Figure 1:** Scheme of the experimental setup and picture of the substrate.

# Unveiling the Potential of Functionalized 2D Janus MXenes

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Janus MXenes are a class of two-dimensional materials (2D) that exhibit unique structural and chemical properties. They consist of atomically thin layers with a Janus-like structure, meaning that one side of the layer has different chemical elements or functional groups compared to the other side. This structural asymmetry grants them diverse applications, such as energy storage, catalysis, sensing, and electronic devices, making them highly promising in the field of nanotechnology.

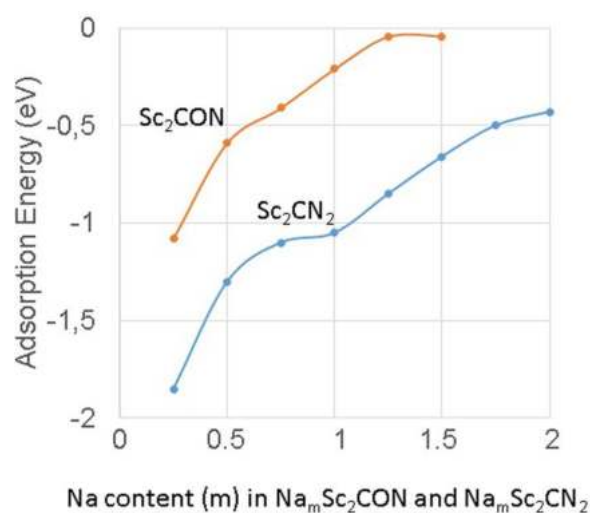
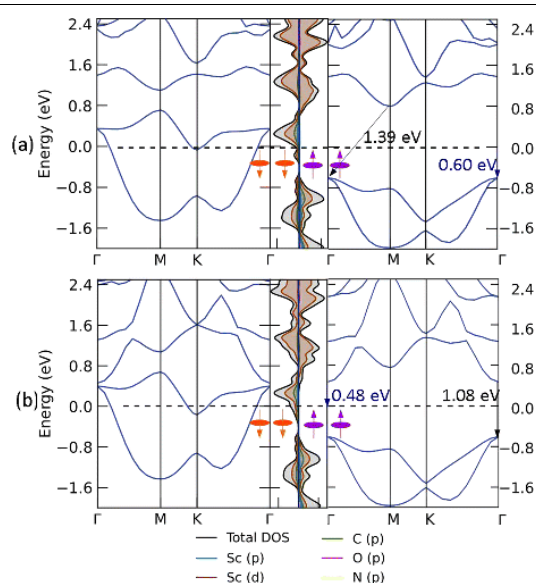
I will show how the Sc<sub>2</sub>C MXene family seems to be particularly suitable to maximize the performance of nanoelectronic devices in, at least, two different aspects. Through Density Functional Theory calculations, we have explored the mechanical, electronic and magnetic properties of 36 functionalized Sc<sub>2</sub>CXT (X = O, F, OH; T = C, N, S) MXenes, revealing interesting aspects such as ferro or anti-ferromagnetism and half-metallicity, depending on the functionalization. On the other hand, the functionalization of Sc<sub>2</sub>CX with N<sub>2</sub>, ON, or O<sub>2</sub> groups shows competitive performance in terms of Na adsorption, diffusion, and capacity as anodes for Na-ion batteries (NIBs).

These findings highlight the remarkable potential of Sc<sub>2</sub>CX MXenes for various applications in 2D nano-, spin-, and energy-related fields.

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## Figures



**Figure 1:** Band and spin-resolved density of states structures of (a) Sc<sub>2</sub>CFC and (b) Sc<sub>2</sub>COHC.

**Figure 2:** Variation in the adsorption energy with increasing Na content on Sc<sub>2</sub>CN<sub>2</sub> and Sc<sub>2</sub>CON.

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Securing communications over long distances requires bright single photon sources emitting in the telecom band in a well-defined spatial and polarization mode.

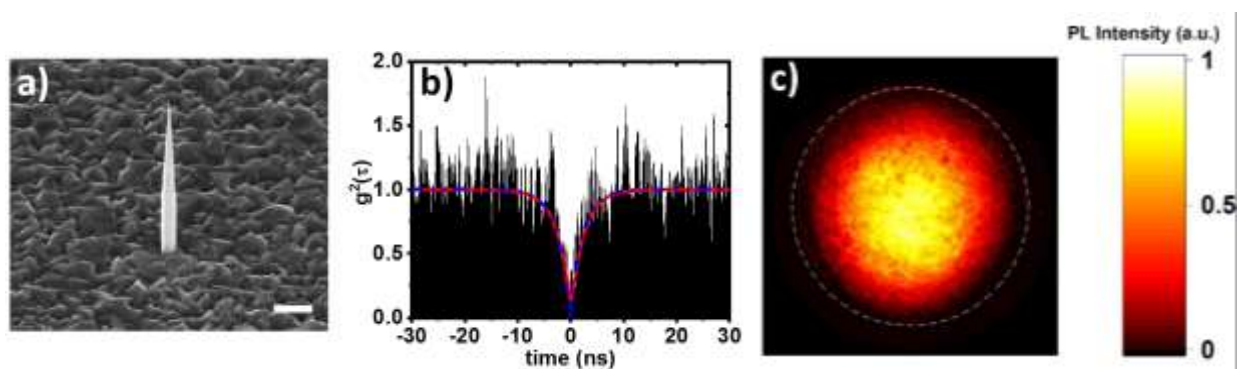
First, we report our efforts to obtain single photon emission and a Gaussian far-field radiation pattern in the telecom O-band from single quantum dot-nanowires (QD-NWs) monolithically grown on silicon. The InAs/InP QD-NWs were grown on silicon (111) substrates by Vapor-Liquid-Solid assisted solid-source Molecular Beam Epitaxy using In-Au droplets as a catalyst in-situ deposited at 500°C [1]. Low QD-NW density was obtained by a careful control of the In/Au catalyst flux ratio to achieve density  $<1$  NW/ $\mu\text{m}^2$  [2]. The growth conditions have been tuned (Fig 1.a) to optimize the source brightness and reduce the far-field divergence. The control of the nanowire geometry allows us to demonstrate a Gaussian far field emission profile with an emission angle  $\theta \approx 30^\circ$  (Fig 1.c) from a single QD at room temperature in the telecom O-band and the observation of single photon emission with  $g^2(0) = 0.05$  (Fig 1.b) at cryogenic temperature [3].

Secondly, we have optimized the growth procedure to achieve InAs/InP QD-NWs with an elongated top-view cross-section. Polarization-resolved photoluminescence measurements have revealed a significant influence of the asymmetric shaped NWs on the InAs QD emission polarization with the photons being mainly polarized parallel to the NW long cross section axis [4]. A degree of linear polarization (DLP) up to 91% is obtained, being at the state of the art for the reported DLP values from QD-NWs.

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## Figures



**Figure 1:** a) Single InAs/InP QD-NW with a needle-like geometry. b) Second order correlation measurement of a single QD emitting at 1328 nm at cryogenic temperature. c) Far-field emission profile of a single QD-NW at room temperature [3].

# Ion implantation and irradiation as a tool to engineer 2D transition metal carbides (MXenes)

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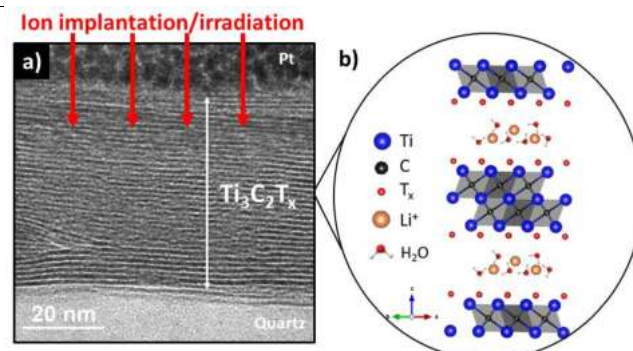
Ion implantation is among the most versatile approaches to modify, in a controlled way and with possible access to out-of-equilibrium states, the structure and physical properties of solids. This technique is widely used in the semiconductor industry for doping or for engineering electronic devices. More recently, it has been extended to 2D materials, such as graphene, MoS<sub>2</sub> or WSe<sub>2</sub> [1]. Among these materials, MXenes is an expanding family of layered transition metal carbides and nitrides, with very promising properties for a large number of applications, including energy storage, transparent electronics, sensors, or electromagnetic interference shielding [2].

In this work, and focusing first on the benchmark Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene (T<sub>x</sub>=F, Cl, or O(H) and x≈2) elaborated as ~100 nm thick spin-coated films (Fig. 1), we show that ion implantation/irradiation offers high flexibility for the design of MXenes, allowing to shape their properties on demand which is a unique asset for applications. By investigating a wide damage range, and using XRD and Electron Energy Loss Spectroscopy in a Transmission Electron Microscope to investigate structural changes and damage together with electronic structure modifications, we demonstrate that ion irradiation can be used to tune the MXene architecture at different levels: modification of the interlayer spacing, tuning of the functionalization groups and control of the structural defects in the MXene sheets. Further, we show that ion implantation can be used to incorporate foreign species (Mn) in Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> sheets up to several percent [3]. Moreover, focusing on the V<sub>2</sub>CT<sub>z</sub> MXene, and using a bottom up approach, we show that the defects introduced by irradiation of its MAX phase precursor V<sub>2</sub>AlC, facilitate the chemical etching and drastically reduce the etching time to synthesize macroscopic nanolayered V<sub>2</sub>CT<sub>x</sub> MXenes [4].

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## Figure



**Figure 1:** (a) HR-TEM micrograph of a Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> thin film (b) Schematic representation of a multilayer stack.



# Preparation of F-diamane-like nanosheets via exfoliation

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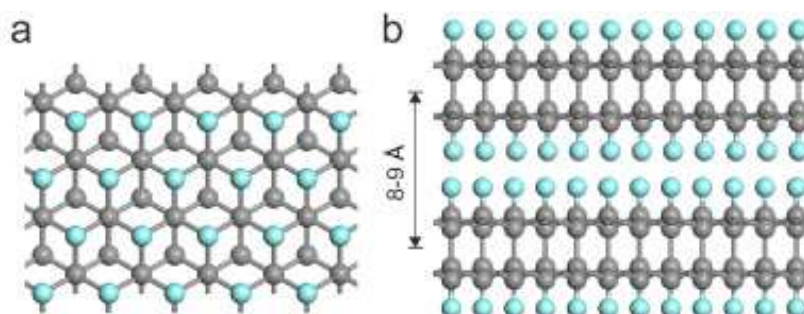
Atomically thin diamond ("diamane") has recently emerged as a new two-dimensional carbon allotrope. Theoretical studies first predicted the conversion of AB-stacked few-layer graphene into diamane films through sufficient formation of carbon-fluorine (C–F) or carbon-hydrogen (C–H) bonds on the two free surfaces. In the present work, poly(dicarbon monofluoride)  $(C_2F)_n$  which is essentially made of stacked layers of "F-diamane" (Fig. 1) has been synthesized and exfoliated in a variety of solvents to yield well-dispersed ultrathin sheets. Microscopic and spectroscopic analyses revealed that the exfoliated nanosheets retained the "F-diamane"-like structure. The experimental results are also supported by density functional theory (DFT) calculations.

To fully exploit the properties of diamane, further advances in the synthesis methods for its large-scale production are required. So, we propose another route for the efficient and high-yield production of fluorinated diamane (F-diamane)-like nanosheets. This is achieved by direct fluorination of expandable graphite or thermally expanded graphite with molecular fluorine to form stage-2 graphite fluoride  $(C_2F)_n$  made of stacked layers of F-diamane. Subsequently, mild sonication is implemented to exfoliate the layers into F-diamane-like nanosheets of hundreds of nanometers to a few micrometers in lateral size, with a thickness of mostly < 10 nm.

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## Figures



**Figure 1:** The proposed (a) top-view and (b) side-view crystal structure of  $(C_2F)_n$  type graphite fluoride.

# Optical nanotweezers for single cell deformability measurements

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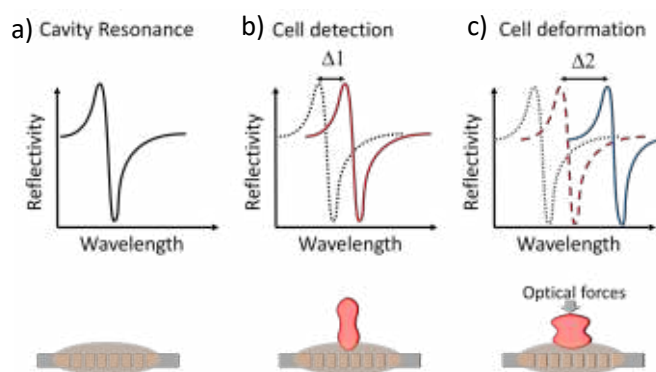
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It is now well recognized that mechanical phenotype of biological cells are related to their physio-pathological state. For example, variation of Red Blood Cells (RBCs) deformability is associated with malaria [1] and increase deformability of metastatic cancer cells [2] have been observed. Hence, a better understanding of cell deformability may imply enormous developments in disease diagnostics, therapeutics and drug screening assays. For this purpose, we propose to implement a new bio-photonic approach applied to the characterization of cell deformability. Its originality relies on the all-optical reading of cell deformability using the resonant mode of photonic crystal (PhC) micro-cavities [3]. It has been demonstrated that the presence of an object on top of a PhC micro-cavity induces a local change of refractive index associated with a spectral shift of the resonance spectrum [4]. We propose to extend this concept to the measurement of cell deformability in order to get the mechanical signature of RBCs. In this work, we demonstrate the proof of principle of our approach by the detection of RBCs deformability using a PhC micro-cavity. Moreover, we have shown for the first time that the spectral response changes of the PhC could allow discriminating between healthy and artificially mechanically impaired RBCs. This work has been funded by the French National Research Agency (ANR) under the project CELLDance (ANR-21-CE09-0011).

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## Figures



**Figure 1:** Schematic view of the optical response of a) an empty PhC cavity b) a cavity in presence of a RBC and c) a cavity in presence of a RBC deformed by applied optical forces.

# Understanding thermal transport in 2D Transition Metal Dichalcogenides

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Layered Transition Metal Dichalcogenides (TMDs) have garnered considerable attention in recent years due to their remarkable characteristics, which differ from those of 3D-bonded material. Gaining insight into their thermal properties is of utmost importance for various applications, such as electronics and thermoelectrics [1]. In this study, we present a theoretical investigation focused on the heat transport properties of WS<sub>2</sub>, WSe<sub>2</sub>, MoS<sub>2</sub>, and MoSe<sub>2</sub>, in monolayer and bulk configurations. By solving the Boltzmann Transport Equation for phonons and utilizing inputs derived from first principles calculations, we determine the thermal conductivity of those TMDs. To obtain the phonon structure and phonon-phonon interactions, we employ the SIESTA method [2,3], based on Density Functional Theory, and utilize the Temperature Dependent Effective Potential package for lattice dynamics calculations at finite temperatures [4]. We compare the obtained thermal properties with experimental data, demonstrating the reliability and efficiency of our computational approach [5]. By comparing the outcomes for different TMDs, we arrive at a comprehensive understanding of heat transport in 2D-bonded semiconductors, offering valuable insights for future technological advancements.

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# Diameter-dependent stacking of dye molecules inside single-wall carbon nanotubes

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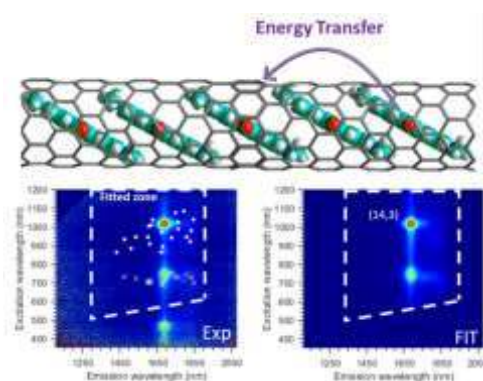
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Thanks to the extensive variability of chiral structures of SWCNT, a large variety of electronic and optical properties can be accessed, making them extremely promising for diverse applications such as solar energy harvesting and high-performance (opto-)electronic devices. Besides these very peculiar intrinsic properties, SWCNTs also exhibit a hollow core, which can be filled with dyes giving rise to new one-dimensional hybrids that merge the properties of the nanotube with those of the dyes<sup>1-2</sup>. In this work<sup>3</sup> we report for the first time the combination of extensive chirality-sorting<sup>4</sup> and dye filling, leading to the isolation of nearly single chirality squaraine-filled SWCNTs as shown in the photoluminescence-excitation (PLE) map presented in Figure 1. For each dye@SWCNT chirality combination, we observe a different absorption wavelength of the confined dyes, originating from the different dye stacking driven by the diameter of the surrounding SWCNT. This diameter-dependent dye absorption followed by an energy transfer, is experimentally determined through the measurement and detailed fitting of fluorescence-excitation maps of different chirality-sorted dye-filled SWCNT samples. We, therefore, demonstrate that the diameter of the SWCNT is a lever to tune optical properties of the hybrids, paving the way for future applications in optoelectronics. Moreover, comparison with molecular models provides access to the possible different stacking configurations of the dyes inside the hollow space of SWCNTs with different diameters.

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## Figures



**Figure 1:** (top) Schematic view of the new hybrids (bottom) Example of a PLE map and the corresponding fit for one of the 15 samples. (left) experimental PLE maps, the white dots represent all the chiralities that have been fitted and the crosses represent the energy transfer. (right) Fitted PLE map, the most abundant chirality is labelled.

# Enabling practical two-dimensional spintronic circuits

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## Abstract

The rise of atomically thin two-dimensional (2D) materials brought new excitement in nanotechnology, particularly the field of spintronics got a fresh boost with 2D materials presenting diverse spin-linked abilities. In terms of exploring spin-polarized electrons or spin currents, graphene stands out as a material where spin currents can travel over tens of microns at room temperature, up to hundreds of times longer than in typical metals. However, charge transfer and spin-orbit coupling at the contact interfaces cause spin relaxation, lowering the spin diffusion length and spin lifetime in graphene. In addition, a key challenge towards practical circuits is their large-scale realization using scalable chemical vapor-deposited graphene, determining eventual high current densities that graphene can sustain, and achieving a cleaner, stable, and more resilient system that can serve as a base platform for 2D material spintronic applications. In this talk, I will explain our efforts in this direction, in particular, device engineering techniques to minimize the contact-induced spin relaxation that led us to the observation of the highest spin parameters with the longest spin communication of 45  $\mu\text{m}$  at room temperature[1], high current carrying capacity[2], and other unique effects of widely used metal-oxides on charge transfer in graphene[3] and how such oxide layers can be used for surface passivation with enhanced performance. Further, I will discuss how these results augment our recent developments of flexible ferromagnetic nanowires [4] and flexible graphene spin devices with high diffusive spin transport [5], providing new opportunities for flexible-integrated large-scale 2D spintronic circuits.

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# Colloidal synthesis of transition metal dichalcogenides – from nano-monolayers to heterostructures.

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The past few years a tremendous attention has been given to 2D materials and in particular to Transition Metal Dichalcogenide (TMDC) compounds ( $\text{MoS}_2$ ,  $\text{WSe}_2$ ...) driven by their remarkable electronic and optical properties. TMDCs offer a compelling combination of the transport properties of graphene with the optical properties of semiconductors. As compared to other semiconductor quantum wells, pristine single layers of TMDCs -which can be as wide as several micrometers- can be obtained by a simple mechanical exfoliation from the bulk material. As a result, TMDCs have been explored as optoelectronic materials for a broad range of applications, such as photo-detection, lighting and lasing, single photon emission, nanosensing, memories...

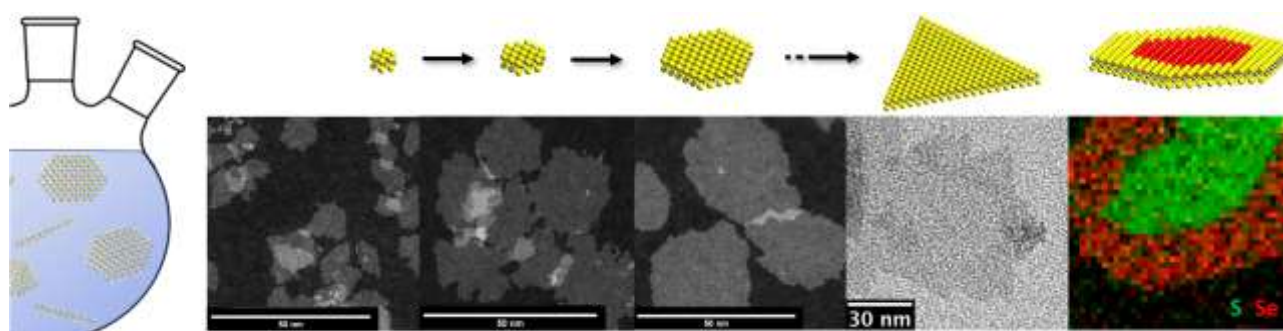
Colloidal synthesis (CS) can offer multiple advantages over other growth methods to produce 2D nanomaterials, the most obvious one being the quantity of free-standing monolayers that can be produced at once (square meters of monolayers for a typical CS). Furthermore, this method could produce numerous nanostructure types from alloyed or doped monolayers, to in-plane and out-of-plane heterostructures. Finally, CS can give access to a size range rarely explored -forming nano-monolayers (NMLs)- where lateral confinement arises, thus becoming an additional tool to tune the optoelectronic properties of colloidal monolayers.

Based on our previous work on colloidal  $\text{WS}_2$  monolayers synthesis,[1] we are currently developing a new strategy to synthesize colloidal TMDC NMLs with a control over their size, size dispersion, composition, crystallinity and shape. The approach consists in addressing these problems separately. A first synthetic scheme has been developed using a nucleation/growth mechanism, allowing the fabrication of monodisperse small (few nm) colloidal NMLs.[2] The size can then be tuned by continuous injection of precursors during growth. The shape can be modified using a second growth step in a different chemical environment. Finally, the crystal structure can be changed post synthetically through annealing either in solution or on a substrate. This strategy also allows for composition modifications, and has been successfully applied to produce alloyed  $\text{WSe}_{2x}\text{S}_{2-2x}$  NMLs.[3]

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## Figures



**Figure 1:** synthetic scheme and associated HR-STEM pictures obtained for  $\text{WS}_2$ -based NMLs.

# Controlling thermal transport in 2D materials and their heterostructures

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In-plane, phonon thermal conductivity ( $\kappa$ ) in 2D materials spans over wide range, from very high in graphene (2000 W/mK) and hBN (700-450 W/mK) to below 100 W/mK in transition metal dichalcogenides (TMDs). For instance, molybdenum disulfide ( $\text{MoS}_2$ ), one of the most representative TMD exhibits the thickness dependent  $\kappa$  which increases from  $\sim 25$  W/mK to  $\sim 100$  W/mK with the thickness increasing from single layer to bulk. Therefore, 2D materials offer an interesting platform to study thermal transport in the nanoscale. The current understanding of thermal transport by phonons will be reviewed considering a few exemplary cases.

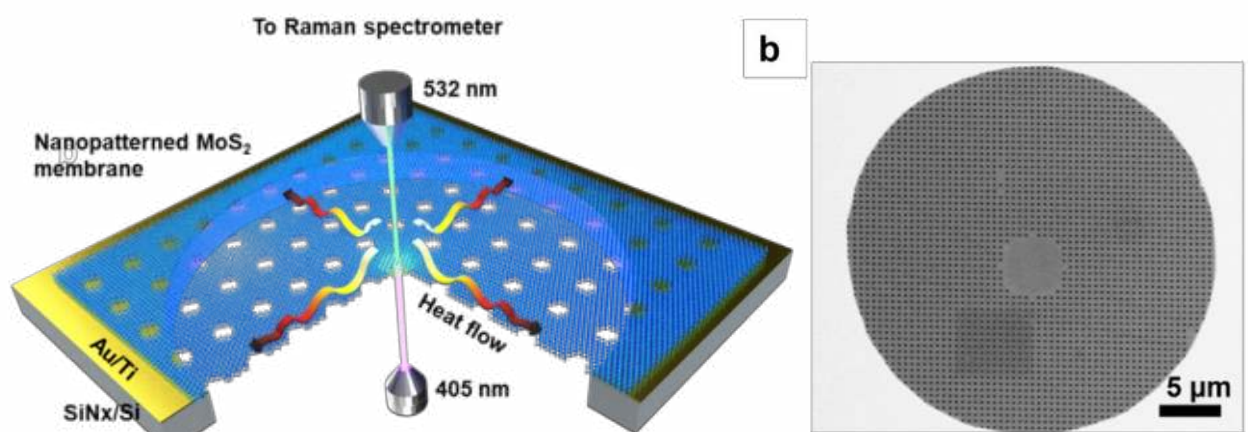
I will discuss the case of few-layer, single crystal  $\text{MoS}_2$  and  $\text{SnSe}_2$  membranes in which the sample preparation is crucial to eliminate effects of imperfections and contamination focusing on the thickness dependence of  $\kappa$  [1, 2]. Two-laser Raman scattering thermometry (2LRT) was used for determining  $\kappa$ , combined with real time measurements of the absorbed laser power.

In the second part of the talk, I will discuss various strategies on tuning the thermal transport in 2D materials, such as creation of heterostructures using the example of  $\text{MoS}_2/\text{hBN}$  [1]. Furthermore, I will explain the effects of phonon scattering on the defects, such as the effect of nanopatterning in 2D materials [3].

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## Figures



**Figure 1:** (a) Schematics of the thermal conductivity measurement set-up (2-laser Raman thermometry) (b) SEM image of the nanopatterned  $\text{MoS}_2$  membrane [3]

# Thermal contact resistance measurements on metal-semiconductor structures by scanning thermal microscopy and $3\omega$ method

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Reduced size of current electronic devices involves boundaries that play a crucial role in heat transfer inside such components. In particular, metal-semiconductor interfaces are widely present. Understanding the mechanisms of thermal transport undergone by energy carriers at the junction regions requires the determination of both thermal conductivities of materials in contact and thermal contact resistance between them [1].

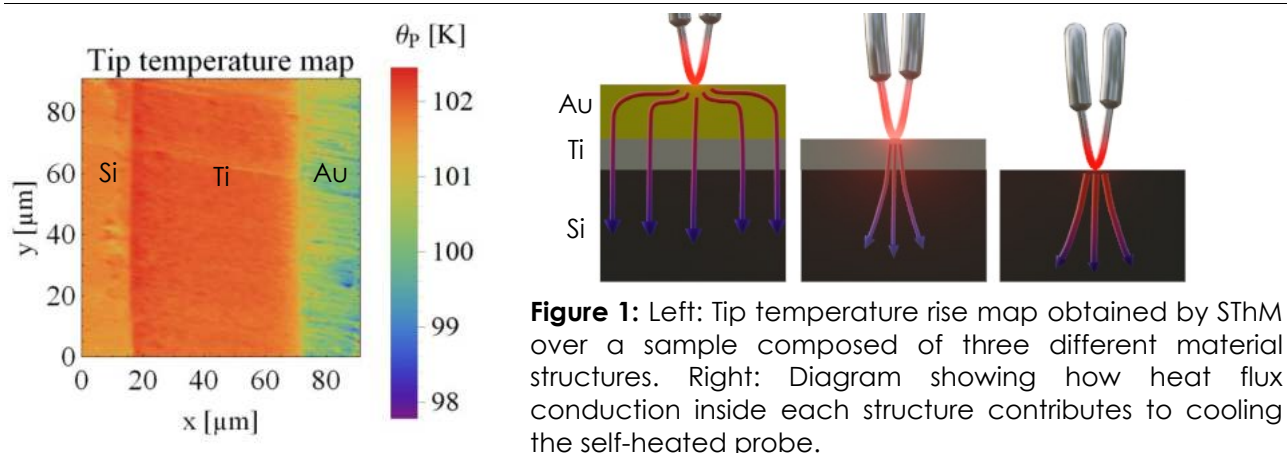
We study experimentally metal-semiconductor structures by means of scanning thermal microscopy (S<sub>Th</sub>M) and  $3\omega$  method. S<sub>Th</sub>M is based on a self-heated metallic thermal sensor that is part of a movable AFM tip and enters in contact with the sample surface [2]. This technique allows to perform thermal imaging with a spatial resolution down to the nanometric scale, at sample temperature close to ambient. The  $3\omega$  method is based on the deposition of a metallic resistive wire on top of the sample and whose electrical resistance is measured as a function of an alternating power input [3]. In contrast to S<sub>Th</sub>M, which is hardly able to be performed as a function of sample temperature, the  $3\omega$  method can provide thermal data over a wide temperature range through the use of a cryogenic system, while it does not allow for spatially-localised measurements.

Figure 1 shows an example of S<sub>Th</sub>M image over a sample containing a silicon substrate on top of which two metallic nanolayers were successively deposited. In order to estimate the thermal boundary resistances involved in the sample, the obtained data are compared to FEM simulations. In addition, in order to better know the semiconductor thermal properties, we perform thermal conductivity measurements of thin layers deposited over silicon substrates by means of the  $3\omega$  method. In this case, a sensitivity analysis is detailed and the experimental results are compared to a semi-analytical model [4].

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## Figures



**Acknowledgements:** We acknowledge the support of ANR project EFICACE (ANR-20-CE09-0024).

# Quantum transport properties of gas molecules adsorbed on Fe doped armchair graphene nanoribbons

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Graphene, when doped with transition metals, is considered, both experimentally and theoretically, as a good candidate for the detection of gas molecules as CO, CO<sub>2</sub>, NO or NO<sub>2</sub> [1]. This opens new perspectives for gas sensor set-ups considering that devices based on 2 dimensional graphene are more sensitive to detect molecules than solid-state gas sensors. The state of the arts on gas adsorption on Fe doped armchair graphene [2] nanoribbons (Fe-AGNR) is still in its starting phase and thorough investigations of the mechanism of the adsorption on graphene need to be done.

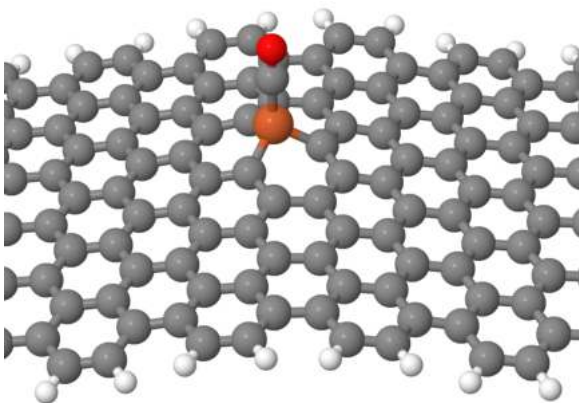
In the present work, the electronic and transport properties of molecules adsorbed on Fe-AGNR (see Fig. 1) are scrutinized using *ab-initio* calculations [3]. We observe that the adsorption of gas molecules on Fe-AGNR changes significantly the electronic properties of both the valence and the conduction band (see Fig.2). Besides, The adsorbed molecules change the local electron density of states of the graphene nanoribbons, modifying thus the conductivity, being one of the main output quantity of the gas sensors. We also observe that the adsorbed molecules induce specific impurity bands which play a role in the transport properties.

Finally, considering the observed variations of electrical conductance induced by the molecules, we propose several strategies to set-up gas sensors for CO, CO<sub>2</sub>, NO and NO<sub>2</sub> molecules. These strategies are either based on the measurement of the conductance in the valence or the conduction band (using either p or n-doped Fe-AGNR) or to the spin polarization induced by the NO and NO<sub>2</sub> molecules.

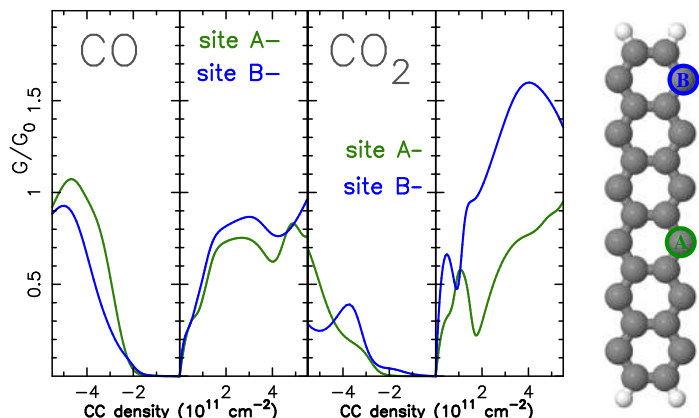
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## Figures



**Figure 1:** Armchair graphene nanoribbon with a CO molecule adsorbed on top of a Fe atom in substitution



**Figure 2:** Electrical conductance as function of the charge carrier density



# SINGLE CRYSTAL MONOLAYER GRAPHENE AND HEXAGONAL BORON NITRIDE BY INDUCTIVE HEATING CVD

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The reduced dimensionality of 2D materials induces all surface accessible defects which play a critical role in materials' properties and device performance. One common defect in 2D materials is the grain boundaries (GBs) consisting of a series of pentagon, heptagon, and hexagon rings formed at the stitching region between two domains with different orientations (Fig 1a). To control the orientation of these domains, monocrystalline Cu(111) is used for graphene growth due to the absence of GB and the small mismatch (Fig 1b). In our approach, centimeter-scale single crystal Cu(111) is produced by applying a controlled thermal gradient to a commercial polycrystalline copper substrate using inductive heating. A 25  $\mu\text{m}$  thick copper foil was transformed into a single-crystal copper foil by inductively heating to  $\sim 1030^\circ\text{C}$ . Unlike Roll to Roll (R2R) methods where the copper is continuously passed in a hot furnace region [1], in our approach, the induction coils are moved at the speed of 1 cm/min (Fig 1c). An edge of the Cu sheet was tapered into a tip shape, which ensured the nucleation of a single Cu(111) grain at the tip. The sliding of the coils across the copper foil caused the movement of the grain boundaries between the single crystal and polycrystalline regions and the grain of single crystal Cu(111) reached the width of the copper sheet. X-ray diffraction of the copper obtained showed the presence of the (111) preferential direction (Fig 1d). 3D calculation demonstrated the driving force of the thermal gradient for the Cu(111) formation (Fig 1e). Consequently, graphene and hexagonal borane nitride were synthesized using inductive heating. From the optical microscopy image (Fig 1f), we can see that all the hexagonal graphene domains are oriented in the same direction and the Raman spectrum shows the total absence of defects (inset f). By applying the same concept to CVD h-BN growth on Cu(111) from ammonia borane, triangular and oriented domains of hexagonal boron nitride are obtained (Fig 1g). During the growth, the adjacent flakes coalesce or compete for adatoms during the growth following the point-to-edge model [2].

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## Figures

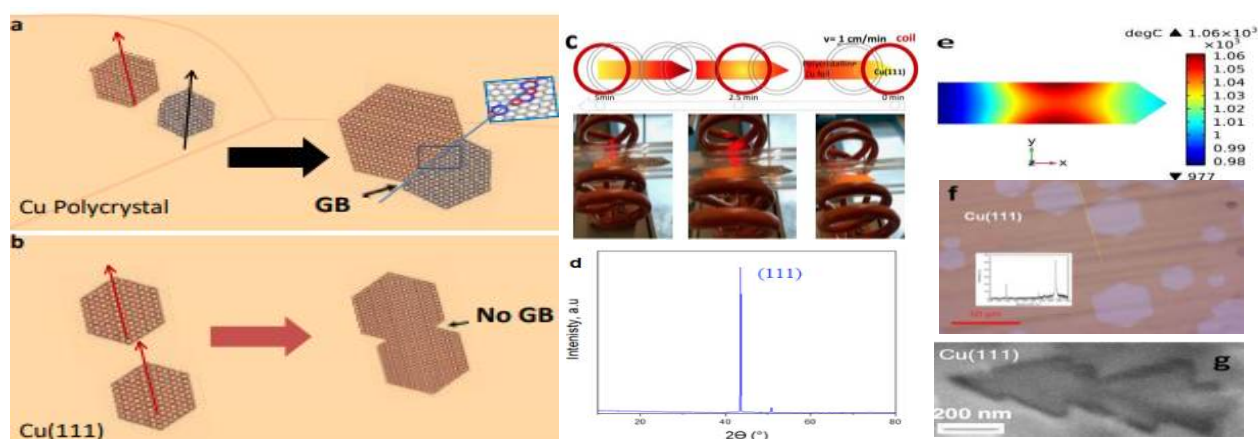


Figure 1: **a,b** Effect of Cu crystallinity on Gr grain boundaries (GB); **c** Inductive heating synthesis of Cu(111); **d** XRD spectra of Cu(111); **e** Comsol 3D calculation of thermal gradient for Cu(111); **f** Optical image of oriented graphene domains on Cu(111); Inset **f** Graphene Raman spectra obtained with 473 nm laser excitation on copper foil; **g** Oriented triangular hBN domains.



# Atomic Structure and Electronic Trap States in Individual CdSe Colloidal Nanoplatelets by Low-Temperature Scanning Tunneling Microscopy

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Among the colloidal nanostructures available, nanoplatelets (NPL) are the most impressive material since they offer a compelling combination of the flatness 2D semiconductors to the richness of the versatile world of colloidal nanostructures [1]. The growth along the confinement dimension, ie the thickness, of all the NPLs in the solution can be controlled at the atomic layer scale. This tour de force in the chemical growth is evidenced by a nearly kT-limited emission linewidth in ensemble measurements at room temperature. By contrast with standard 2D semiconductor materials (MoS<sub>2</sub>, WTe<sub>2</sub>...), the properties of NPLs can be further tailored by selectively changing their thickness or the in-plane dimensions. In addition, NPL are also used as seed material to form heteronanostructures that have striking optical properties.

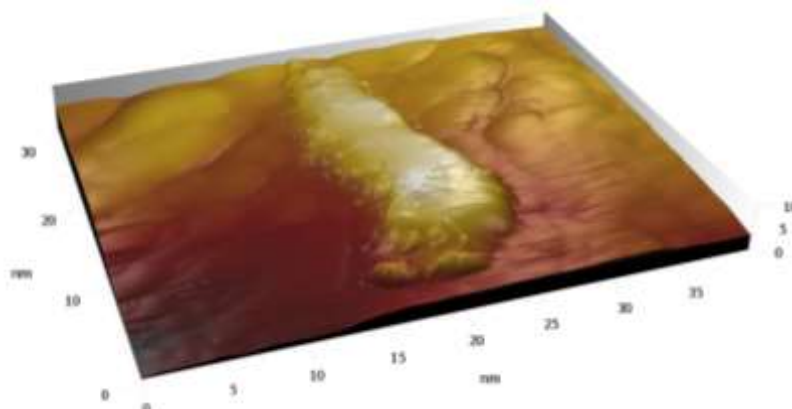
To date CdSe NPLs have been the workhorse of the field and have been used as a playground to investigate the changes of charge carrier's dimensionality in nanostructures [2] or surface-related interactions [3]. While advanced properties of CdSe NPLs are constantly discovered, basics information on their structural properties (shape, trap states) are still missing, which hampers establishing direct correlations between structural and electronic/optical properties.

By studying individual CdSe NPL with a scanning tunnelling microscope (STM) we unveil for the first time their real morphology, their edge shape, as well as the spatial and energetic position of electronic trap state at their surface. These results are of tremendous importance to understand the growth mechanism, the nature of the interface for NPL-based HNS or the origin of trap states in NPLs.

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## Figures



**Figure 1:** 3D STM image of an individual CdSe nanoplatelets on gold substrate

# High-dimensional neural network potential for borophene on metallic surfaces

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Single layer materials have drawn a lot of attention due to their peculiar physical properties (opto-electronic properties, high conductivity, flexibility...). In particular, it has been predicted that boron could exist as a single atomic layer in distinctive crystallographic configurations (allotropes), called *borophene* – in reference to the carbon equivalent, graphene. Borophene is one of the only 2D material with metallic behaviour, among other interesting properties [1]. Recent studies have focused on the synthesis of such material under various allotropic forms, the obtained allotrope depending on the substrate used and experimental parameters such as synthesis temperature [2–5].

To identify and assess borophene allotropes synthesised on metallic substrates, we propose to produce an extended database of simulated structures and their corresponding STM images, allowing a facilitated allotrope identification from experimental STM imaging using image classification. For that purpose, one needs a large database of accurate extended models comprising several units cells of substrate and borophene – such large models are needed to allow describing Moiré patterns and/or borophene corrugation. In the first stage of this work, we have developed a new atomic potential using a machine learning approach [6–8], which allows us to explore multiple structural arrangements of borophene allotropes on metal substrates. The developed potential presents the advantage of performing fast simulations with a level of accuracy comparable to ab initio calculations [9] – moreover, no classical potential pre-existed for this type of system.

Here, we will present the methodology to develop this machine learning potential as well as the various borophene allotropes that have been simulated on Ag surfaces. We will also show how structural properties of given allotropes can be retrieved from their STM images.

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# From electronic state to atomic orbital mapping in graphene in the transmission electron microscope

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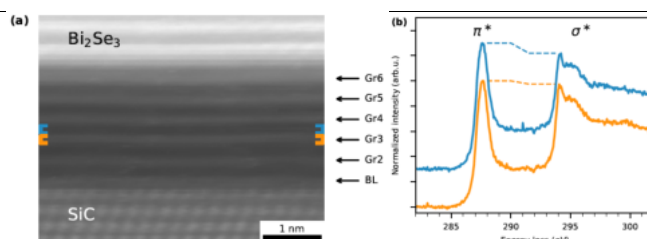
Mapping individual molecular orbitals has been demonstrated in scanning tunneling microscopy for a couple of decades, with impressive signal to noise ratio, albeit with surface sensitivity only [1]. There is strong scientific interest to achieve a comparable feat in transmission electron microscopy (TEM): understanding chemical bonding at interfaces and defects to foster defect engineering and the development of novel materials in, e.g., photocatalysis or microelectronics. Recently, we demonstrated real space imaging of atomic orbitals in bulk rutile TiO<sub>2</sub> [2] using electron energy-loss spectroscopy (EELS) in TEM. Here, we explore the capabilities of STEM-EELS to map electronic states and corresponding orbitals in a crystal presenting a discontinuity due to its inherent 2D nature: graphene.

The simple picture of expected state localization ( $\pi^*$  states out-of-C-planes,  $\sigma^*$  states in-C-planes) does not account for the beam geometry nor beam propagation, which play an important role on the experimental fine structure maps. The graphene layers are probed in side-view, i.e., the electron beam is parallel to the graphene layer, in a few-layer stack of epitaxial graphene grown on SiC. The interpretation of the experimental data is achieved with simulated maps obtained from inelastic channeling calculations, accounting for both the electron beam propagation and the inelastic scattering. The strong agreement between experimental and simulated  $\pi^*$ ,  $\sigma^*$ ,  $\pi^*/\sigma^*$  fine structure maps confirms that the experimental contrast is a signature of the corresponding  $p_z \sim \pi^*$  orbitals [3]. These results also demonstrate that the effect of electron beam channeling hinders the visualization of atomic orbitals, and highlight some of the key limitations to mapping orbitals in TEM [4].

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- [4] The electron microscopy work was supported by the EPSRC (UK). SuperSTEM Laboratory is the EPSRC National Research Facility for Advanced Electron Microscopy. Parts of this work were supported by the French National Research Agency (ANR-22-CE29-0019) and the Austrian Science Fund (FWF) under grant no. I4309-N36.

## Figures



**Figure 1:** STEM-HAADF image (a), and C-K edges extracted from in- and out-of-C-plane (b).

# Hot electron dynamics in graphene –a linear-scaling atomistic approach

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Graphene holds significant promise for a variety of applications. In particular, graphene photodetectors have been shown to be very fast, highly sensitive, and consume minimal power, making them extremely promising for next-generation optical communication technologies[1].

Hot electrons – electrons whose temperature is higher than the surrounding lattice – play a fundamental role in such graphene photodetectors. A variety of theories and measurements have been developed and conducted to understand the main factors controlling the dynamics and relaxation of hot carriers in graphene, but fundamental questions remain to be examined [2].

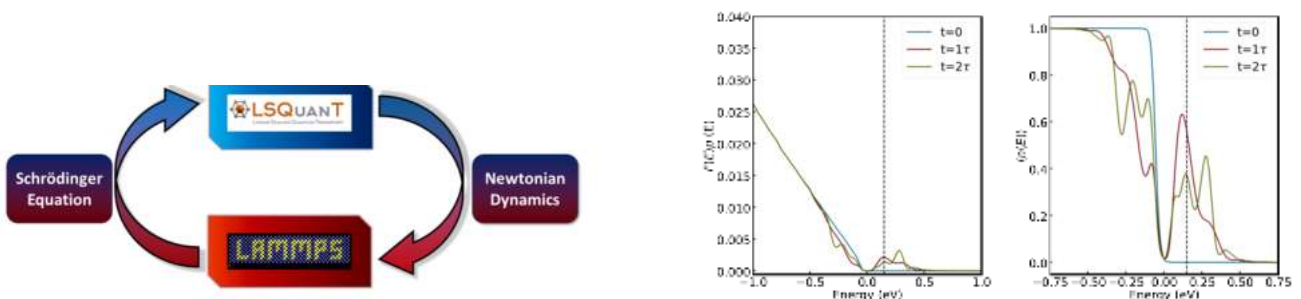
Here, we present our development of a numerical simulation tool that can capture the dynamics of hot carriers in graphene with arbitrary lattice vibrations, defects, and disorder. Our methods are linear-scaling, meaning we can simulate systems with millions of atoms – this permits an atomic description of the system while allowing for system sizes that approach the experimental scale. Such a tool will allow for a deeper fundamental understanding of hot carrier dynamics in graphene, as well as reveal strategies for the control of such dynamics, with an eye toward future applications in photodetection, optical communications, and energy conversion.

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## Figures



**Figure 1 Left:** Schematic representation of the self-consistency cycle for the atomistic simulation of coupled charge and ion dynamics. **Right:** Time and energy resolved phonon absorption in monolayer graphene.

# Real-time millikelvin thermometry in a spin qubit architecture

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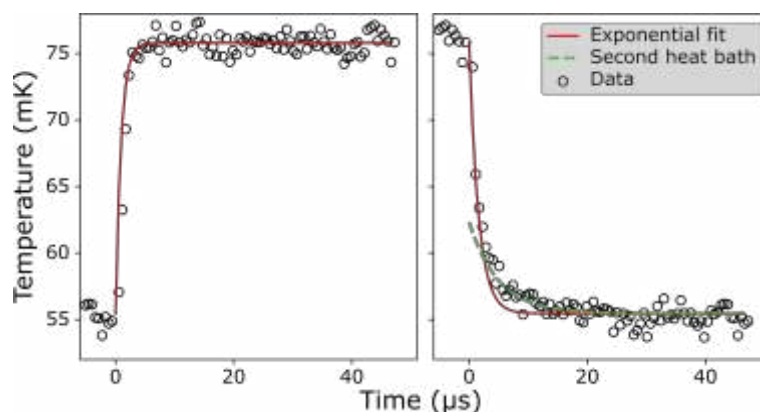
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In the worldwide efforts to build the first useful quantum processor, semiconductor quantum dots[1] are attracting increasing interest owing to their scalability prospects[2]. In this approach, the qubits can be encoded in the spin degree of freedom of individual electronic charges localized in gate-defined potential wells. Recent works indicate that the heat generated by the manipulation and read-out of qubits constitutes a bottleneck for the efficient operation of large-scale quantum processors[3,4]. We present time-domain temperature measurements in the immediate environment of a semiconducting spin-qubit architecture. We take advantage of the temperature dependence of quantum capacitances in a silicon nanowire quantum dot array, which we read out via a radio-frequency tank circuit. Using two measurement configurations, we access the temperatures of both the local electron and phonon heat baths, respectively, with a noise equivalent temperature of  $3 \text{ mK}/\sqrt{\text{Hz}}$ , possible futures improvements of which are discussed. We illustrate (Fig.1) the time-domain capabilities of this thermometry technique by detecting the  $\mu\text{s}$ -scale temperature variations in response to short microwave bursts. This work represents a starting step towards the understanding and mitigating of the detrimental impact of dissipation on spin based quantum processors.

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## Figures



**Figure 1:** Real-time thermometry. Recording of the phonon temperature in a silicon nanowire, while (left panel) and after (right panel) irradiating a microwave burst as used for qubit manipulation.



# Design and Numerical Simulation of a Quantum Graphene Gyroscope

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Today, most personal navigation devices rely on the Global Positioning System (GPS). This system is quite accurate under open sky, but this accuracy can be significantly degraded when satellite signals are blocked by terrain or buildings, or when the receiver is indoors or underground. In everyday situations these issues are mostly a minor inconvenience, but they can become critical in situations such as disaster relief or medical emergencies.

For this reason, there is a need for personal location and navigation systems that do not rely exclusively on GPS signals. Such a system can be constructed with a combination of accelerometers and gyroscopes – by tracking changes in velocity and in orientation, this would provide accurate location information from a known starting point. This system would also ideally be lightweight, compact, robust, low power, and highly accurate, making it practical for personal handheld devices. The goal of our current research is to develop a gyroscope based on graphene that meets all of these requirements.

In this talk, I will present an analysis of graphene gyroscopes that can detect rotation through purely electrical means. This is accomplished via the Sagnac effect, which is a quantum mechanical effect where angular rotation induces quantum interference that results in a modulation of current through a ring structure. This is analogous to the Aharonov-Bohm effect in electrically conductive systems, with angular momentum replacing the magnetic field, and can be implemented in both optically and electronically.

The optical Sagnac effect has been used for decades in aerial navigation, but these optical gyroscopes tend to be quite bulky and heavy. This arises from the tautological fact that light moves at the speed of light, and thus very large optical path lengths are required for the gyroscope to be sufficiently sensitive to rotation. In contrast, electrons in solids move much more slowly, allowing for much smaller structures and potentially enabling their incorporation into handheld devices.

We use a combination of numerical simulations and device modeling to design and evaluate the sensitivity of gyroscopes based on the electrical Sagnac effect in graphene. Our numerical simulations are carried out using the *Kwant* and *pybinding* simulation packages. We find that a gyroscope based on a simple graphene ring structure requires extremely demanding criteria to reach the sensitivity needed for handheld applications. We will discuss the criteria that must be met, and offer a perspective on the practicality of such a gyroscope design. Time permitting, we will then describe alternate designs that appear to be much more promising.

# A QM/MM-NEGF approach to address electrified metallic/water interfaces

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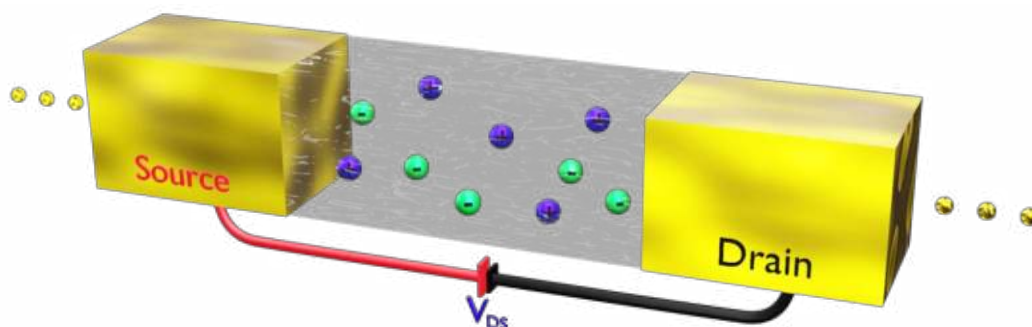
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Several macroscopic observations are intrinsically related to processes occurring at the nanoscale. In that regard, molecular modeling stands as a crucial tool in investigating many problems in nanotechnology. Most of those problems involve water in contact with metallic - often electrified - surfaces, especially when dealing with electrochemical processes. Nonetheless, traditional molecular modeling approaches, such as standard density functional theory, have limitations in realistically addressing the systems needed to simulate an electrochemical cell. Here we propose using a hybrid quantum mechanics/molecular mechanics (QM/MM) approach [1] combined with the non-equilibrium Green's functions (NEGF) formalism [2,3] implemented in the SIESTA code [4,5] to tackle electrified metallic/water interfaces. Using the NEGF allows us to mimic an electrochemical cell very closely to an experimental setup, where two metallic electrodes are kept under different chemical potentials, sandwiching a central cell containing liquid water, as sketched in Figure 1. To get a good cost-accuracy compromise, we describe the water molecules using a classical force field while the metallic electrodes are fully ab-initio. We demonstrate the effectiveness of the proposed method by applying it to a system containing liquid water in contact with gold electrodes. The approach is first validated by comparing the structural properties of water (layering and angle distribution) extracted from our QM/MM molecular dynamics (MD) against full ab-initio MD simulations. We then apply the method to perform QM/MM-NEGF MD simulations to these systems, where we demonstrate that our approach can correctly capture the changes in the structural properties of water and in the electronic structure of gold due to the voltage applied to the electrodes. Finally, we reveal that the performance reached by the proposed approach paves the way for applying it to way larger systems, containing as much as 7,500 atoms, where realistic electrolytes could be addressed.

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## Figures



**Figure 1:** Sketch of the setup used to perform QM/MM-NEGF molecular dynamics.

# Wet-jet milling exfoliated hexagonal boron nitride for anticorrosive coating

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Corrosion of metals poses significant challenges to the durability and longevity of various metallic substrates in industrial applications.[1] To mitigate this issue, researchers are focusing on the development of advanced protective coatings with enhanced anticorrosion properties. Amongst the emerging strategies, the integration of two-dimensional (2D) materials has gained significant attention due to their physicochemical properties.[2]

In this work, wet-jet milling (WJM) exfoliation [3] was used to produce few-layer hexagonal boron nitride (*h*-BN) flakes [4] as a corrosion-protection pigment in polyisobutylene (PIB)-based composite coatings for marine applications.[5] This study highlights the benefit obtained by the incorporation of *h*-BN, yielding a corrosion rate of the protected structural steel as low as  $7.4 \times 10^{-6}$  mm year<sup>-1</sup>. The 2D morphology and hydrophobicity of the *h*-BN flakes, together with the capability of PIB to act as a physical barrier against corrosive species, are the main reasons behind the excellent anticorrosion performance of the as-designed composite coating.

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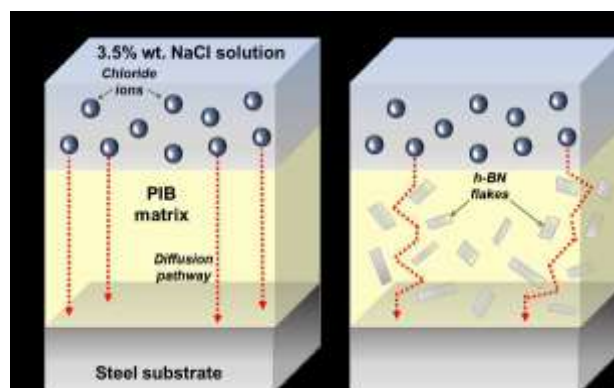
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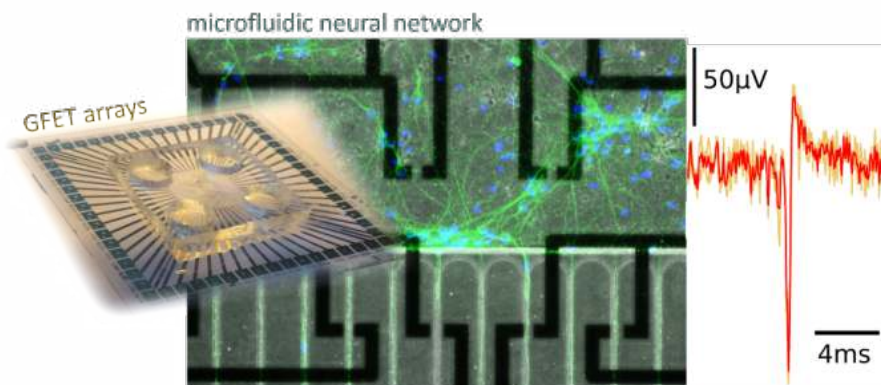
**Figure 1:** Schematic diagrams of diffusion pathways through a) pristine PIB and b) *h*-BN/PIB coatings.

# Graphene nanoelectronics meets neurofluidics for versatile labs on chip

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New methods and new technology are currently required to interrogate neuronal cells by many means and at multi-scale, in-vivo and within model neural networks in-vitro. In particular, to understand how neural circuits operate, we need access to activity of large numbers of neurons at the same time, and record their activity at the single cell level regarding the lot of information which relies at the level of synapses and ion channels. In that race, Graphene offers an ideal platform for recording and culturing neural networks, regarding its exceptional neuronal affinity and the presence of readily accessible surface charges which give the unprecedented possibility to realize a direct coupling with cells to detect ion fluxes at the nano<sup>1,2</sup> and mesoscale.<sup>3,4</sup> Here, we report on a novel and versatile approach that combines array of graphene field effect transistors (GFET) and microfluidic platforms for culturing and sensing neurons in designable network architecture.<sup>5</sup> The fluidic microchannels, somatic and synaptic chambers enable to define the neuron network topology, while the graphene devices provide localized, highly sensitive and optically transparent sensing sites. The efficient cell-sensor alignment obtained by the microfluidic circuit enables to reach the highest reported signal-to-noise ratio for single-units detection with GFETs, revealing additional information that remain hidden from recordings when using conventional microelectrode arrays (MEAs). Thus, the combination of graphene sensors and microfluidic circuits leverages the advantages of two state-of-the-art technologies for highly efficient sensing of model neural networks. Being fully transparent and therefore compatible with optogenetic tools and high-resolution microscopy, this novel platform could provide a versatile lab-on-chip for diagnosis and treatment of tomorrow, and open avenues of investigation for studying topological neuron network and living matter in general.



**Figure 1:** Neuron-gated GFET arrays with microfluidic circuits (left) allows for highly efficient extra-cellular detection of action potential (right). The graphene sensing site being optically transparent, cells can be observed in real-time during the culture (several weeks) providing multiple way to follow both structural and functional changes within model neural network (center).

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# PtSe<sub>2</sub> films grown by molecular beam epitaxy for high frequency optoelectronics

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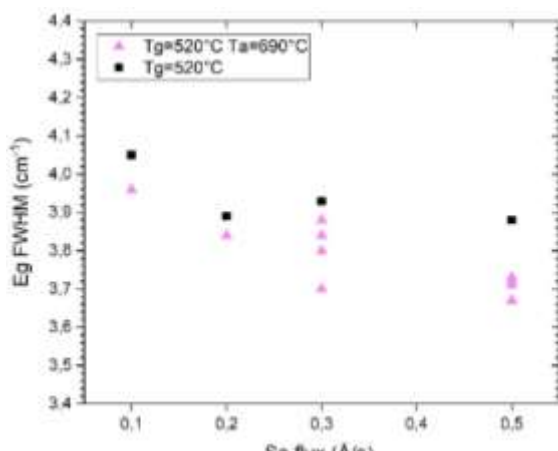
PtSe<sub>2</sub> is a 2D material with high intrinsic qualities suitable for high frequency IR optoelectronics [1], exhibiting a bandgap varying from 1.2eV (monolayer) to 0.2eV (bilayer) and becoming semi-metallic for few layers and in bulk form [2]. We investigated the synthesis of PtSe<sub>2</sub> films on sapphire substrates by molecular beam epitaxy. In particular, we studied the impact of a post-growth annealing for various Se fluxes on the full width at half maximum (FWHM) of the PtSe<sub>2</sub> Eg Raman peak (Figure 1): thinner is the Eg peak width, higher is the crystalline quality [3] which is essential for high (opto)electronic performances. PtSe<sub>2</sub> was also grown on vicinal sapphire(0001) surfaces and we demonstrated a large improvement of film crystallinity using grazing incidence X-ray diffraction (GIXRD) and transmission electron microscopy (TEM) techniques. Conductivity and carrier mobility measured by Van der Pauw experiments on 20x20 mm samples are also improved.

We synthesized a 7.5nm-thick PtSe<sub>2</sub> film on a 2 inches sapphire substrate and fabricated coplanar waveguides integrating a 4x4 μm PtSe<sub>2</sub> channel. The channel was illuminated with a 1.55μm laser beam modulated in intensity at frequencies varying between 2 and 67 GHz. Our PtSe<sub>2</sub> photodetector exhibits a record 3dB bandwidth of 60GHz (Figure 2).

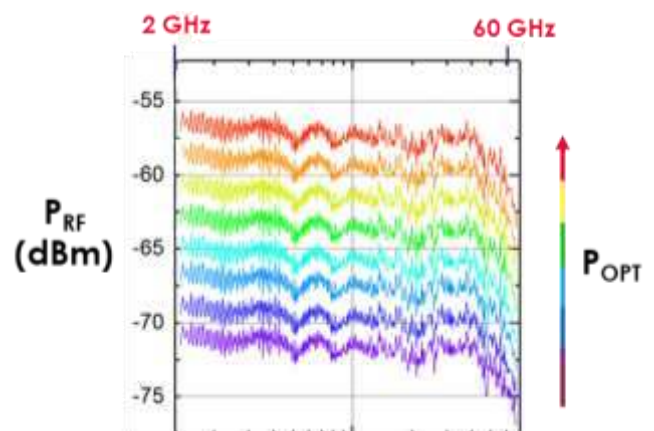
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## Figures



**Figure 1:** FWHM of Eg RAMAN peak of PtSe<sub>2</sub> films grown at T<sub>g</sub>=520°C with a post-growth annealing at T<sub>a</sub>=690°C (purple triangles) or without annealing step (black squares), under different Se fluxes.



**Figure 2:** High frequency 1.55μm photodetection with a 7.5nm-thick PtSe<sub>2</sub> channel inserted in a coplanar waveguide. A 60GHz bandwidth photodetector is demonstrated.



# Magnetic Anisotropy of Ultrathin Co-Layers Deposited by Electron Beam Evaporation in Moderate Vacuum Conditions

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Perpendicular magnetic anisotropy (PMA) in Co/Pt multilayers has been broadly studied for decades due to their potential for technological applications, particularly in the field of high-density magnetic storage and spintronics.[1] The main approach to fabricate these materials is magnetron sputtering,[2] offering high quality thin films and good control on critical growing parameters. However, its deposition geometry makes difficult to integrate with nanopatterning, often giving rise to problems with the quality of the edges of the nanostructures. Electron beam evaporation (EBE) is an accessible and a non-conformal physical vapor deposition technique to easily create ultra-thin film nanopatterns with a high degree of PMA for spintronic applications. There are not many studies using this technique, and those existing are based on very low vacuum pressures ( $<10^{-8}$  mbar).[3] Pressure control is a crucial parameter for roughness and epitaxiality control of deposited layers and, therefore, for a good thin film quality and a high degree of PMA. In this work, we explore the magnetic and structural properties of ultra-thin Co/Pt multilayers (below 1 nm thick) evaporated in lower vacuum conditions compared to previous literature (up to  $\sim 10^{-5}$  mbar). Results show that a Cu buffer layer between the Si substrate and the Co/Pt heterostructure is key to promote a high degree of PMA in the aforementioned vacuum conditions. The proper engineering of the Cu layer thickness dramatically changes the magnetic properties of the multilayer, such as the coercivity or the loop squareness. This work provides with an easy path to develop magnetic heterostructures compatible with nanolithography, tunable magnetic properties and high degree of PMA even on rough pressure environments.

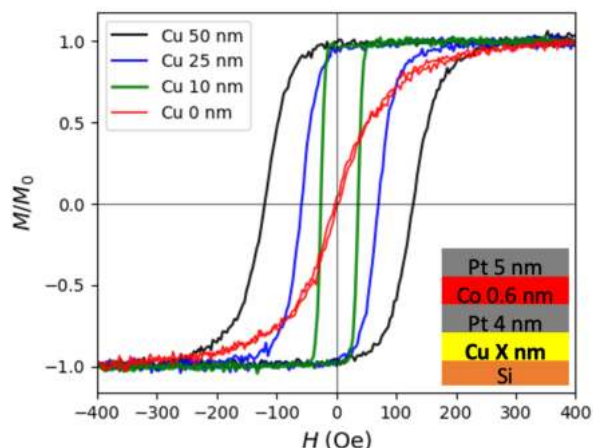
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## Figures



**Figure 1:** Normalized polar Kerr hysteresis loops of e-beam evaporated Si/Cu(x)/Pt(4)/Co(0.6)/Pt(5) ultra-thin films (units given in nm). All samples were fabricated in the same run.

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The 2D materials have attracted a huge scientific interest owing to their reduced dimensionality as well as the predicted properties interesting for the applications in electronics, optics and spintronics [1-3]. However, the synthesized materials often contain inevitable structural anomalies that induce the deviation from the theoretically predicted properties. The knowledge about the structural defects in these materials is thus essential for the understanding of growth mechanisms as well as for the insight into the properties of the synthesized materials.

Up to now, the structural information of the synthesized materials has been most often assessed by means of cm-scale grazing incidence X-ray diffraction giving statistical information about crystal quality or nm-scale aberration-corrected (scanning) transmission electron microscopy giving access to high resolution imaging of atomic defects. Recently, a new imaging technique called 4-dimensional scanning transmission electron microscopy (4D-STEM) has been demonstrated where a 2D diffraction pattern in reciprocal space is captured at each 2D real space electron beam position [4]. The generated 4D datasets contain a huge amount (~GB) of information that can be processed in order to reconstruct micrometer scale real space 2D images of relevant crystal information.

In this work we demonstrate the use of 4D-STEM for the large scale imaging of crystal orientation, polar direction, crystal polymorphs or twist angle for the layered systems synthesized by different growth processes. By carefully selecting the diffraction spots in reciprocal space, specific crystal information can be targeted and retrieved in form of a reconstructed 2D image. Contrary to the x-ray diffraction, the information obtained by 4D-STEM is spatially and quantitatively resolved allowing for the imaging of the distribution of misoriented and/or polar inverted domains, crystal phases and stacked layers. In this way, the spatial distribution of associated crystal defects such as grain boundaries as well as heterojunction interfaces can be imaged and the full structural information on large scale materials is obtained [5].

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# Carbon nanodots driven coating of WS<sub>2</sub> nanotubes improves hydrogen evolution reaction

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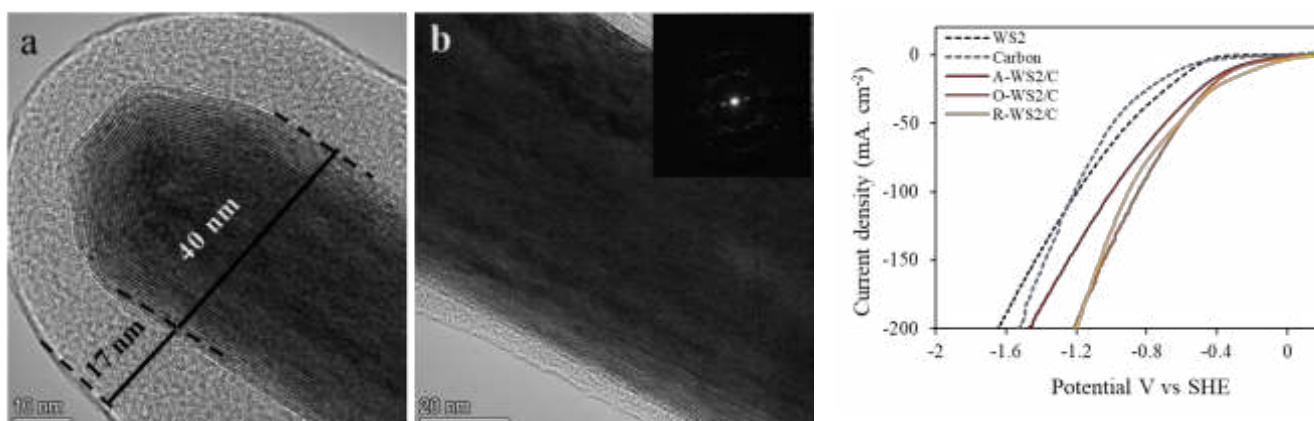
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## Abstract

Transition metal dichalcogenides have recently been proposed as an excellent catalytic substitute for noble metals for hydrogen evolution reaction (HER). However, these alternatives often suffer from inferior performance. The poor performance of WS<sub>2</sub> nanotubes attributes intrinsically inert basal plane and lack of active edge sites which causes less electron transport and low conductivity. In this work, tungsten disulfide nanotubes (WS<sub>2</sub> NT) are coated with nitrogen-doped graphitic carbon, in three steps. Excess carbon from the sample is removed by CO<sub>2</sub> gas which acts as a mild oxidizer. Finally, recrystallization at 800° C is done by thermal annealing in presence of N<sub>2</sub>. Products from each reaction step are chemically analyzed. The heterostructure with carbon after recrystallization shows significantly improved HER performance showing an onset potential of 172 mV compared to 540 of the uncoated NTs. The improved activity was confirmed in different pH electrolytes. Moreover, stability measurements prove enhanced efficiency of the composites upon prolonged electrochemical reaction. The formation of carbon-coated INT-WS<sub>2</sub> nanostructure provides a promising way to obtain a pH-universal, cost-effective electrocatalyst for energy conversion.

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**Figure 1.** (Left) TEM magnification image of WS<sub>2</sub> nanotube coated by carbon layers. (Right) LSV curves showing H<sub>2</sub> evolution reaction in 0.5 M H<sub>2</sub>SO<sub>4</sub>.

# Substrate and environment roles on the high pressure tuning of carbon low-dimensional system's properties

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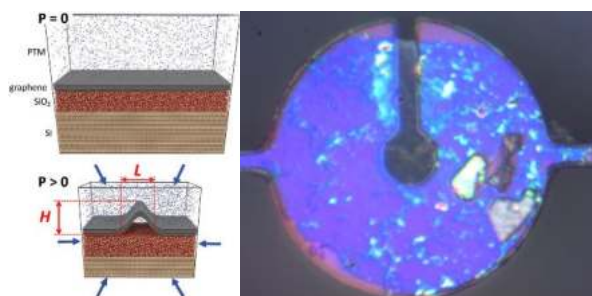
Carbon based materials such as graphene and carbon nanotubes came under the spotlight due to their extremely promising properties and potential, for technological advancements. Moreover, their properties are extremely tuneable by applying external perturbations such as external electric, strain and doping [1-3]. Largely less explored is the use of pressure as a tuning parameter. When low-dimensional materials are submitted to high-pressure their physical properties can be drastically modified, as in the case of phase transitions [4], as well as smoothly altered by tweaking their strain and doping levels [5,6]. Environment has a massive impact in the pressure response of those materials at the point that their behaviour can be desirably controlled by pressure environment engineering.

We will present here a series of experiments where we explored the environmental effects on the pressure response of carbon nanotubes, graphene and graphene stackings. Raman spectroscopy as well as optical microscopy allowed to probe the samples during the high pressure runs. For what concerns graphene and graphene stackings we showed that the substrate plays a fundamental role governing the dynamics of phase transitions as well as establish a fine equilibrium with graphene and the surrounding environment. We discovered in our recently published work [7] that, using SiO<sub>2</sub> substrates, it is possible to detach graphene from its substrate depending on the environment that envelops it. On the same line phase transitions can be induced by selecting different environments in graphene stacks or carbon nanotubes. In order to get the unaltered environmental response, we engineered micrometric substrates for graphene suspension compatible with high pressure experiment and studied the pure graphene environment interaction.

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## Figures



**Figure 1:** On the left, schematic representation of the environment mediated multilayer graphene detachment with pressure. On the right, a sample of bilayer graphene deposited on a substrate for high pressure suspended measurements.

# Phonon Mean Free Path - Thermal Conductivity Relation of Beta Form Gallium Oxide

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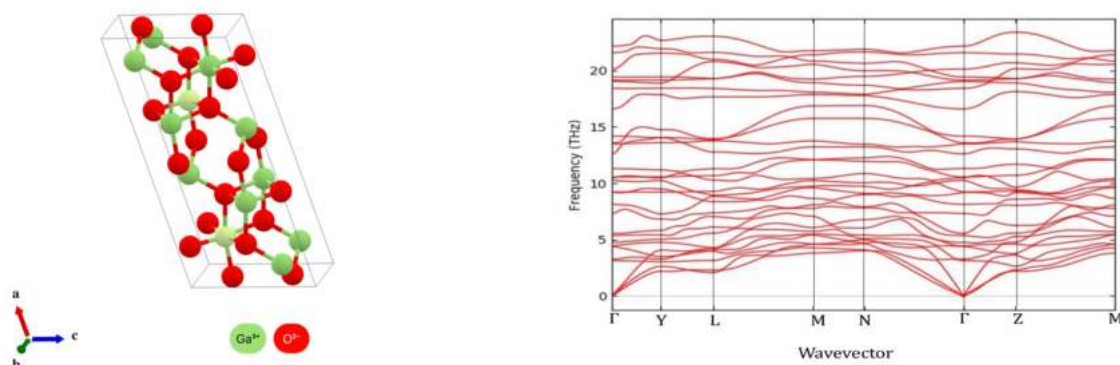
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Beta-gallium oxide ( $\beta\text{-Ga}_2\text{O}_3$ ) is an ultra-wide bandgap semiconductor material that has gained significant attention in recent years. With its wide bandgap over 4.5 eV it is found highly promising for high power and optoelectronic applications. Other uses include dielectric coatings for solar cells, deep-ultraviolet transistors, light-emitting diodes, and lasers [1]. The pressing issue of local heat build-up and narrowing thermal pathways in such high-performance miniature devices is a significant challenge and demands innovative solutions. This can be done by investigating the properties of dominant microscopic energy carriers in materials, in this case lattice vibrations (i.e., phonons). Such properties can help to understand the thermal behaviour of materials at the nanoscale. One of the critical properties that characterize this behaviour is the phonon mean free path (MFP). With its distinctive monoclinic lattice structure,  $\beta\text{-Ga}_2\text{O}_3$  exhibits three-dimensional anisotropy in its thermal conductivity [2]. Therefore, additional problems in design and optimization of high-performance electronic devices made from this material are expected. The significantly lower conductivity (16-27 W/m.K at room temperature) compared to other wide-bandgap semiconductor materials like SiC and GaN [3] only complicates these problems. In this study, the phonon MFP and thermal conductivity relationships for ( $\beta\text{-Ga}_2\text{O}_3$ ) at different lattice temperatures were theoretically derived through ab-initio simulations and phonon interaction computations, using up to third-order force constants. Our results reveal that the isotopic disorder of gallium atoms is the main factor that affects the phonon mean free path, while anharmonic phonon-phonon interactions cause a plateau-like behaviour in thermal conductivity at low temperatures.

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## Figures



**Figure 1.** (Left) The unit cell and (Right) Phonon dispersion of  $\beta\text{-Ga}_2\text{O}_3$



# Lab-On-Fiber: Wearable Multi-Sensing Device Enabling the Assessment of Wound Healing

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Chronic wounds such as venous and diabetic foot ulcers affect 1-2 % of the population and represent 2-4 % of healthcare expenses. Management of chronic and acute wounds remains challenging: available methods based on visual signs and symptoms provide limited accuracy and strongly rely on the practitioner's experience. Moreover, wound care technologies lack sufficient evidence of their impact to objectively support their utilization.

We designed a non-invasive lab-on-fiber multi-sensing device for monitoring physiological parameters in wound exudate that are relevant to evaluate the healing process, such as the pH level and the concentration of glucose and proteinase[1]. Each of the three polymeric optical fibers (POF) forming the device was functionalized with specifically designed fluorescent-based sensing chemistries for the targeted analytes. Whereas the fabrication of pH-sensitive fiber was relatively straightforward, the preparation of glucose and proteinase-sensitive fibers required firstly the design of suitable fluorescence-based detecting methods[2] which were then used to functionalize POFs. The detection sensitivity and selectivity was determined for each fiber confirming their suitability for monitoring pH, glucose, and proteinase in the ranges relevant to the wound environment. As expected the use of POF allowed to increase the detection sensitivity for both glucose and proteinase detection of respectively 5.9 and 2.6 times. The selectivity and robustness of the multi-sensing device were confirmed by testing it with complex solutions having different pH (5, 6, and 7) and different concentrations of glucose (1.25, 2.5, and 5 mM) and MMP (1.25, 2.5, and 5 µg/mL). Further studies are planned to evaluate the stability of the sensing chemistries over time and to test the efficacy of the proposed device using wound exudate samples from hospitalized patients. The simple set-up of the multi-sensing POF-based devices is versatile and can be further implemented to detect other parameters that are relevant for the rapid and accurate assessment of wound healing (e.g. uric acid, bacteria). We believe that such a simple set-up and the sensing chemistries proposed in this work could represent a game changer in the non-invasive management of wounds.

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# Investigation of Heat Transport in an Individual Nanostructure by Dual Scanning Electron and Thermal Microscopies

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## Abstract

A novel combined setup, with a Scanning Thermal Microscope [1] (SThM) embedded in a Scanning Electron Microscope [2] (SEM), is used to characterize a suspended silicon rough nanowire, which is epitaxially clamped at both sides and therefore monolithically integrated in a microfabricated device [3]. The rough nature of the nanowire surface, which prohibits vacuum-SThM due to loose contact for heat dissipation, is circumvented by decorating the wire with periodic platinum dots. Reproducible approaches over these dots, enabled by the live feedback image provided by the SEM, yielded a strong improvement in thermal contact resistance and a higher accuracy in its estimation. The results – thermal resistance at the tip-sample contact of  $188 \pm 3.7$  K/W and thermal conductivity of the nanowire of  $13.7 \pm 1.6$  W/m·K – are obtained by performing a series of approach curves on the dots [4]. The work highlights the capabilities of the dual SThM/SEM instrument, in particular the interest of systematic approach curves with well-positioned and monitored tip motion.

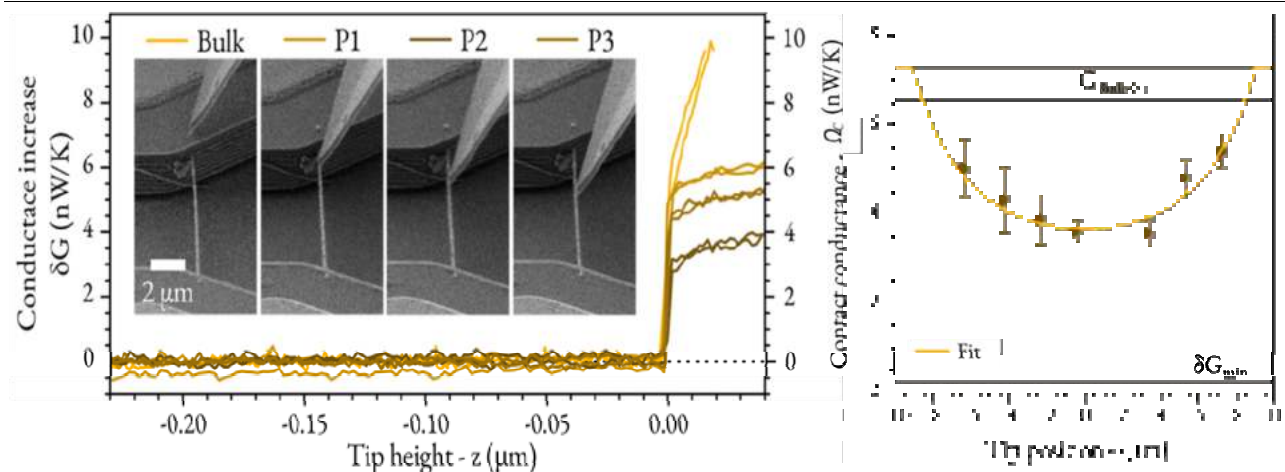
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## Figures



**Figure 1:** Thermal conductance increase vs. tip height  $z$  for approaches over different deposited Pt nanodots along Si NW (on the left) and in contact with the measured nanowire at different locations along the nanowire (on the right).

# One-dimensional hBN/CNT Van der Waals Heterostructures Fabricated by Atomic Layer Deposition

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Graphene's isolation has led to a strong interest in two-dimensional (2D) materials and the ability to stack them into van der Waals (VdW) heterostructures has opened up a wide field of applications based on these new materials. Neither too weak nor too strong, VdW coupling allows connecting two different materials to combine their intrinsic properties and/or to create new ones. The interest in this coupling is currently extending beyond 2D materials, with 1D VdW heterostructures that consist of coaxial stacking of two or more distinct materials. The two-dimensional electron confinement associated with VdW stacking is expected to improve/modify the physical and chemical properties of the final material compared to the initial ones. In particular, Hexagonal Boron Nitride (hBN) is generating much interest as it is isostructural to graphene with a large bandgap, excellent thermal stability, and photoluminescence intensity in the visible or UV spectral regions; thus, coaxial stacking of hBN onto carbon nanotubes (CNTs) can enrich optoelectronic properties of the initial structures [1]. Fabricating these high-quality hBN/CNT heterostructures requires a synthesis approach capable of precisely controlling the epitaxial deposition onto supports at the atomic scale. Based on self-limiting gas-surface reactions, Atomic Layer Deposition (ALD) has proven to be ideally suited for fabricating functional hetero-nanostructures, such as carbon nanotube-based materials [2]. Herein, a two-step ALD process of hBN is utilized for fabricating hBN/CNT heterostructures based on polymer-derived ceramics chemistry [3]. Briefly, a pre-ceramic layer of polyborazine is successfully deposited on single-wall or multi-wall CNTs within the first ALD step and then annealed at high temperatures in the second step to convert the polyborazine into crystalline hBN. The resulting BN-coated CNTs are thoroughly investigated employing advanced characterization techniques. Specifically, high-resolution transmission electron microscopy exhibits the fabrication of highly crystalline hBN/CNT heterostructures, and electron energy loss spectroscopy permits us to observe a conformal and homogeneous coating of hBN layers onto single-wall and multi-wall CNTs. The influence of the ALD parameters and post-annealing treatment on BN growth (thickness, number of layers, homogeneity) and structure (amorphous, turbostratic, hexagonal phase) is explored in detail as well as the impact of the starting carbon material on the final heterostructures in terms of morphology and crystallinity. Particular attention is paid to successfully fabricate 1D VdW heterostructures made of few-layer hBN coated-single wall carbon nanotubes. The Raman and photoluminescence spectroscopies are performed to evaluate the structural and optical properties of the obtained heterostructures.

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# Boron-carbon thin films deposited via plasma enhanced atomic layer deposition (PE-ALD)

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Boron carbide ( $B_xC$ ) finds diverse applications due to its superior hardness, high neutron absorption, and semiconducting nature. Magnetron sputtering [1], and high temperature ( $\geq 1000$  °C) chemical vapor deposition (CVD) are the conventional processes to obtain boron carbide thin films. CVD involves boron hydrides [2] or halides [3] as precursors along with dihydrogen or simple hydrocarbons. Such precursors come with challenges such as high toxicity and/or corrosive by-products. Furthermore, conformality and thickness control of these films is still a challenge. To overcome it, atomic layer deposition (ALD) appears as a technique of choice, however,  $B_xC$  has never been synthesized by this technique so far.

From triethylborane (TEB) and hydrogen gas ( $H_2$ ) as precursors, amorphous  $B_xC$  thin films with atomic-level thickness control on Si (100) substrate using plasma-enhanced atomic layer deposition (PE-ALD) are successfully obtained. The use of hydrogen plasma to remove ethyl groups of TEB to deposit  $B_xC$  films at low substrate temperatures ( $\leq 200$  °C) is demonstrated. It should be noted that in this process the expected by-products are non-toxic and non-corrosive.

Here, the influence of the deposition parameters on the film growth rate, composition and structure will be discussed. The ALD reaction temperature is being investigated between 80 °C and 300 °C alongside spectroscopic ellipsometry. Additionally, the pulse/purge of precursors is optimized to ensure a saturated self-limited surface reaction, and the role of  $H_2$  concentration and plasma power in the composition and growth of the deposit is being explored.

In-situ optical emission spectrometry (OES) is also performed to detect and compare the intensity of hydrogen lines, and to look at species responsible for etching and deposition during the ALD cycle. The impact of plasma-activated hydrogen species (as a function of plasma power and  $H_2$  concentration) on the morphology and B:C ratio of the deposits is preliminarily assessed via secondary electron microscopy (SEM) and energy dispersive spectroscopy (EDS), respectively. Moreover, surface-sensitive quantification and bonding information are obtained via time-of-flight secondary-ion mass spectrometry (ToF-SIMS) and ex-situ x-ray photoelectron spectroscopy (XPS).

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# Multiplexed Extended-Gate Field-Effect Transistor-Based Immunosensor with Gold Nanoparticle-Amplified Potentiometric Response

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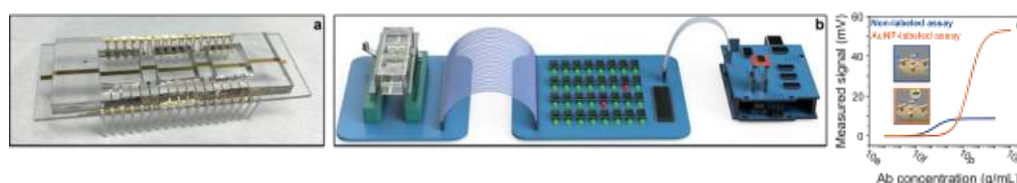
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To clinically evaluate complex diseases at the point of care (POC), it is crucial to have multiplexed quantitative sensing of biomolecules. This need has led to the development of ultra-sensitive and cost-effective biosensors. Electronic biosensors based on extended gate field-effect transistor (EGFET) are promising candidates for multiplexed biosensing due to their excellent sensitivity, facile integration, and straightforward interfacing with the readout electronics. Although some high-performance biosensing applications of EGFET systems have been demonstrated [1,2], current EGFET-based biosensors still need to overcome practical issues to reach broad use in POC settings, such as readout at low current levels ( $\sim$ nA), limited multiplexing ability, and complex customized nanofabrication of FET transducers. We demonstrate a custom standalone multiplexed EGFET-based potentiometric biosensing platform relying on modular electronics constructed with off-the-shelf components and an innovative assay format employing bioconjugates of gold nanoparticles (AuNPs) and antibodies (Abs). Our platform comprises a disposable sensing chip containing an EG electrode array functionalized with bioreceptor molecules, a multiplexing module enabling reproducible scanning of up to 32 electrodes, and a readout module based on a commercial FET operating in constant charge mode to enable indirect monitoring of gate surface potential shifts caused by analyte binding. We observe a remarkable 5-fold amplification of the potentiometric response due to the labeling of target antibodies with AuNPs in comparison with the traditional non-labeled assay. We investigate the amplification mechanism by analyzing and modeling the impedimetric response of the system and propose that AuNPs act as localized regions of high surface charge mediating the diffusion barrier layer disruption. The AuNP-enhanced response brings the sensitivity of our platform to a level comparable with fully customized potentiometric nanobiosensors while avoiding complex nanostructuring processes and enabling accurate readout with conventional electronics. Furthermore, our EGFET-based platform exhibits  $\sim 10^4$ - $10^6$  times lower detection limits than gold-standard optical methods. Our findings indicate great promise for the development of highly sensitive and low-cost EGFET-based electronic biosensing systems suited for use at the POC.

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## Figures



**Figure 1:** a) EG sensing chip; b) Multiplexed EGFET platform illustration; c) Response of the biosensor.



# An innovation on deterministic graphene origami

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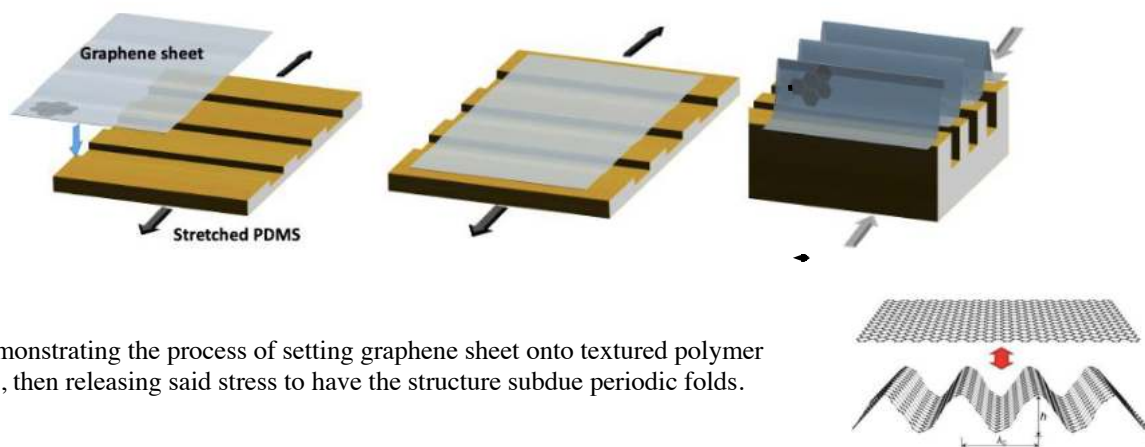
Graphene planes exhibit physical and chemical properties that depend on its curvature [1,2]. The creation of deterministic or stochastic graphene folded fields or n-layer graphene stacks is an active research area with different approaches[3,4].

The goal of this project is to create an original method for the realization of surface fields with tunable multiscale texturing, relying on deterministic and reversible graphene folds. The idea comes from the Japanese art of origami, where we take a 2D surface that when folded transforms into a 3D structure. With the capability of repeating the process of folding and unfolding perfectly. The aim is to develop novel nano devices or surfaces with tunable physical properties. Our strategy will allow us to transform a graphene surface supported through the uniaxial or biaxial compression of an elastomer substrate. The latter will have been previously etched using ultra-fast laser or Focus Ion Beam texturing to create the micrometric structures that will serve as a "pattern" for the expected folds of the graphene that will be deposited.

We present here the first results on this innovative approach. We demonstrate the creation of wrinkles on the graphene surface with a deterministic, reversible, and even repeatable (several fold/unfold processes) behavior. Atomic Force Microscopy was used to characterize the height profile of graphene under varying levels of elastomer stress. By analyzing the height profile as a function of stress percentage, we were able to demonstrate control over the height of the graphene folds. Raman Spectroscopy was also employed, to determine the induced defects (or lack there of) present.

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**Figure 1 :** Fig. demonstrating the process of setting graphene sheet onto textured polymer with a given stress, then releasing said stress to have the structure subdue periodic folds.

# Amorphous Boron Nitride: Atomistic Characterization and Performances

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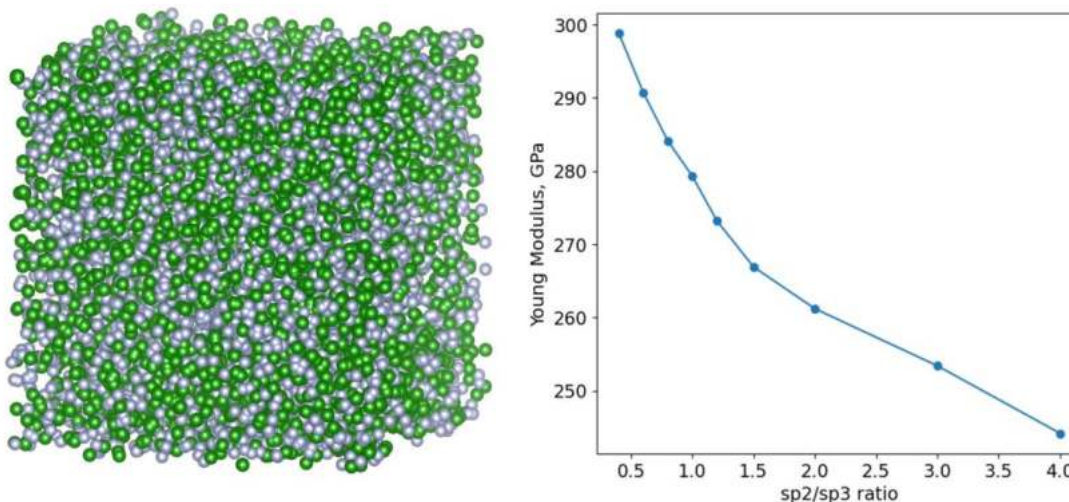
## Abstract

Amorphous boron nitride (aBN) has been revealed as an ultralow dielectric constant material ( $\kappa < 2$ ), with strong thermal stability and mechanical properties, making it highly suited for next generation interconnects technologies [1, 2]. The uniqueness of amorphous materials derives from their complex structure, which can to some degree be controlled at the fabrication level, and allows the tuning of specific properties useful for applications. In this respect, new fabrication strategies to modify the structural properties and a systematic theoretical characterization of the impact of the thermal, mechanical and electronic properties are urgent. In this work, we present a theoretical investigation of thermal and mechanical properties of aBN as a function of external parameters such as temperature, quenching rate, presence of unwanted or dopant atoms. Using machine learning interatomic potentials, we ensure the reliability of our calculations by describing the atomic interactions more accurately, introducing Gaussian Approximation Potentials [3] which are trained on a large dataset of atomic structures generated with ab-initio calculations [4,5]. We found that the incorporation of dopant atoms causes a significant change in the structure of aBN, which is strongly reflected in the resulting the thermal and mechanical properties of the compounds [4]. Further, we will discuss the anticorrosive properties and dielectric constant of aBN films. Our simulations will provide some recipe to design most suitable amorphous boron nitride-based coatings and metal diffusion barriers.

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## Figures



**Figure 1:** A ball-and-stick picture of aBN sample (left) and Young's Modulus of aBN samples with varying sp<sup>2</sup>/sp<sup>3</sup> bond ratio (right).

## Acknowledgement

This project is conducted under the REDI Program, a project that has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 101034328 and has been supported by Samsung Advanced Institute of Technology and ICN2 acknowledges the Grant PCI2021-122092-2A funded by MCIN/AEI/10.13039/501100011033 and by the "European Union NextGenerationEU/PRTR". Simulations were performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility, supported by the U.S. DOE, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. Additional computational support was received from the King Abdullah University of Science and Technology-KAUST (Supercomputer Shaheen II Cray XC40) and Texas Advanced Computing Center (TACC) at The University of Texas at Austin.

# Room-temperature single-photon emitter in the blue-green spectral range using a CdSe/ZnSe nanowire quantum dot

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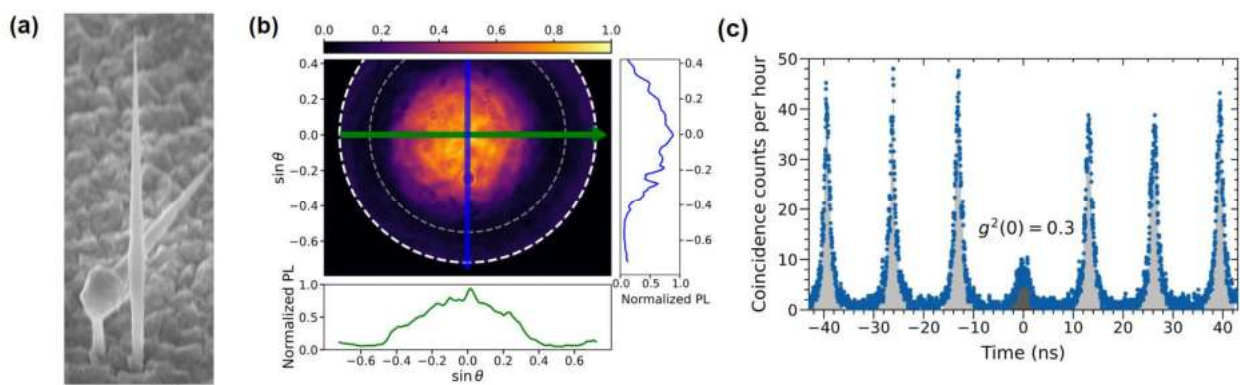
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Single-photon sources are key components for communication ultra-secured by quantum physics laws. In this contribution, we present a promising solid-state system able to emit triggered single-photons at room temperature in the blue-green range. This spectral band allows quantum communications both in free space and underwater.

The active element is a CdSe quantum dot (QD) embedded in a bottom-up core-shell ZnSe nanowire (NW) grown by molecular beam epitaxy. The NW shell acts as a waveguide and confines the fundamental optical mode HE<sub>11</sub>, channelling the photons emitted by the QD along the NW axis. We present a thorough study of a single nanowire using a whole range of characterization thanks to markers made on the growth substrate. The studied NWQD has a base diameter of 140 nm and a length of 5  $\mu\text{m}$  (Fig. a). The conical ending adiabatically expands the guided mode and reduces the divergence angle, thus increasing the collection efficiency [1]. This is confirmed by the far-field diagram (Fig. b) collected along the NWQD axis (Fig. a) where a Gaussian mode profile with small divergence angle is observed. Photocorrelation measurements on the excitonic lines show anti-bunching with  $g^{(2)}(0)$  value down to 0.3 (Fig. c) [2]. Complementary measurements done at cryogenic temperature have helped to understand the phenomena that degrade the single-photon purity at room temperature. We found that the single-photon emitter shows a promising brightness with a potential emission rate of 13 MHz with a 76 MHz excitation rate. This work paves the way for development of on-chip single-photon sources operating at non-cryogenic temperatures.

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**Figure :** (a) SEM image of a vertical and tapered ZnSe NW embedding a CdSe QD; (b) Radiation pattern of the QD-NW displayed in (a) through a microscope aperture of NA=0.72; (c) autocorrelation histogram of the NWQD at 300K with a  $g^{(2)}(0)$  value of 0.3.

# Thermoelectric and thermal properties of supported few layers 2D materials

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## Abstract

Two-dimensional (2D) materials have a great potential in the domain of energy conversion due to their unique structure and physical properties [1-3]. However, application of 2D materials as thermoelectric materials depends on the ability to fully explore their physical properties once implemented in real devices, requiring heat flow control at the nanoscale. We present here a complete thermoelectric characterization of devices based on thin flakes of tungsten diselenide (WSe<sub>2</sub>) and multilayer graphene (MLGN) deposited on hexagonal boron nitride (h-BN), by coupling electric and thermoelectric measurements with modulated thermorefectance (MTR) [4]. Our work demonstrates selective non destructive measurements of thermal conductivities and Seebeck coefficients in 2D materials thin flakes embedded in a device configuration. We provide also evidence that nanostructuring can improve the thermoelectric performances of 2D materials by reducing thermal conductivity and increasing Seebeck coefficient without changing electronic transport.

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## Figures



**Figure 1:** 2D material based device for electric and thermoelectric measurements



# Atomic scale characterization of carbon nanotubes combining transmission electron microscopy and deep learning image analysis

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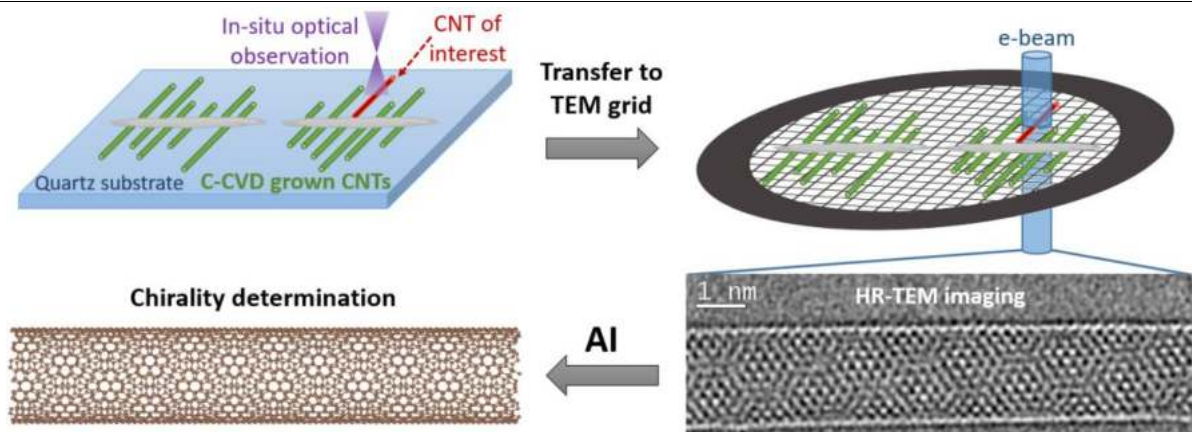
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In the recent years, major breakthroughs were accomplished in single wall carbon nanotubes (SWCNTs) based microelectronics, which has become one of the best candidates to produce beyond-silicon electronic systems [1]. This new technology requires a high level of control over the chirality of SWCNTs, which determines their semiconducting properties. Recently, advanced in-situ optical observations evidenced the complex relationship between the growth rate and chirality of SWCNTs grown by catalytic chemical vapour deposition (C-CVD) [2]. In-depth structural analysis of the SWCNTs identified by the in-situ analysis is now needed for further understanding of the chiral selectivity related to the growth kinetics. High-resolution transmission electron microscopy (HR-TEM) is the most powerful technique to assess local chirality of SWCNTs at the atomic scale. However, combining in-situ optical observations and ex-situ TEM characterization faces two main challenges: i) observation of a single SWCNT of interest by both techniques and ii) a fast determination of chirality from TEM images for high information throughput. Here, we present a unique and powerful characterization process for chirality assessment. This includes an original sample transfer protocol, which allows the localization of a targeted SWCNT inside the TEM. Then a deep learning algorithm [3] enables the fast chiral determination as well as their detailed atomic models directly from single TEM phase images. These observations are expected to help refine our current CNT growth models, by correlating CNTs' local structure with their growth kinetic.

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## Figures



**Figure 1:** Experimental process steps for determining the chirality of a particular CNT grown by C-CVD on a quartz substrate.

# New two-dimensional nanomaterials and devices for phototherapy

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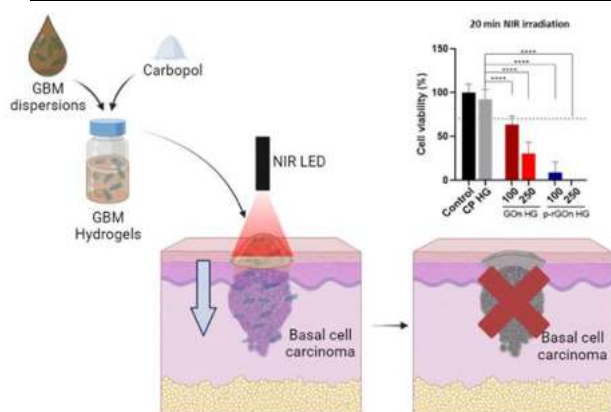
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Nanosized graphene oxide (GOn) is stable in aqueous dispersion, due to the oxygen functionalities on its surface, but possess low photothermal efficiency in near infrared (NIR) region. GOn total reduction originates reduced nanographene oxide (rGOn) that presents high NIR absorption, but poor water stability. In this work, we produced a never before reported partially-reduced nanographene oxide (p-rGOn) by GOn photoreduction using light irradiation, yielding nanometric particles that preserve the original water stability, but acquire high light-to-

heat conversion efficiency. GOn and p-rGOn presented mean particle sizes of  $170 \pm 81$  nm and  $188 \pm 99$  nm, respectively. 8 h of light irradiation allowed to obtain a p-rGOn stable for up 8 months in water, with a zeta potential of  $-32.3 \pm 1.3$  mV. p-rGOn water dispersions have shown to absorb NIR radiation, reaching  $57.2$  °C ( $250 \mu\text{g mL}^{-1}$ ) after 30 min of irradiation. Chemical characterization of p-rGOn showed a decrease in the number of characteristic oxygen functional groups, confirming GOn suitable chemical modification. Additionally, p-rGOn ( $150$ – $250 \mu\text{g mL}^{-1}$ ) has been proven not to have impact on human skin fibroblasts (HFF-1) cell viability, after 24 h of incubation. Furthermore, an innovative custom-built NIR LED-system has developed and validated for 2D-nanomaterials photothermal effect evaluation. Nanomaterials were included in pharmaceutical formulations, and proven effective for skin cancer cells complete eradication, revealing to permeate across human skin. This is the 1st pharmaceutical formulation ever reported to deliver graphene through skin for cancer therapy. A general perspective on the work of our team will be presented, focusing on applications of graphene-based nanomaterials and also of other never before explored 2D-nanomaterials in phototherapy, immunotherapy and 3D-printing for tissue regeneration [1-3].

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# h-BN crystal growth: from synthesis to functional properties

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Whether used as a substrate or as an active layer, high quality 2D hexagonal boron nitride (hBN) holds great promise for future research and applications, especially in optoelectronics. Vapor-phase processes such as Chemical Vapor Deposition can achieve large scale coverage, but selfstanding hexagonal boron nitride crystals provide exfoliated nanosheets (BNNS) of unrivalled purity and crystal quality which are still preferred for demanding applications.

In order to obtain high quality and large size BNNSs, we propose a synthesis route coupling the Polymer Derived Ceramics (PDCs) process with a specific sintering step. [1,2] The hBN obtained by this method has already demonstrated a very high crystalline quality attested by a Raman FWHM value of  $7.6 \text{ cm}^{-1}$ , one of the best reported in literature to date. [2] Our study aims at understanding the mechanisms of hBN crystals growth and the generation of crystalline defects in order to better control the synthesis and to provide hBN with the desired quality. X-ray tomography and SEM observations (Figure 1b, c) provide insights into nucleation and growth orientation. To search for defects in the crystal, its optical (see Figure 1a) properties and the electrical properties of encapsulated graphene are explored. BNNSs exfoliated from these crystals have been used to fabricate graphene field effect transistors showing a mobility up to  $70\,000 \text{ cm}^2/\text{Vs}$  [3]. Such functional measurements allow the assessment of the overall crystal quality and prove to be a powerful tool for the optimization of the process parameters.

These BNNSs have also been used to encapsulate Transition Metal Dichalcogenides (TMDs). Such van der Waals heterostructures have been tested by optical spectroscopy. The photoluminescence widths of  $\text{WSe}_2$  and  $\text{MoSe}_2$  neutral exciton lines at 4K were measured within the 2-3 meV range [2], while non-encapsulated TMD monolayers exhibit photoluminescence line widths of a few tens of meV. These results demonstrate that these BNNSs are relevant for future electronic and opto-electronic applications.

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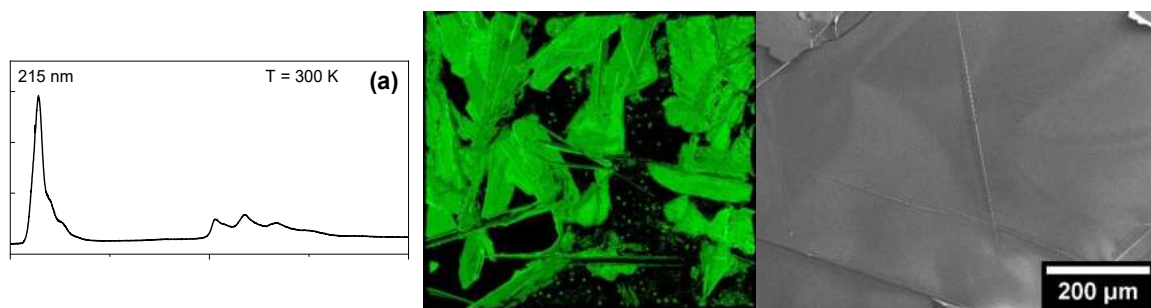


Figure 1: (a) Cathodoluminescence measurement of a PDC hBN crystal [2]; (b) 3D extracted view of entangled crystals inside the as-obtained ingot from X-ray tomography; (c) low magnification SEM view of the crystal surface.

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# Synthesis of ultra-high temperature nanoparticles and nanowire ceramics for spatial applications

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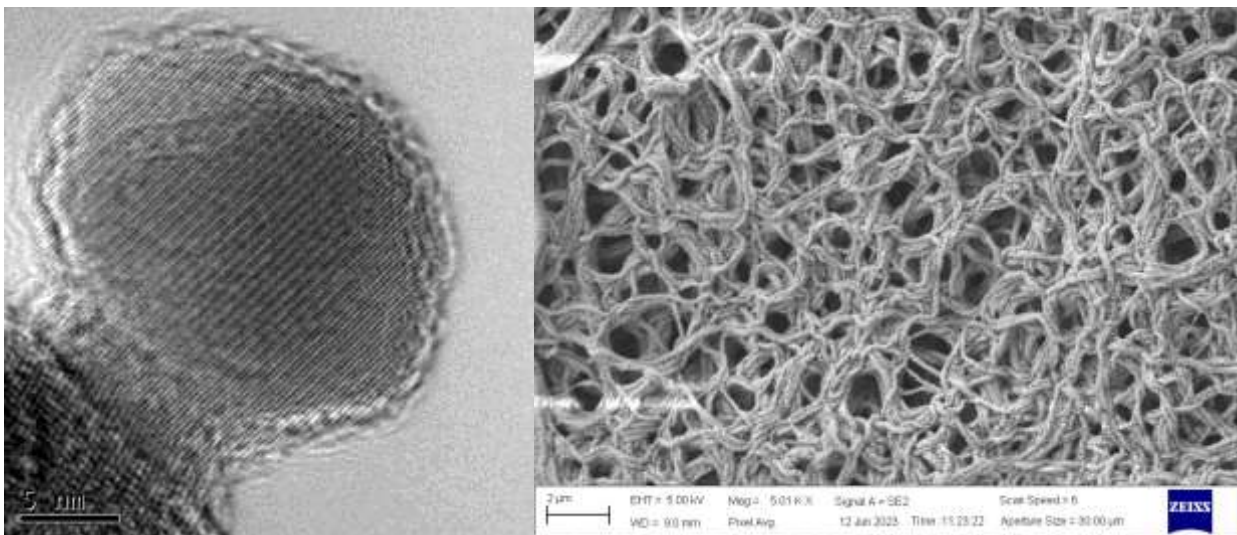
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## Abstract

We are investigating different synthesis routes to produce elemental bricks for the manufacture of ultra-high-temperature ceramic matrix composites for space applications. The aim is to produce materials of controlled composition and size, in the form of nanoparticles and fibres, which can then be assembled to form ceramic matrix composites.

The aim of these materials is to improve both their mechanical strength and their resistance to high temperatures in ablative atmospheres, such as re-entry conditions in the Earth's atmosphere. To this end, the different synthesis routes are all based on a two-step process. First, the synthesis routes are based on Zr, B and C precursors that are intimately mixed. Second, such as the polymer-derived ceramics route, a high temperature step allows pyrolysis of the precursors and reactivity to form ZrC or ZrB<sub>2</sub>.

## Figures



**Figure 1:** left : ZrC nanoparticles synthesized at 1400°C. Right : Nanofibers obtained at 1200°C



# Direct surface structuration and functionalization using localized Atomic Layer Deposition

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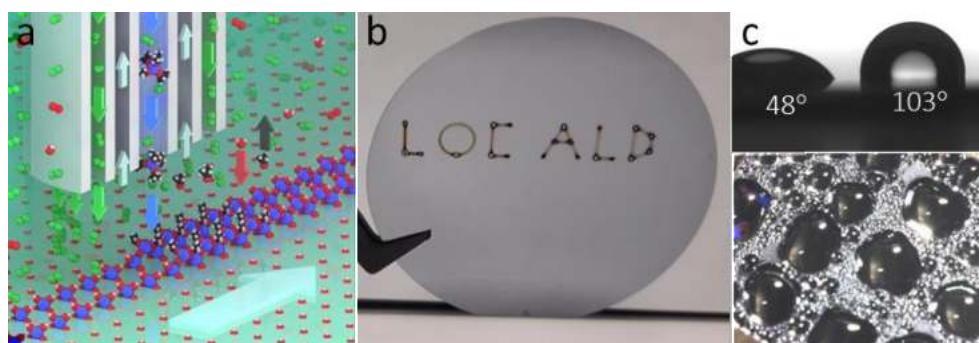
Precise designs of micro- and nanostructures are sought after for many devices and applications such as thin films transistors, diodes, electrocatalysts, solar cells, sensors, or membranes. Additive and subtractive technologies are nowadays areas of extensive research. In particular, additive approaches permit the controlled stacking of layers made of different materials. However, they display limitations either in thickness of the deposited material, in lateral resolution, or structuring scale. Combining control of at least one dimension at the nanometer level with large-scale patterning is still challenging in the direct write approach. Atomic Layer Deposition (ALD) is a technique of choice for depositing thin films with a thickness control at the atomic scale. In particular, direct patterning can be realized using spatial ALD (SALD). [1–3]

Herein, maskless deposition of uniform and homogenous oxide thin films is successfully demonstrated with a lateral resolution tuned from millimeters to hundred micrometers range (Fig1b) while keeping a film thickness in the range of a few to hundreds of nanometers with a control at the nanoscale. A modified open-air SALD head (Fig1a) is employed to fabricate complex oxide patterns on various substrates. [4] The co-reactant being kept in the surrounding atmosphere *i.e.* water from relative humidity in the present case, a simple injection head that consists of three concentric nozzles with only one precursor outlet has been designed. An easy and reversible modification in the diameter of the metal precursor outlet that permits direct patterning with different lateral sizes is demonstrated. This maskless SALD approach also enables controlled surface functionalization. In particular, using alkyl silane, it is possible to locally modify the surface properties (hydrophilic/hydrophobic character...). This is particularly of interest to control water condensation and drop displacement (Fig. 1c).

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## Figure



**Figure 1:** a) Scheme of localized ALD principle and b) photograph of a 76 nm thick  $\text{TiO}_2$  pattern deposited on Si wafer with sub-millimetre lateral resolution. Photographs of c) drops and water condensation on surfaces locally functionalized by an alkyl silane.



# *In situ* Transmission Electron Microscopy experiments on individual nanoparticles

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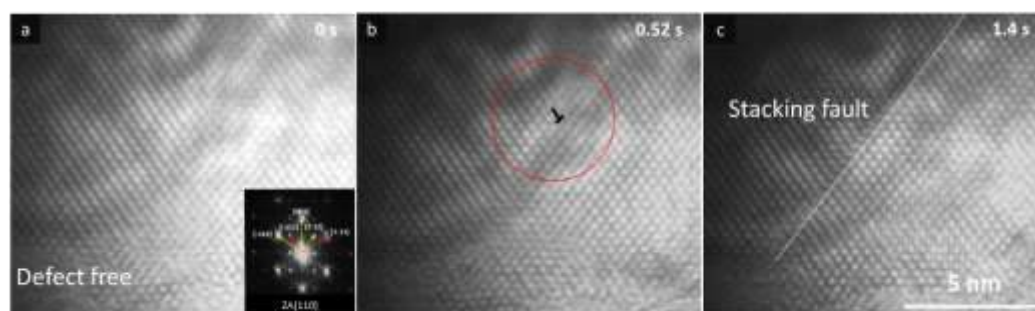
## Abstract

The behavior of oxides at the nanometer scale strongly differs from the one of the corresponding bulk materials. Indeed, large plasticity has already been reported, even at room temperature [1, 2]. Yet, the plasticity of nanoparticles has not really been exploited, probably because the mechanisms are usually not evidenced. We will present *in situ* mechanical tests on individual oxide nanoparticles, using Transmission Electron Microscopy. The key steps, from sample preparation to data processing, will be presented. The case of cerium oxide (CeO<sub>x</sub>) nanoparticles with sizes between 20 and 130 nm will be described. Interestingly, the same particles can be tested with two different structures (bixbyite / fluorite), depending on irradiation conditions (high / low dose rate) and gaseous environment (under vacuum / in air). The deformation mechanism will be evidenced for each crystal structure and compared with simulations results. The differences in the mechanisms will be discussed as a function of the fraction and arrangement of oxygen vacancies. Finally, the evolution of the yield stress vs the nanoparticle size will be analyzed for both crystal structures, similarly to what was performed on MgO [3, 4].

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## Figures



**Figure 1:** *In situ* generation of a stacking fault in a CeO<sub>1.5</sub> nanocube that was initially defect free.

# Enhancing alkaline media nitrogen reduction reaction through formation of 2D/2D hybrid structures of MoS<sub>2</sub>/rGO

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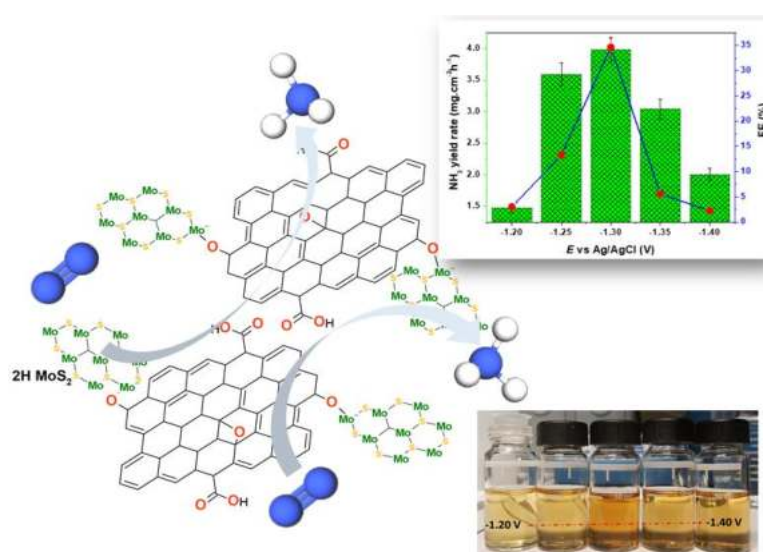
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Given the challenging task of constructing an efficient nitrogen reduction reaction (NRR) electrocatalyst with excellent ambient condition performance, properties such as high specific surface area, fast electron transfer, and design of the catalyst surface, constitute a group of key factors to be taken into consideration to guarantee outstanding catalytic performance and durability[1]–[3]. Thereof, this work investigates the contribution of the 2D-2D heterojunction interface between MoS<sub>2</sub> and reduced graphene oxide (rGO) on the electrocatalytic synthesis of NH<sub>3</sub> in an alkaline media. The results revealed remarkable NRR performance on the MoS<sub>2</sub>@rGO 2D-2D hybrid electrocatalysts, characterized by high NRR sensitivity (Faradaic Efficiency) of 34.7 % with NH<sub>3</sub> yield rate of 3.98 ± 0.19 mg.h<sup>-1</sup>.cm<sup>-2</sup> at the overpotential of -0.3 V vs RHE in 0.1 M KOH solution. The hybrid electrocatalysts also exhibited selectivity for NH<sub>3</sub> synthesis against the production of hydrazine (N<sub>2</sub>H<sub>4</sub>) by-product, excellent hindrance of the competitive hydrogen evolution reaction (HER), and good durability over an operation period of 8 h. In hindsight, the study presented a low-cost and highly efficient catalyst design for achieving enhanced ammonia synthesis in alkaline media via the formation of defect-rich ultrathin MoS<sub>2</sub>@rGO nanostructures, consisting predominantly of HER-hindering hexagonal 2H-MoS<sub>2</sub> phase.

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## Figures



**Figure 1:** Graphical presentation of NRR process on MoS<sub>2</sub>@rGO hybrid nanocatalysts.

# Dielectric properties of 2D water confined in gypsum.

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## Artem Mishchenko

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## Abstract

We investigated how two-dimensional (2D) water sheets behave when confined within the layered mineral gypsum. Our observations revealed that the O-H stretching modes of water localise on two types of O-H dipoles, which exhibit distinct vibration frequencies due to varying hydrogen bonding strengths. This allowed us to independently study the dielectric behaviour of these confined O-H dipoles, which show a distinct vibrational anisotropy, indicating the orientation of O-H dipoles within the 2D confinement. By analysing the vibration frequency under different confinement geometries of O-H dipoles in the presence of external electric field, we uncovered the dielectric polarization of nanoconfined water.

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## Abstract

There is a tremendous need to find new properly functional mimics of natural organelles or cells to address both early diagnostics and efficient therapeutics or to understand in more details cell behavior, if they can be made sufficiently flexible and capable. In particular, soft synthetic nanocompartments can be combined with biomolecules in order to develop artificial organelles. Here we present how DNA-directed arrangement of soft synthetic nanocompartments serves to generate super-assemblies with emergent properties, which can be loaded with biomolecules and/or imaging agents in order to develop medical applications [1]. The size and stability of the resulting DNA-linked compartment clusters have been controlled by manipulating molecular factors such as compartment membrane composition and DNA surface density [2]. These clusters can interact selectively with different cell lines, opening a new strategy to modify and expand cellular functions by attaching them on cell surfaces. To display the breadth of therapeutic applications attainable with our system, we encapsulated medically established enzymes within the inner compartment and demonstrated their activity within the clustered compartments. A step forward has been achieved when such DNA-zipped compartments were able to serve as segregated nanospaces containing therapeutic enzymes (Dopa decarboxylase, DDC) and fluorescent probes for development of nanotheranostics [3]. The diagnostic compartment provides a twofold function: tractability via dye-loading as the imaging component and the ability to attach the cluster construct to the surface of cells. The therapeutic compartment, loaded with active DDC, triggers the cellular expression of a secreted reporter enzyme via production of dopamine implicated in atherosclerosis. The architecture of the DNA-zipped clusters of nanocompartments equipped with biomolecules can be expanded by integrating Janus nanoparticles as core components to induce a specific location of the nanocompartments[4]. Such DNA-mediated clusters of soft or soft-hard components allow a large variety of medical applications by diversifying the types of utilizable active molecules.

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# Universal method for preparing two-dimensional metal dihalides

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## Abstract

Crystal in a reduced dimension exhibits extraordinary characteristics that bring important insights into materials properties and ways to develop high efficiency devices. Being in atomic thicknesses, two-dimensional (2D) materials have revolutionized the materials science and opened a new era for 2D devices (1, 2). Metal halide is an exceptional group of layered materials received extensive attention in the recent decade as a promising 2D system to access low-dimensional physics. While there are several literature reports on the metal trihalide, there has been an increase in the reports on metal dihalide family - a group of layered materials which have excellent electrical and magnetic characteristics that are predicted theoretically to be sustained down to the two-dimensional limit. Here we report a mechanical exfoliation method for a series of 2D metal dihalides, from bulk layered crystals and characterize them by Raman spectroscopy, optical measurements and photoelectron spectroscopy.

Current synthesis methods mostly rely on catalysts/substrates to induce the crystal growth or chemical deposition. Moreover, the stringent requirements for the parent crystals (i.e., high purity, optimization of the sublimation temperature for each crystal and seek for an appropriate catalyst) calls for a unified synthesis methodology when it comes to a wide range of metal halide families. On the other hand, mechanical exfoliation is a simple method to produce 2D materials with high quality; it is a simple and robust method which led to exploration of several 2D materials. To expand the research into the metal dihalides, we need such simple methods which can yield pure crystals and by exfoliation can produce 2D materials with ease.

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# Femtosecond laser induced creation of color centers on the silicon-on-insulator platform and control of their emission directivity with Mie resonators

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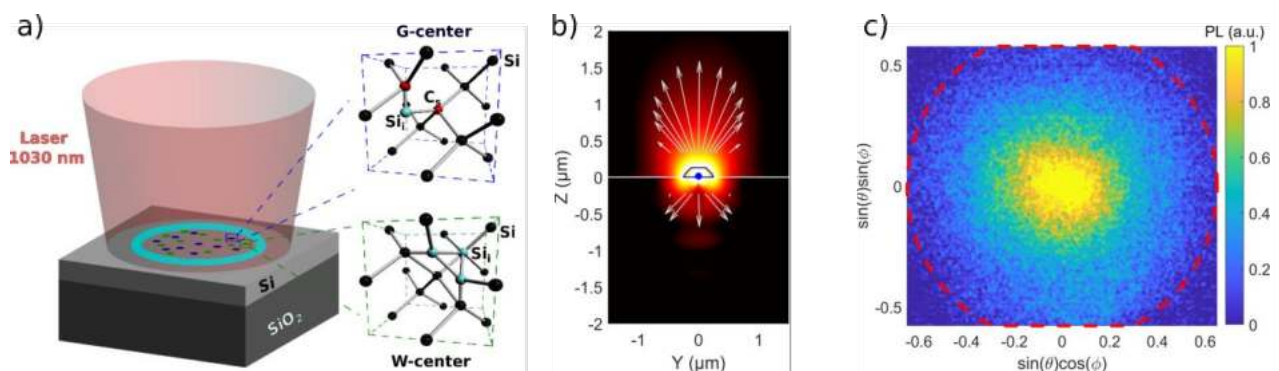
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Researchers and engineers have been exploring ways to integrate light sources in silicon photonics for decades. Recently, fluorescent point defects in Silicon, also known as color centers, have been explored as promising candidates for such light sources. Moreover, individual defects act as single photon sources which paves the way towards the integration of quantum photonic devices with existing silicon-based electronics platforms. However, the current processes for creating such defects are complex, commonly requiring one or two implantation steps. In this work, we have demonstrated implantation-free G and W-centers in commercial silicon-on-insulator substrates using femtosecond laser annealing (see Fig. 1a). Furthermore, we have observed that a low-temperature annealing annihilates the G-centers while slightly enhancing the emission of the W-centers. This allows us to isolate W-centers in a restricted area of a size close to the cross section of the femtosecond laser spot [1]. Furthermore, we have found a way to improve color center emission directivity by embedding them into silicon Mie resonators (see Fig.1 b and c) fabricated by dewetting, achieving an extraction efficiency exceeding 60% with standard numerical apertures. This approach could lead towards ultra-bright telecom band single photon sources in silicon [2].

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## Figures



**Figure 1:** a) Schematic representation of the femtosecond laser irradiation process used to create G and W-centers. b) FDTD simulation of the Poynting vector of the emission of a dipole representing a color center embedded in a Mie resonator. c) Experimental far-field emission profile of G-centers embedded into Mie resonators obtained by angle-resolved photoluminescence spectroscopy.

# Spin-Density Interactions in Metal-Organic Networks/Graphene Heterostructures

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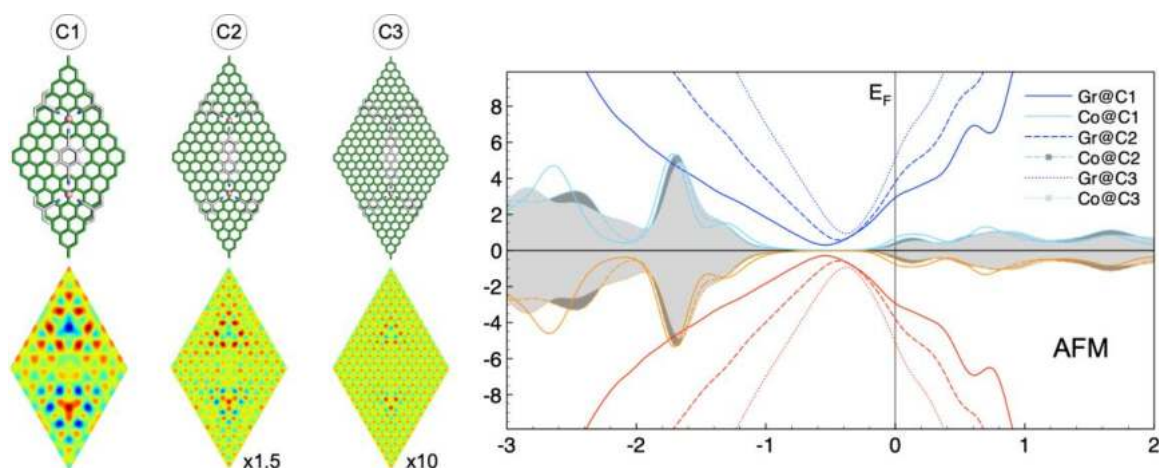
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## Abstract

The influence of a graphene substrate on the electron interaction within two-dimensional metal-organic networks (2D-MON) has been studied with the help of first principle DFT and DFT+U calculations. We have investigated a class of 2D-MON where magnetic Co atoms are bonded to polyphenyl-dicarbonitrile (PPDCN) linkers with different polyphenyl lengths ( $C_n$ ,  $n = 1-3$ ) to modulate the distance between Co atoms from 11.4 (C1) to 19.9 Å (C3). The freestanding 2D-MONs show a ferromagnetic (FM) behaviour that slowly turns to paramagnetic (PM) from C1 to C3 as the Co-Co distance increases. In contrast, the 2D-MON with short linker (C1) adsorbed on graphene demonstrates an antiferromagnetic (AFM) character that also gradually turns into a PM character for longer linkers (C2, C3). The presence of graphene drastically improves the spin interaction between Co atoms of the 2D-MON, and we can clearly observe a magnetic signature in the graphene substrate with spin-polarized scanning tunnelling microscopy (STM) simulations (Figure 1). Moreover, the Co atoms of the 2D-MON are strongly coupled to graphene and contribute to modify its electronic and magnetic properties. This work finally shows that 2D-MON can be used to introduce a magnetic character into graphene and to modify its electronic properties through a non-invasive process.



**Figure 1.** Top view of the unit cell (upper panels) used for the C1 to C3 models, and corresponding simulated STM images of the backplane of graphene (lower panels). Projected DOS of Co atoms and graphene for the AFM phase of C1 to C3 complexes.

# Electron tomography of hydrated beam-sensitive samples

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Beam sensitive samples, such as hydrogels or biological objects, are challenging samples for electron microscopy characterizations. Up to now, it has always been almost impossible to study them in native states by electron tomography. Of course, such materials are characterized in 3D but in cryo or embedded in a resin.

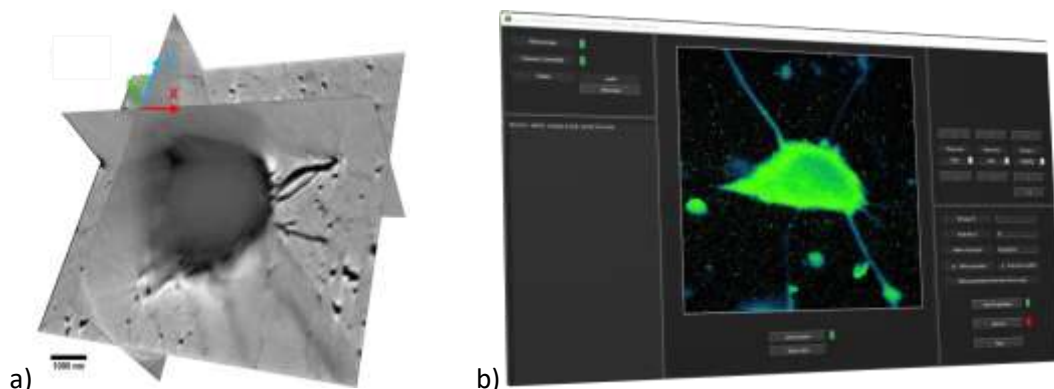
We will present the development of electron tomography of beam sensitive materials close to their native state. Here, the samples are not enclosed in an environmental cell, they are instead preserved in liquid state by cooling the sample at around 1-4°C, while 7-10 mbar of water vapor are insert in the chamber of an environmental electron microscope. [1] We will show developments made to analyze in 3D a full hydrated NIH-3T3 cell. The cell was cultivated on a gold TEM grid and then fixed – but not stained- and imaged in 3D as an entire and fully hydrated object (Figure 1 a)). [2]

Because low beam electron tomography requires fast manipulation of the microscope that become difficult even for most experimented users, we will also describe the principles of a Python code dedicated to fast electron tomography at multi scale at low electron dose. The code is compatible with both E-SEM and E-TEM electron microscopes and enables the 3D characterization of electron beam sensitive materials in native states (Figure 1 b)). Examples will be shown and discussed. [3]

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- [3] The authors acknowledge the CLYM ([www.clym.fr](http://www.clym.fr)) for the access to Quattro ESEM and Titan ETEM (80-300 keV) electron microscopes. This work was funded by ANR (project ANR-20-CE92-0014-01).

## Figures



**Figure 1:** **a)** 3D model of a full hydrated NIH-3T3 cell obtained by BF-STEM electron tomography by using a dedicated E-SEM. **b)** Front image of a Python script developed for low beam electron tomography images recording for E-SEM and E-TEM enabling environmental electron tomography at multi scale.

# Hydrocarbon Contamination in Angström-scale Channels

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Abstract

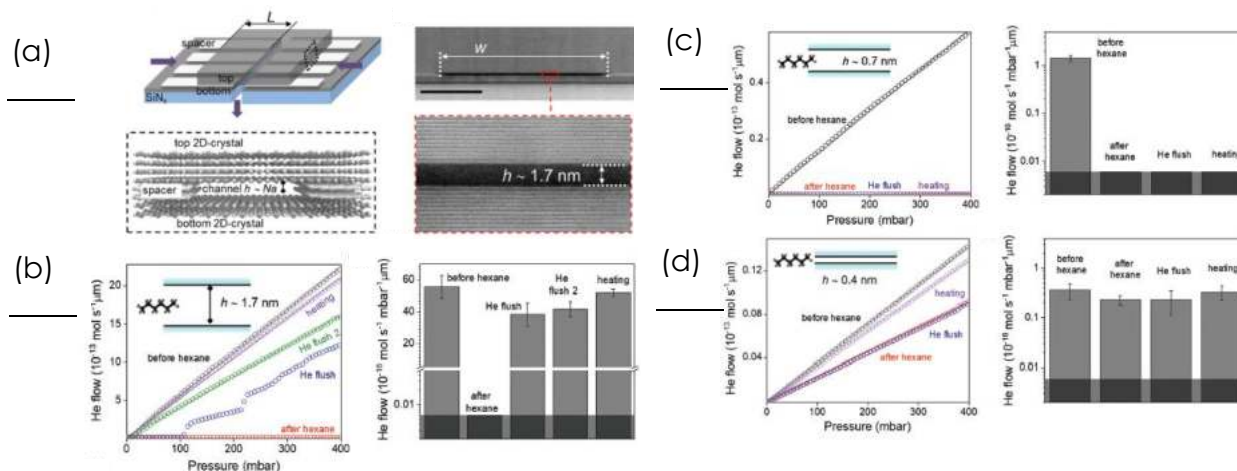
Nanopores and nanochannels made of 2D materials play an important role both in fundamental studies of confined molecular transport [1] and mimicking biological channels. Nonspecific molecular adsorption like airborne contamination occurs on most surfaces including 2D materials and alters their properties. While the surface contamination is well studied, the effect of contamination in a confined system such as nanochannels/pores leading to their clogging is still lacking. We report a systematic investigation of hydrocarbon adsorption in the angstrom ( $\text{\AA}$ ) slit channels of varied heights where hexane is chosen to mimic the hydrocarbon contamination. A dynamic transition of the clogging and revival process is shown in sub-2 nm thin channels and long-term storage and stability of our  $\text{\AA}$ -channels is demonstrated [2]. This study highlights the importance of the nanochannels' stability and demonstrates self-cleansing nature of sub-2 nm thin channels enabling a robust platform for molecular transport and separation studies. We provide a method to assess the cleanliness of the nanoporous membranes, vital for the practical applications of nanofluidics in various fields like molecular sensing, separation and power generation.

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Figures



**Figure 1:** (a) Schematic of a device showing a silicon nitride (SiNx) membrane with angstrom slit channels on top and their length  $L$  is noted. Purple arrows indicate the flow directions of the gas through the device. The below inset shows a schematic representation of a channel displaying the top, bottom and spacer layers, with channel height  $h$  labelled.  $N$  is the number of layers of graphene spacer, and  $a$  is the interlayer distance in graphite. Cross-sectional TEM dark field image of a 5-layer channel, with a magnified view shown below. Horizontal bright lines represent individual layers of graphite, and the dark space is the  $\text{\AA}$ -channel. Scale bar of the top image, 50 nm. (b, c, d) Comparison of helium leak rate before and after exposure to hexane through various graphite  $\text{\AA}$ -channel devices with heights, (b)  $h \sim 1.7$  nm, (c)  $h \sim 0.7$  nm, and (d)  $h \sim 0.4$  nm. The insets show the schematics depicting the relative size of the hexane molecule to the channel in each case. The bar graphs in (b), (c), and (d) represent normalized He flow per unit pressure. Grey shaded area indicates the limit of detection. All the graphs represent the flows normalized per single channel and per  $\mu\text{m}$  length of the channel. Error bars are from two measurements on the same device, and where there was only measurement (e.g., He flush), it represents uncertainty in the best fit to the measured data.



# Thermal radiation across a water nanobubble induced by a heated gold nanoparticle

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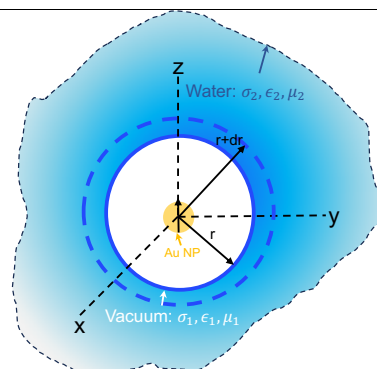
With advancements in nanoscience, precise control of light within the visible and near-infrared ranges has been achieved at the nanoscale, leading to the development of diverse technologies [1]. Metallic nanoparticles (NP) offer a versatile approach to adjusting radiation characteristics through modifications in morphology, size, material, and aggregation. One method for localized heating without physical contact involves introducing metallic NPs into a liquid medium. Steady-state or pulsed illumination generates nanobubbles around the nanoparticles, enabling applications such as optical hyperthermia, microbiology, and solar thermal water heating [1]. Bubble formation involves complex processes like vaporization, heat transfer, and multiple scattering [1]. However, studying thermal radiation between nanoparticles and a liquid has been limited due to the small size of the nanoparticles compared to Wien's wavelength. Accurate evaluation of sub-wavelength thermal radiation requires precise calculations using fluctuational electrodynamics (FE), revealing that small objects can have an effective emissivity exceeding unity [2]. Radiative transfer occurs also through photon tunneling in the near field, which can also be analyzed using FE. This study focuses on evaluating the contributions of radiative heat transfer using the dipole approximation, encompassing both electric and magnetic dipoles within a cavity immersed in a dissipative medium. Considering spherical geometry and employing the Mie theory, we highlight the strong deviation to macroscopic thermal-radiation estimates and underline wave effects. Volumetric near-field absorption in water follows a sixth power relationship with the distance from the origin and a third power relationship with the cavity radius. Observable interferences arise as the system approaches the far-field regime, with spectral signature resonances of water dominating radiative exchange. The findings contribute to a better understanding of radiative exchange in nanoparticle-liquid systems, advancing thermal engineering, bioengineering, and biomedical applications.

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## Figures



**Figure 1:** Au NP- Water nanobubble system approximated as an electromagnetic dipole in a cavity immersed in a dissipative medium i.e. water.

We acknowledge the support of ANR project CASTEX (ANR-21-CE30-0027) and discussion with S. Merabia.



# A flexible and biocompatible nanostructured NbN@Ni foam supercapacitor towards implantable energy storage applications

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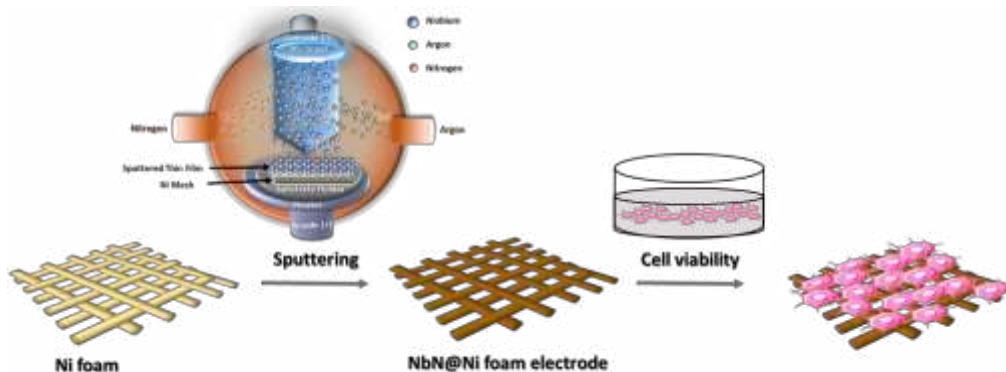
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## Abstract

As the demand of implantable and wearable electronic devices is becoming prevalent, the development of flexible and biocompatible energy storage is imperative. In this study, we have successfully fabricated a flexible and biocompatible electrode towards supercapacitor application. We used DC magnetron sputtering to deposit niobium nitride (NbN) on the nickel foam (Ni foam) substrate to fabricate NbN@Ni foam. The fabricated NbN@Ni electrodes demonstrates highly porous structure with uniform distribution of NbN on nickel foam substrate. The in-vitro biocompatibility of the electrode was assessed using cell viability studies on human embryonic kidney (HEK 293) cell line. The biocompatibility tests revealed no significant cytotoxic effects on the cell lines. The electrode demonstrated excellent electrochemical stability and efficient electrochemical performance.

## Figures



**Figure 1:** Schematic for the fabrication of biocompatible NbN@Ni foam electrode

# Tuning the crystallinity of Boron Nitride using Chemical Vapor Deposition

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2D materials are excellent candidates for current and future electronic devices. Among them, hexagonal boron nitride (hBN) is proving to be a key material for future graphene-based optoelectronic devices,<sup>1</sup> as it is an insulator and an isostructural of graphene. It appears to be a substrate of choice to boost the properties of graphene and thus enable the implementation of this later in real-life applications. Recently, it has been shown that controlling the degree of crystallinity of BN can have a significant impact on its intrinsic properties. For example, amorphous BN displays an ultra-low dielectric constant of 1.16, whereas a value of 4.0 at 1MHz is observed for hBN.<sup>2</sup> Therefore, tailoring the structure of BN and thus its properties would permit widening its application areas, from isolating interconnects and high-performance electronics in optoelectronic to spintronics.<sup>3</sup>

Among the synthesis approaches, Chemical Vapor Deposition (CVD) of hBN has been widely reported in the literature and thin films have been obtained from different precursors such as ammonia-borane, diborane, BCl<sub>3</sub> and borazine (formula B<sub>3</sub>N<sub>3</sub>H<sub>6</sub>).

In the present contribution, BN films with different degrees of crystallinity deposited by CVD are introduced. The impact of the different growth parameters on the final material is presented using the borazine as a single source precursor. Four different gases are investigated: Ammonia, Nitrogen, Ar/H<sub>2</sub> 95/5 and Ar/H<sub>2</sub> 90/10. Particular attention is paid to the influence of the carrier gas flow rate, the type of substrates and the deposition temperature. The obtained films are characterized by ellipsometry, X-ray diffraction, scanning electron microscopy, electron dispersion, Raman and Infra-red spectroscopy.

As expected, the deposition temperature plays a crucial role, although the nature of the carrier gas strongly influences the reactivity of the borazine and thus the final structure of BN. The results show a stoichiometric B:N ratio of 1:1 with very low carbon and oxygen contamination on the films deposited with an Ar/H<sub>2</sub> mixture on the copper foil, while higher oxygen impurities and lower crystallinity are noted on Si(100). Films grown at 1000°C show the presence of small crystallites. Control of the crystallinity of BN films can be achieved by regulating the temperature during the process, allowing the deposition of films within a wide range of crystallinity. Not only copper but also Si 100 has been used as a substrate with similar results without cleaning nor treatment of the substrates.

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# Graphene nanodevices for biochemical detections: from neural spike to ion channel detection within living cells.

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Several types of electronic devices have been developed to detect ions and electrical signals through cell membranes. In the 1950's, patch-clamp was a pioneer method to record either spiking activity (e.g. neural cells) or ion channel currents. Then, because they are easily interfaced with cells, microelectrodes (MEs) appeared as robust and less damaging method to follow neural activity. But these devices are still limited in term of electrical sensitivity and spatial resolution. Over the past decade, this sensitivity was enhanced by developing field-effect detection. Indeed, field-effect transistors (FETs) allow to reach higher electrical sensitivity while reducing the channel length. Meanwhile, bioelectronics sensing has been also improved by using graphene to design microelectrodes or FET channels. Because of their high sensitivity and chemical stability in liquid media, the graphene FETs, we have developed, are an ideal platform for biomolecular and ion sensing. These devices are used to detect analyte composition[1] or pH[2] changes, proteins activity such as ion channels[3] and electrical signals within electrogenic cell[4][5]. Here we show our recent works about (1) hybrid biosensors to transduce biological signals from *Xenopus* oocytes with ultra-high sensitivity down to individual ion channels and (2) on real-time opto-electrical recordings within neuron network that open avenue of investigations for sensing living matters and ionic fluids in general.

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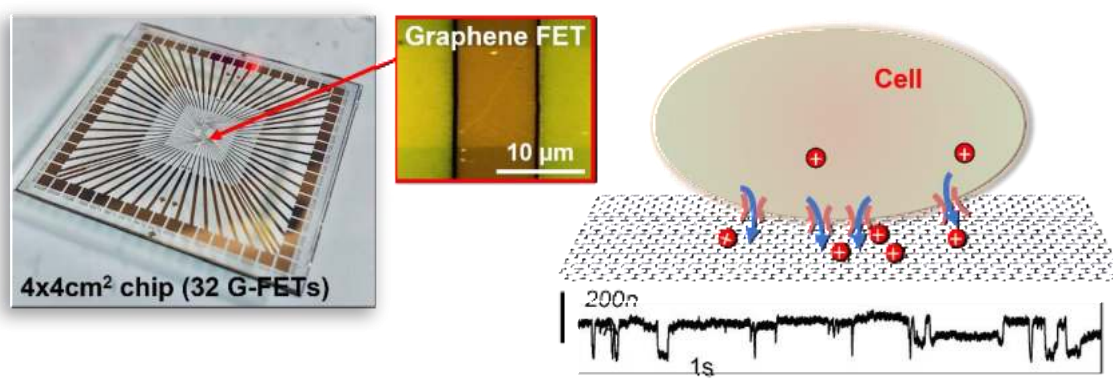
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## Figures



**Figure:** Graphene-FET detection of ion channel activity at the cell interface

# Surface/Interface effects for size-selected FeRh nanomagnets deposited on perovskite oxide crystals

## F. Tournus

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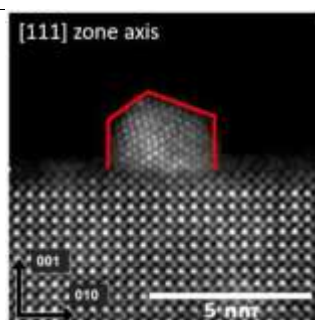
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The major importance of surface atoms in small nanoparticles (NPs) offers the opportunity to tailor magnetic properties by playing with the interface between a nanomagnet and its surrounding. FeRh alloy has attracted a lot of attention because the bulk material presents an antiferromagnetic to ferromagnetic order (AFM-FM) transition close to room temperature, for the chemically ordered B2 phase. Inspired by epitaxial FeRh film studies on perovskite oxide [1], and motivated by the possibility to obtain hybrid multiferroic nanosystems, we have studied the structural and magnetic properties of size-selected FeRh clusters (diameter < 10 nm) deposited on perovskite oxide surfaces. For this system, a strong interplay between surface configuration, morphology and magnetic state is taking place [2,3]. FeRh nanomagnets have been deposited on BaTiO<sub>3</sub> thin films and SrTiO<sub>3</sub> single crystals, using the mass-selected low energy cluster beam deposition technique (MS-LECBD) under ultra-high vacuum. Using synchrotron radiation, we have observed the chemical ordering of FeRh nanoparticles into the B2 crystalline phase upon annealing, which is also accompanied by a Fe magnetic moment evolution visible from X-ray magnetic circular dichroism (XMCD) measurements. The orientation dependence of x-ray diffraction FeRh peaks indicates that particles, despite their random deposition, are finally adopting preferential orientations. In addition to the usual epitaxy relationship met for thin films, a novel orientation is observed (corresponding to a 45° in-plane rotation), as well as other favorable coincidences for particles on SrTiO<sub>3</sub>. At the same time, X-ray spectroscopy at iron edges reveals that NPs assemblies, systematically appear to be (partially) oxidized after transfer in air while FeRh nanoparticles can be reduced thanks to in situ vacuum annealing. Concerning magnetic behavior, as for previous FeRh NPs embedded in carbon matrix [2], no metamagnetic (AFM-FM) phase transition has been observed from XMCD measurements.

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## Figures



**Figure 1:** cross section image (STEM-HAADF) of a FeRh nanoparticle on the SrTiO<sub>3</sub> surface.

# Synthesis and surface modification of Quantum Dots for solid-state lighting applications

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In the past decades, thanks to their low toxicity, InP QDs have been extensively studied as replacements for Cd-based QDs materials in display and lighting applications. However, InP QDs have low stability under photonic/thermal stresses and their synthesis remains a challenge. I will describe a new method to tune the size of InP QDs using a novel precursor reactivity approach. Using several amino phosphine precursors with ethylenediamine substituents, the reactivity could be adjusted and the size of tetrahedral QDs controlled (edge lengths from ~ 3 to 6 nm). The underlying mechanisms were clarified by combining <sup>31</sup>P liquid NMR and UV/Visible spectroscopies. [1]

The passivation of InP QDs using anhydrous n-alkylammonium fluoride was used to improve the PLQY and luminescence linewidth. n-Alkylammonium fluoride etches the QD liberating PH<sub>3</sub> and phosphorus oxides from the surface. The product surfaces are stabilized by metal fluorides and ammonium fluorides, which narrows the absorption and luminescence linewidth (FWHM as low as 42 nm) and increases the PLQY. The small size and the electron withdrawing properties of fluorine leads to a high surface coverage, which supports excellent surface passivation.

In order to protect the QDs in using conditions, a layered double hydroxide (LDH) matrix was designed to host red-emitting InP/ZnS core-shell QDs, yielding original high-performance functional QD-bola-LDH hybrids. The easy incorporation into silicone-based resins makes these hybrid phosphors attractive for high-tech applications. A proof-of-concept LED prototype has proven to be very promising, displaying a high color rendering index, suitable for implementation in high CRI white LEDs. [2]

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# Fully-Printing Methods for Flexible Supercapacitors and Soft Sensors

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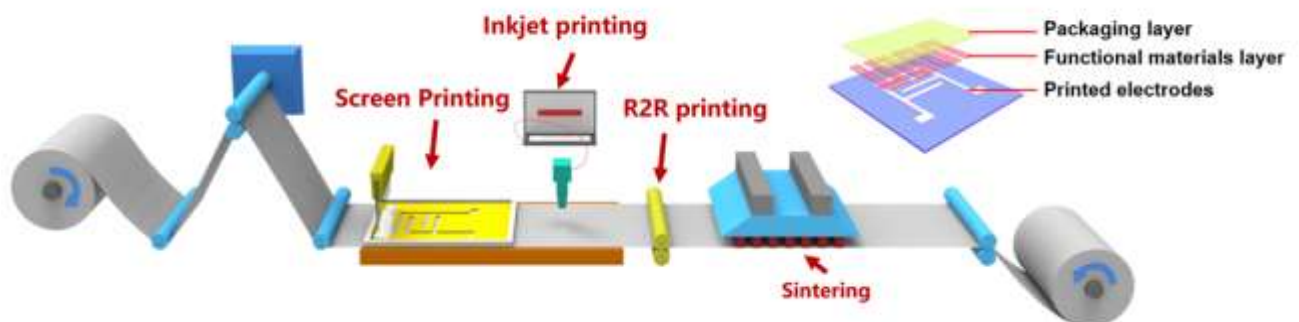
## Abstract

The rapid development of printed electronics technology has promoted the development of flexible electronic devices. Among them, fully-printed electronic technology is expected to further reduce the manufacturing cost of flexible electronic devices, and play a huge advantage in the pattern construction of special-shaped devices. The development of novel printable functional materials and the preparation of functional inks with good printability are prerequisites for the fabrication of printed electronics. Based on large-area screen printing technology, it will focus on the progress in printed sensors and flexible energy devices, and clarify the development and application prospects of fully printed electronic devices.

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## Figures



**Figure 1:** Schematic illustration of fully-printing process for multilayer flexible electronic devices

# Photo magnetism in glasses doped with cobalt

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By doping glass, a non-magnetic material, with cobalt, a magnetic material, their individual properties combine, resulting in the emergence of new properties [1]. This study aims to investigate the magnetic and magneto-optical (MO) properties of cobalt thin films and cobalt-doped Soda Lime Glass (SLG). An in-situ simultaneous MO measurement and oxidation via laser irradiation of a cobalt thin film was performed.

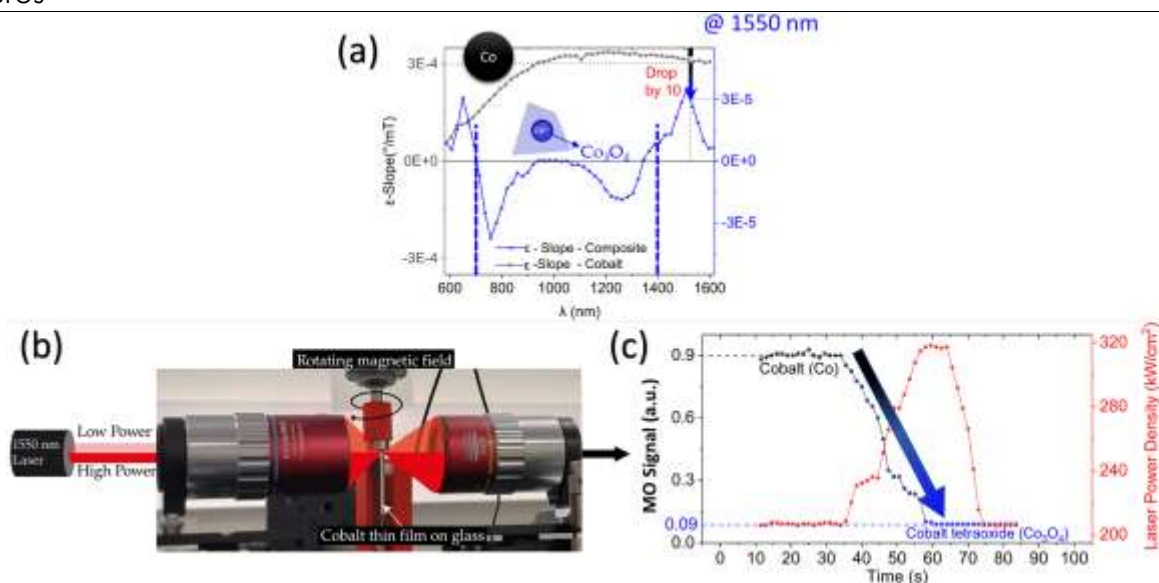
Figure 1(a) illustrates the MO spectral behavior, showing a smooth increasing of the Faraday ellipticity for cobalt thin films, similar to the Drude dispersive model for metals [2]. Conversely, in the case of glass doped with cobalt, the spectrum exhibits two distinct bands. These bands correspond to the MO dipolar transitions of  $\text{Co}^{2+}$  ions in tetrahedral sites, which exist in the  $\text{Co}_3\text{O}_4$  structure only[3]. Notably, the overall MO effect of cobalt, after its diffusion into the glass matrix, decreases tenfold, specifically at 1550 nm. To investigate the oxidation of a cobalt film, in-situ measurements were performed by simultaneously heating the cobalt thin film with a 1550 nm continuous wave laser, as depicted in Figure 1(b-c). The detected oxidized phase was confirmed to be  $\text{Co}_3\text{O}_4$ , as evidenced by the tenfold drop in measurements.

We are currently investigating the reversible transformation of  $\text{Co}_3\text{O}_4$  to  $\text{CoO}$  in the glass doped with cobalt using the in-situ experiment presented in Figure 1 (b), exploring its potential for photomagnetic features in data storage and optical MO switching applications.

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## Figures



**Figure 1:** Magneto-optical spectral behaviour of cobalt and cobalt-glass composite (a). Simultaneous in-situ laser treatment (b) and magneto-optical oxidation measurement (c).

# Excitons in disordered Boron Nitride

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Hexagonal Boron Nitride (hBN) is a two-dimensional material well-known for its strong excitonic effects. Recently, defects in hBN have attracted considerable attention for application in optoelectronics, such as single-photon emitters. Concurrently, *amorphous* Boron Nitride (aBN) has been identified as an ultralow dielectric constant material with potential for next generation interconnects [1]. There is thus at present a need for methods to compute the excitonic properties of large disordered systems, and investigate the interplay between disorder, electron-hole Coulomb interaction and dielectric screening. Using BN as a prototypical system, we start from a tight-binding (TB) description of its electronic structure and perturbatively map the Bethe-Salpeter equation onto an effective TB Hamiltonian [2]. We are then able to extract relevant properties of large systems at a low computational cost by means of real-space linear scaling techniques (KPM, recursion...) [3,4]. As proof of concept, we discuss optical absorption in hBN in the presence of Anderson disorder as well as a toy model of structurally disordered BN based on aBN geometries obtained by molecular dynamics [5].

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## Acknowledgements

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This presentation has received funding from the PETITE project, under grant by EIG CONCERT-Japan. This project has been supported by Samsung Advanced Institute of Technology, the European Union's Horizon 2020 research and innovation program under grant agreement No 881603 and the REDI Program, a project that has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement no. 101034328. ICN2 acknowledges the Grant PCI2021-122092-2A funded by MCIN/AEI/10.13039/501100011033 and by the "European Union NextGenerationEU/PRTR". Molecular dynamics simulations were performed at the King Abdullah University of Science and Technology-KAUST (Supercomputer Shaheen II Cray XC40). The ICN2 is funded by the CERCA programme / Generalitat de Catalunya and supported by the Severo Ochoa Centres of Excellence programme, Grant CEX2021-001214-S funded by MCIN/AEI/10.13039/501100011033.



# Controlling magnetic anisotropy in graphene spinterfaces

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Graphene-ferromagnet heterostructures have acquired significant attention for their use in two-dimensional spintronic circuits as spinterfaces. Because of its tunable electrical properties, long-spin diffusion length, and scalability [1–3], graphene stands out as an ideal material for engineering new spinterfaces [4]. In this study, we investigate the controllability of graphene spinterfaces by characterizing the magnetic properties of the cobalt thin films grown over graphene through magneto-optic Kerr effect (MOKE) measurements. We observe drastic changes in magnetic anisotropy and coercivity of the thin film heterostructures under different interface conditions achieved by intermediate ultrathin metal-oxide layers. We conduct a comprehensive microstructural analysis of the heterostructures to gain insights into the underlying mechanisms that lead to the modifications induced by interface conditions. Furthermore, we also explore the electrical control of magnetic anisotropy in such graphene-ferromagnet heterostructures. This investigation opens unique pathways for new tunable spintronic interfaces.

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# Different approaches for nanocomposite characterization: the role of organization of the nanoparticles

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Dispergation of nanoparticles in a polymer matrix is a key task in the preparation of nanocomposites. Atomic force microscopy (AFM) can be used for the detection of the homogeneity of the nanoparticle distribution, assessing the quality of their dispersion inside the bulk material or on its surface as well as checking that the incorporation procedure has a minimal impact on the morphology of the nanoparticles. In this study, we focused on the comparison of several types of nanoparticles, i.e. (1) in situ-prepared fully oriented layers, (2) nanolayers having a house-of-card architecture in the matrix and (3) randomly or oriented nanolayers in the matrix. The shape and the size of the primary nanoparticles were characterized after spin-coating of their dispersion in the solvent as well as in a matrix with the identical dispergation method as used for the nanocomposite. The results are compared to the cut and surface of the nanocomposite.

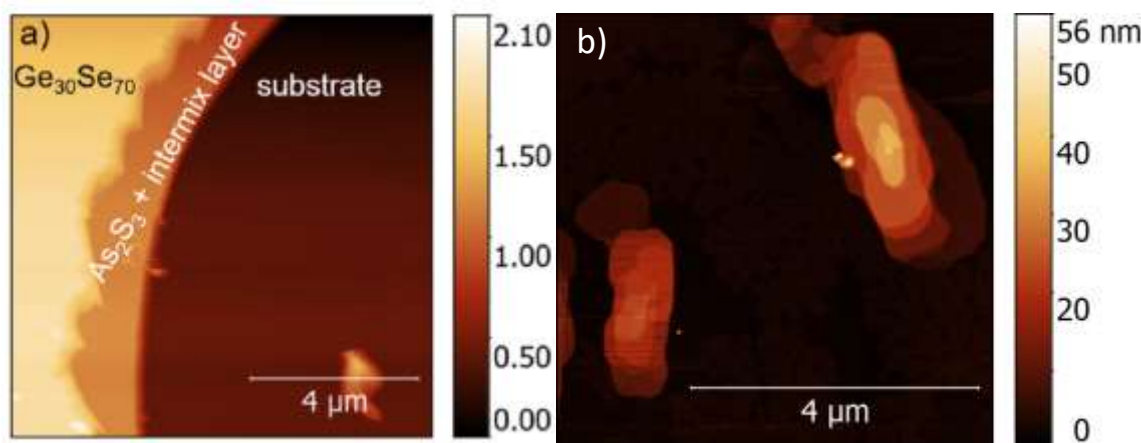
The comparison of the fully oriented nanocomposite (layered chalcogenides prepared by a photo-induced solid-state reaction of chalcogenides [1]), non-reactive nanomaterials (calcium phenylphosphonate [2]) and tunable polyborazylene (the size and reactivity are changed by the annealing [3]) enables the illustration of different approaches of the preparation of the samples, AFM measurement modes and necessity of other characterization techniques (BET, spectroscopies, etc.).

The project is financially supported by the Czech Technology Agency (No. FW06010094).

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Figure



**Figure 1:** The illustration of the sandwich-like chalcogenide thin film formed by the solid-state reaction (a) and polyborazylene (annealed at the 700°C) on the substrate (b)



# Ultrafast spin dynamics in graphene-ferromagnet interfaces

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Graphene is an extraordinary material for electronic charge and spin transport, which makes it ideal for spintronic applications[1], and it presents a novel pathway for the exploration of ultrafast graphene spintronics. Metal oxides and ferromagnets form key components of graphene spintronic systems. While metal oxide layers serve as tunnel barriers for efficient spin-polarized tunneling and non-invasive surface charge transfer doping in graphene[1,2], controlling ultrafast spin dynamics in ferromagnets can enable new spintronic and magnonic applications[3]. In particular, ferromagnet interfaces with graphene reveal striking properties[4,5]. In this work, we fabricate graphene-ferromagnetic interfaces with and without oxide tunnel barriers and investigate how such graphene heterostructures can lead to the control of ultrafast spin currents electrically at graphene-ferromagnet junctions. These studies show how interfaces with oxide layers lead to changes in ultrafast spin dynamics in graphene ferromagnet interfaces. Finally, our experiments reveal that doping control of graphene can significantly impact ultrafast spin dynamics. These results provide new ways to influence the growing research and technological fronts in two-dimensional ultrafast spintronics.

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# 3D-AFM imaging of the liquid-solid interface at the nanometric scale

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Solid-liquid interfaces are of great abundance since they occur whenever a solid meets a liquid. Investigating these interfaces is of great importance for the fields of science, medicine and technology. But, regardless of their importance, there are very few techniques to study these interfaces at the atomic and molecular scale. However, a new technique was recently developed for interfacial characterization: the 3D-Atomic Force Microscopy (Figure 1a) [1,2].

In general, AFM is used for surface characterization where a 2D topographical image of the surface is generated. Also, AFM can be used in 1D as force spectroscopy where point-by-point force vs z-distance curves are measured. 3D-AFM is a combination between these two techniques where a 3D image of the phenomena occurring above the surface, i.e. the interface, is generated. In this work, a 3D – AFM system is implemented in a conventional 2D-AFM apparatus (Park System's NX10) and the study is focused on the characterization of gold surfaces functionalized with thiol polymers for tribological and biological applications.

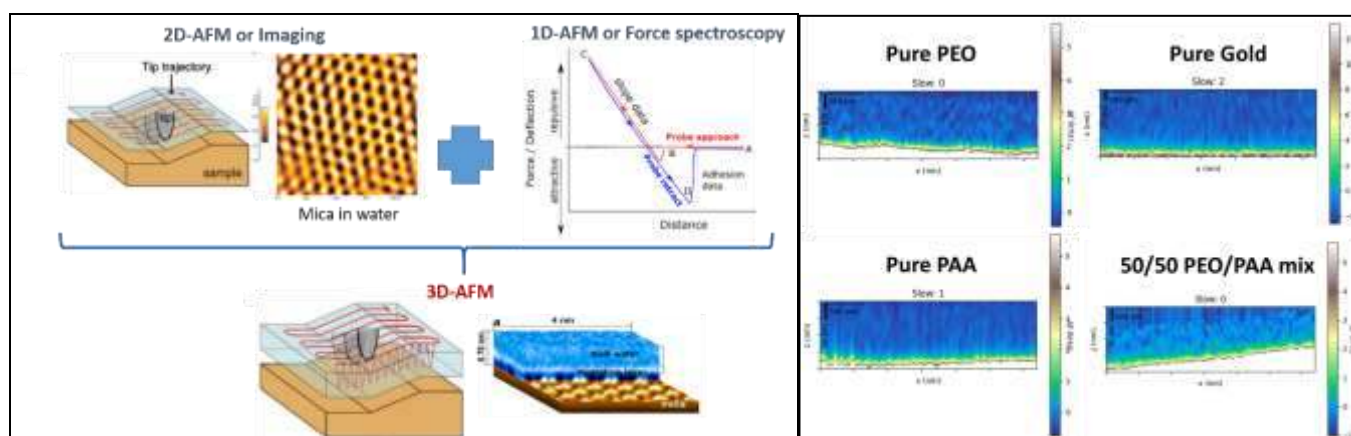
Four samples were used: pure gold, pure Poly(Acrylic Acid) PAA, pure Poly(Ethylene Glycol) PEG, and 50/50 PAA/PEO (figure 1a). We measured these samples in pure water and in a 0.01M PBS solution. The shifts in the frequency  $\Delta f$  recorded during the 3D-AFM scan were used in a Python program to create a 2D (xz) colour coded cross-sectional image of the scanned samples (Figure 1b). Our first experiments tend to show that this 3D-AFM method is appropriate to visualize the difference in behaviour between the samples caused by different polymer chain-tip interactions during the measurement. Our future work consists of generating force/distance curves using the  $\Delta f$  curves and the Sader-Jarvis equation. Then a 3D force map of the sample can be created by combining the several 2D (xz) cross-sectional force maps created.

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## Figures



**Figure 1.** Representation 3D-AFM (left image) and 2D (xz) cross-sectional images of the pure PEO and the mixed PAA/PEO samples scanned in a 0.01M PBS solution by 3D-AFM (right image)

# Tunneling switching mechanism in non-semiconductor materials

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## Abstract

The era of silicon, which can no longer adhere to Moore's Law, is coming to a close. The exponential increase in data due to the development of artificial intelligence (AI) has not been matched by a corresponding increase in the speed of components required for data processing. To overcome these limitations, research is currently underway on switching devices that utilize various 2D materials and switching mechanisms, as well as doping for improved operational speed. One such approach is the metal-insulator-metal (MIM) structure using the tunneling mechanism, which offers many advantages for high-speed operation but suffers from inefficient switching behavior. Researchers are exploring ways to enhance switching efficiency through work function differences [1], geometrical asymmetry [2], and heterojunction tunneling barriers [3], but significant results have yet to be demonstrated.

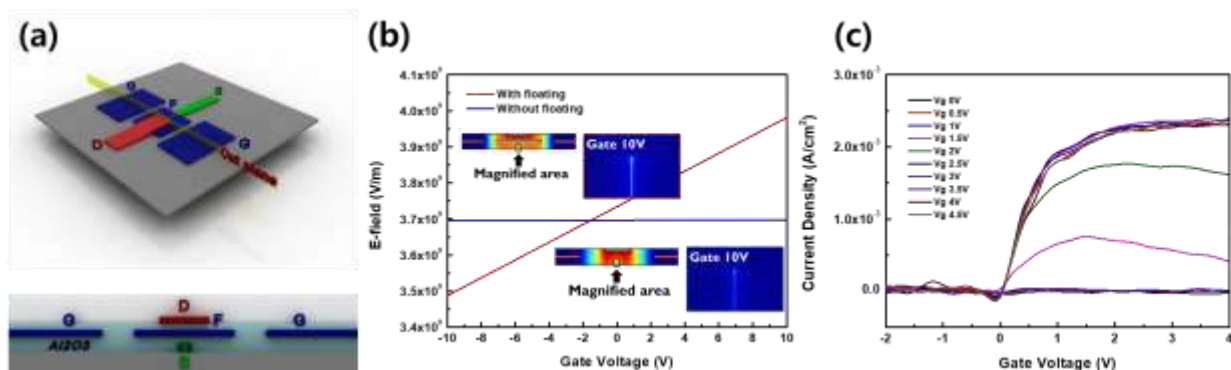
To address this issue, we propose a novel approach that employs geometric asymmetry and a floating electrode to improve switching behavior. Our proposed transistor features a vertical channel and lateral gate structure for controlling step tunneling by the floating electrode, allowing for high-speed operation and high-efficiency switching concurrently. Compared to conventional CMOS transistors, our transistor exhibited an extremely low leakage current and an extremely low capacitance, thanks to its structural advantages.

Overall, this novel approach has the potential to enhance the performance of conventional FETs and contribute to the development of low-power consumption devices and high-speed electrical systems.

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## Figures



**Figure 1:** Tunneling switching device by controlling floating electrode (a) schematic illustration (b) the effect of a floating electrode to tunnelling switching behavior (c) the electrical characteristics of tunnelling device with floating electrode

# Near-Field Radiative Heat Transfer Between a Sphere and a Flat Surface in the Sub-200 nm Regime and Prospects for Energy Harvesting

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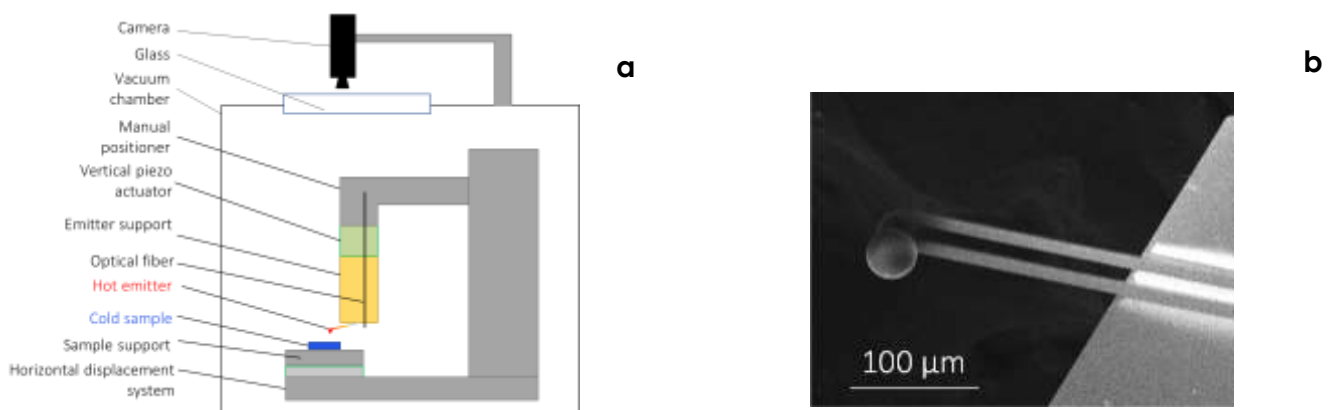
When the distance between objects decreases below the characteristic wavelength of thermal radiation (few micrometres in the 300-1000 K range), the radiative heat exchanged between these objects is increased beyond the blackbody limit imposed by Planck's law in far field. This increase of thermal radiation, which takes place in the near field and is due to the additional contribution of evanescent waves, can reach several orders of magnitude. This phenomenon can be of interest for thermal-energy harvesting. For instance, thermophotovoltaics (TPV) can take advantage of this enhancement of the radiative heat flux in order to increase the electrical output power density when the emitter is brought closer to the cell [1].

As the radiative flux between objects depends dramatically on distance, it is critical to determine it with extreme precision. We report on our recent efforts to evaluate the stability of our experiment. It involves a heated micrometric sphere as the emitter, which is glued on a Scanning Thermal Microscopy probe cantilever. The emitter is moved towards the cold sample or a pn junction (TPV cell or Light Emitting Diode, LED) using a piezoelectric actuator while the radiative transfer is measured throughout the approach. We analyze the vibrations of our cantilever-based system during the approach with combined means of interferometry, optical deflection and resistive thermometry in order to provide accurate data in the sub-200 nm distance regime. We discuss the prospects for energy harvesting by means of TPV or thermophotonics, a technology close to TPV where the emitter is a hot LED.

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## Figures



**Figure 1:** (a) Schematic of the near-field radiative experiment and (b) SEM image of the spherical heated emitter

# Two-dimensional electron system Pt/Ge (111) for Spintronics

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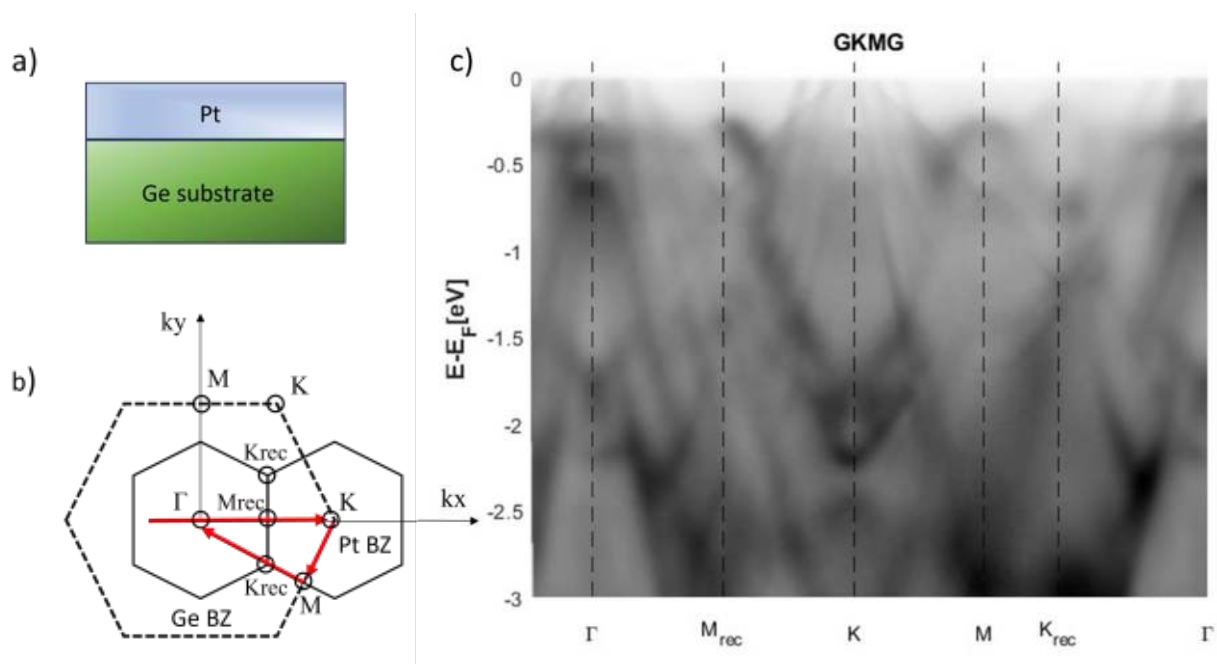
Abstract

Spintronics, which aims to exploit the electrons spin for the development of novel information storage or logic devices [1], is nowadays a major and competitive research field in physics. Exploiting spin degree of freedom increases the functionality of electronic devices and enables such devices to overcome physical limitations related to speed and power. Currently, one of the most promising way to achieve the desired control of the electrons spin is by the application of external electric field in presence of the so called Rashba spin-orbit coupling (SOC). The essential feature of Rashba SOC is that a spin-polarized electron moving in an electric field experiences an effective magnetic field which drives the precession of the spin orientation even without an external magnetic field [2]. In this study, we investigated the electronic properties of Pt single atomic layer on Ge(111) by molecular beam epitaxy (MBE) in an ultra-high vacuum (UHV) environment. Our preliminary results, obtained through angle-resolved photoemission spectroscopy (ARPES), suggest the presence of a possible Rashba SOC in the system. These findings provide valuable insights for the potential utilization of Rashba SOC in Pt/Ge electron system for future applications.

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Figures



**Figure :** a) Scheme and b) reciprocal space geometries of Pt/Ge(111) and c) ARPES results along the red path.



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