

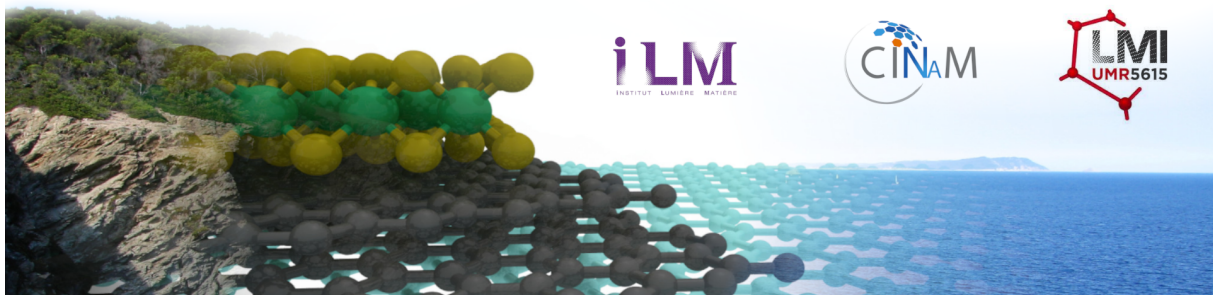
GDR HOWDI Annual Colloquium 2023

May 8th - 12th, 2023
Porquerolles - France

BOOK OF ABSTRACTS



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Van der Waals hetero-structures of low dimensionality is both a national research group (GDR 2112) and an international coordination network (IRN Graphene and co)

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	<u>Mon. 08</u>	<u>Tue. 09</u>	<u>Wed. 10</u>	<u>Thu. 11</u>	<u>Fri. 12</u>
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Monday, 18:45-19:45

Spectroscopy

2D MATERIALS SPECTROSCOPY - A TUTORIAL FROM THE THEORY PERSPECTIVE

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How do we know what we know about the structures and the properties of 2D materials? There are a few methods that enable us to “see” the atomic arrangement “directly”: scanning tunneling microscopy (STM), atomic force microscopy (AFM) and transmission electron microscopy (TEM). Diffraction methods such as X-ray diffraction or low-energy electron diffraction (LEED) give information about the structure in reciprocal space. But for a full characterization of a material’s chemical composition, the number of layers, the interaction with the substrate, doping, impurities, etc., it is a plethora of spectroscopic methods that can provide the missing information.

In many cases, spectroscopic methods need detailed theoretical modeling to get a maximum of information from the measured spectra. In this tutorial, I will explain how this interaction of experiment and theory works for some prototype spectroscopy methods: Optical absorption, luminescence, and Raman spectroscopy. The analysis usually starts with a calculation of the electronic band structure and, in the case of vibrational spectroscopy, the phonons of the material. In many cases, this information is readily available in online materials data bases. A complete understanding of the peak intensities, however, requires the calculation of optical dipole matrix elements, electron-phonon coupling and – in many cases – excitonic effects, which tend to be particularly pronounced in 2D materials. I will try to give an easy-to-follow introduction to all these concepts and about available online tools/data bases. I will talk about the role of symmetries and selection rules and the role of the reduced dimensionality in spectroscopy of 2D materials.

Modern theoretical spectroscopy benefits from decades of intense theory and method development. I will explain some of the theoretical/computational concepts such as density-functional theory and ab-initio many-body perturbation theory and give tribute to the many recent developments in the electronic structure community. Finally, I will make some publicity for the European Theoretical Spectroscopy Facility (ETSF, <https://www.etsf.eu/>), a loose network of research groups in Europe which are heavily engaged in electronic-structure method development and which can provide theory support for various methods of spectroscopy and various materials.

Cross section for phonon assisted absorption, involving excitons with finite wave vector \mathbf{q} :

$$\alpha(\omega) \propto \sum_{\nu} \int_{\mathbf{q}} \sum_{S'(\mathbf{q})} \left| \sum_{S(0)} \frac{g_{S'(\mathbf{q})S(0)}^{\nu} d_{S(0)}}{\hbar\Omega_{S'(\mathbf{q})} + \hbar\omega_{\nu\mathbf{q}} - \hbar\Omega_{S(0)}} \right|^2 \delta(\hbar\omega - (\hbar\Omega_{S'(\mathbf{q})} - \hbar\omega_{\nu\mathbf{q}}))$$

Exciton-Phonon coupling, composed of electron-phonon and hole-phonon couplings:

$$g_{S(0)S'(\mathbf{q})}^{\lambda\mathbf{q}} = \sum_{\mathbf{k},c,v} \left[\sum_{c'} \left(A_{c'\mathbf{k}+\mathbf{q},v\mathbf{k}}^{S'(\mathbf{q})} \right)^* g_{c'\mathbf{k}+\mathbf{q},c\mathbf{k}}^{\lambda\mathbf{q}} A_{c\mathbf{k},v\mathbf{k}}^S - \sum_{v'} \left(A_{c\mathbf{k},v'\mathbf{k}-\mathbf{q}}^{S'(\mathbf{q})} \right)^* g_{v\mathbf{k},v'\mathbf{k}-\mathbf{q}}^{\lambda\mathbf{q}} A_{c\mathbf{k},v\mathbf{k}}^S \right].$$

Figure 1: Some of the advanced formulas that you are going to see in the tutorial. (Don’t worry, you will also see some easy sketches and some colorful figures.)

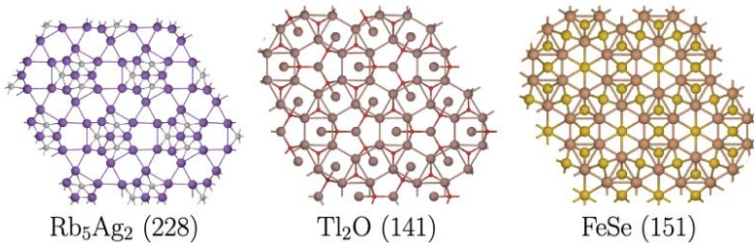


Figure 2: Some novel predicted 2D structures (Hai-Chen Wang, M.A.L. Marques, L.W. A. Romero, et al, [arXiv:2212.03975](https://arxiv.org/abs/2212.03975) [cond-mat.mtrl-sci]). But what do their spectra look like?

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Tuesday, 8:40-10:00

Strain Properties

GENERATION OF NOVEL HETEROSTRUCTURES BY EXTREME PRESSURE CONDITIONS IN LOW DIMENSIONAL SYSTEMS

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The application of pressure, which is by definition a 3-dimensional variable, has opened up new possibilities for studying low-dimensional systems such as nanotubes and 2D van der Waals atomic layers. By subjecting these systems to extreme conditions, changes in geometry and dimensionality are induced, resulting in the emergence of heterostructures. These heterostructures are the product of complex coupling with the system environment, including the substrate, pressure-transmitting media, and other low-D systems. In some cases, these environmental factors become integral components of the structure, leading to the formation of unique and fascinating heterostructures. Our research investigates the generation of these heterostructures, shedding light on the fundamental processes that govern their formation and properties.

We have obtained a comprehensive phase diagram for carbon nanotubes under high pressure, encompassing all diameters and numbers of walls [1]. Through this work, we have discovered that the critical pressure of radial collapse is accurately described by a modified Lévy-Carrier law. Furthermore, we have identified a buckling mechanism that appears to be universally linked to discretization [2,3], with heterostructural molecular filling offering a means of controlling this process [4,5]. At even higher pressures, the tubular geometry of the nanotubes breaks down, giving rise to the formation of ribbons or layers [6] - a phenomenon that can even occur within the tubes themselves.

Our research has uncovered the crucial role played by substrate interaction in the behavior of 2-D van der Waals systems under hydrostatic pressure [7]. This interaction gives rise to a range of phenomena, including anisotropy of strain and charge-transfer between layers [8], strong evolution in the resonance properties [9] or the formation of stochastic folds in response to pressure [10]. These folds can even result in the unbinding of n-layered graphene samples, highlighting the complex interplay between environmental factors and material properties. Excitingly, we have found that combining intercalation and high pressure offers a new pathway for the design of novel 2D systems, as our modeling work demonstrates.

These findings deepen both our understanding of the behavior of low-dimensional systems under extreme conditions and offer new opportunities for the design of novel materials with tailored properties for a wide range of applications, from nanoelectronics to energy storage.

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GDR HOWDI 2023 MEETING: CARBON NANOTUBE MECHANICAL MASS SENSOR WITH SINGLE MOLECULE RESOLUTION AT ROOM TEMPERATURE

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Carbon nanotubes (CNTs) are incredible materials with very unique mechanical, thermal and electrical properties due to their sp^2 -hybridization resulting in nearly perfect atomic structures. Another interesting property of CNTs is their lightness with masses in the attogram range ($1 \text{ ag} = 10^{-18} \text{ g}$). Moreover, CNTs are bottom-up materials and do not suffer from surface defect as their top-down equivalent NEMS which are etched from silicon or nitride substrates [1]. Using those two properties, striking sensitivity was demonstrated in a cryogenic environment with a sensitivity of 1.4 yg [2], which is the mass of a single proton ($1 \text{ yg} = 10^{-24} \text{ g}$). Yet, this sensitivity was reported to be much worse at room temperature, about 25 zg [3] ($1 \text{ zg} = 10^{-21} \text{ g}$). This has prevented the use of CNTs as sensors in real-life applications.

In this work, we demonstrate that CNTs mechanical resonators can scope as well striking sensitivity at room temperature, down to 270 yg . Noise mechanisms that could limit the sensitivity were conscientiously investigated. Such limitations could come from electrical fluctuations, temperature drifts, residual molecules in the gas phase and Brownian motion to name only the most important ones. We established that our set-up operates closely to the Brownian noise limit and is not constrained by external sources of noise. Interestingly, the sensitivity does not seem to degrade when the pressure is increased meaning this sensitivity might be preserved up to ambient pressure. Last but not least, the striking sensitivity observed here is similar for several CNTs, making it a reliable and reproducible asset.

Our work opens up the possibility to implement single-molecule sensing, in various situations such as biological applications, metrology, mass spectrometry or surface sciences [4].

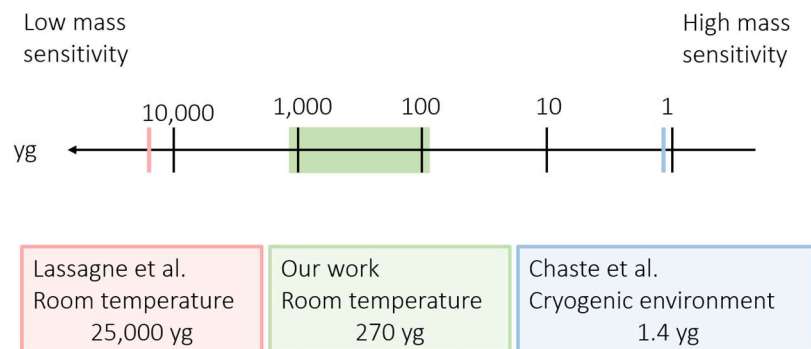


Figure 1: Illustration of the mass sensitivity, found by different research group, using carbon nanotubes mechanical resonators at room temperature or in cryogenic environment.

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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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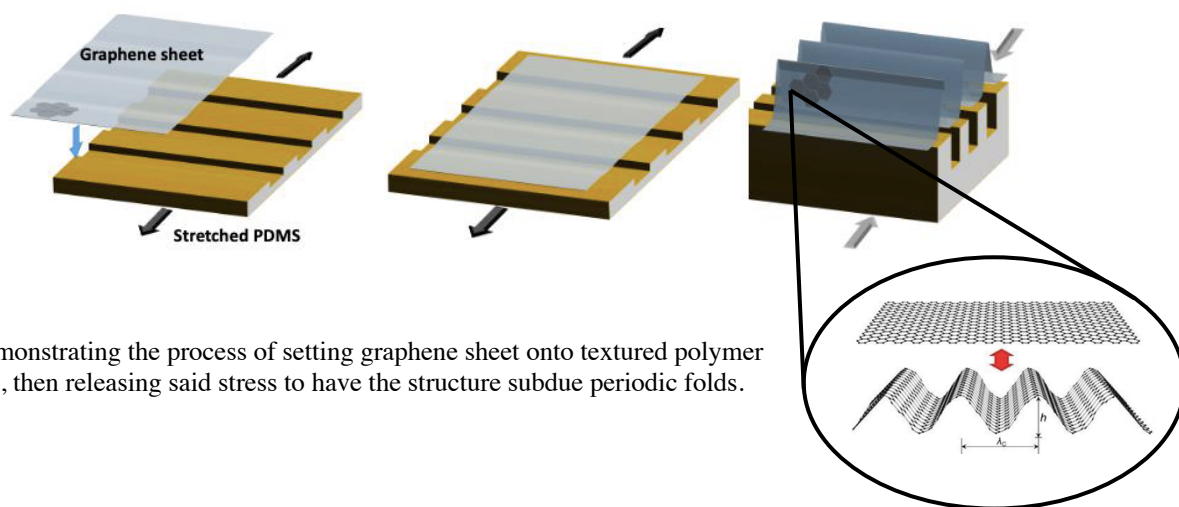


Figure 1 : Fig. demonstrating the process of setting graphene sheet onto textured polymer with a given stress, then releasing said stress to have the structure subdue periodic folds.

MAPPING OF STRONG AND TUNABLE MECHANICAL COUPLING OF 3R-WSE₂ DRUMS

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Straintronics is the use of strain to engineer properties of materials. This field is in constant evolution in 2D materials thanks to their extreme sensitivity to strain variation. All properties of these materials can be modified by strain engineering.

Nanodrums of 2D materials are very sensitive to strain variations. These static variations significantly alter the mechanical vibrations and behaviour of the drums. A simple electrostatic gate effect or a thermal dilatation via Joule heating efficiently tune the vibration of the material¹. We have transferred this tunability to coupled mechanical modes. Coupled Regimes between different vibrational modes could be used for the transfer of information. The quest for coherent and strong coupling regimes is then necessary for these applications. 2D materials have shown very strong coupling at cryogenic temperatures² between separated resonators and at room temperature for coupling of different modes of the same resonator³.

Here we demonstrate the strain engineering leading to a tunable mechanical coupling between two connected circular nanodrums at room temperature. We studied and mapped the shape of the localized modes of each resonator and the coupled, delocalized modes of the system. We used separated local gates to actuate electrostatic forces independently on each resonator (Figure 1-a) and tune the frequency of vibration and the coupling via small strain variations. We demonstrate that we can achieve coupled regime between the drums of 5% of the mode frequency (Figure 1-b) at room temperature. We increase the cooperativity to values greater than 60 at room temperature (Figure 1-c). The simplicity of our model system and the resonant mode maps allow us to play with the coupling and to describe the transition from two localized modes, on two resonators nearby, to a larger resonator with two harmonic modes fully delocalized.

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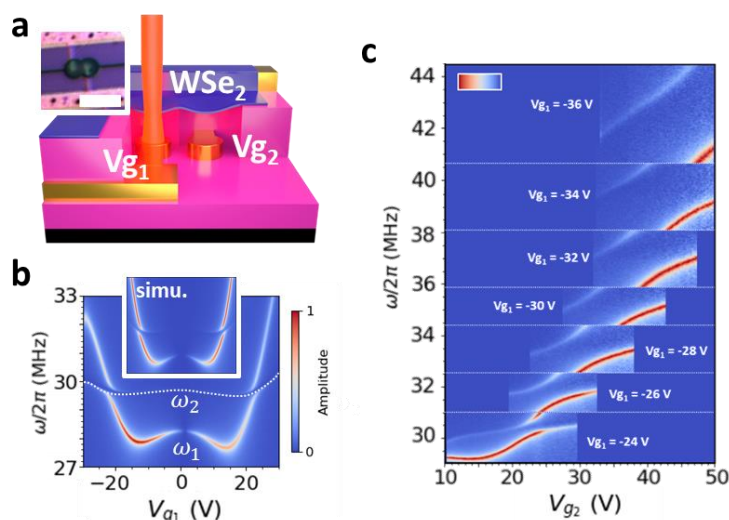


Figure 1: Mode coupling in 2D materials. a) Scheme of the experimental device. 2 membranes of WSe₂ connected mechanically and actuated separately. Inset: optical image of the device. Scalebar: 5 μm. b) Frequency/Vg characteristics of membrane 1. When $f_1 = f_2$, we observe an anti-crossing indicating an effective coupling. Inset: numerical simulation. c) Tunable coupling strength and cooperativity between membranes' mechanical modes.

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Tuesday, 10:30-12:00

Electronic transport

Non-identical Moiré Twins in Bilayer Graphene on hBN

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Assembly of 2D materials into van der Waals heterostructures has recently been a novel technique to deterministically manipulate electronic structures and, thereby, to achieve new properties and states of matter [1,2]. In these heterostructures it is possible to design the novel band structure by mixing materials and then further controlling it by the modification of interlayer spacing and layer rotation [3,4]. In particular, layer rotation has been demonstrated to strongly affect the band structure of graphene, both, on hexagonal boron nitride (hBN) and in twisted bilayer graphene structures. However, little is known on how other factors, such as layer atomic relaxation impact the properties of the heterostructure. In this talk, we present our recent study [5] showing that two moiré superlattices created by bilayer graphene aligned with hBN do not share the same electronic properties, and thus produce non-identical moiré twins. These two moiré superlattices actually correspond to 0° and 60° alignments of graphene and hBN layers. They are indeed shown to be not equivalent in electron transport measurements, although the similar superlattices of monolayer graphene on hBN suggest an identical behavior. In particular, we show the presence of a fully developed valley Hall effect in the 0° case but its complete absence at 60°. We explain these surprising results by numerical simulations, which show that the atomic reconstruction plays an important role on the electronic properties of these moiré superlattices. Indeed, the electronic band structures are very similar for the unrelaxed systems but present significant differences when the atomic relaxation is taken into account, thus giving rise to the valley Hall effect in one case and making it absent in the other. This could be essentially explained by different reconstruction patterns (consequently, different staking patterns) obtained in these relaxed structures.

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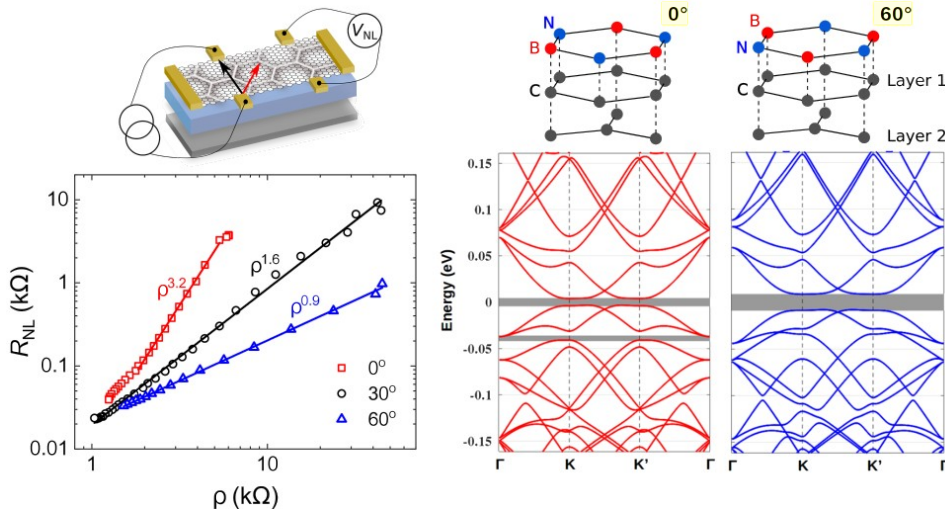


Figure 1: (Left) Non-local resistance as a function of the local resistivity, both at the CNP, for different angular alignments. (Right) Atomic and electronic band structures in two perfectly aligned cases.

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GDR HOWDI 2023 MEETING: PHOTO-FERROELECTRIC VAN DER WALLS NEUROMORPHIC DEVICE

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Recently, 2D ferroelectric materials have attracted interest due to their intrinsic ferroelectric properties.¹ Moreover, their van der Waals (vdW) interfacial coupling capabilities ease their implementation into complex hybrid architecture challenging with standard thin film technology.² Here, I will demonstrate the non-volatile electrical and optical control of the ferroelectric polarization in all-vdW ferroelectric/semiconductor heterostructures.³ The wavelength-dependent study unveils ferroelectric polarization control and decouples the mechanisms that are driven by photogenerated carriers for each material. The vdW Ferroelectric Field-effect transistors show On/Off ratios exceeding 10^7 , large hysteresis memory windows, and multiple remanent states, sorting them as good artificial synapse candidates. Following, long-term potentiation/depression, and spike rate-dependent plasticity are shown using electrical control. Moreover, the synaptic functionalities were complemented by the unique dual optical and electrical control, enabling optically stimulated and optically assisted synaptic devices. We benchmark our device with a simulated artificial neural network and achieve an excellent accuracy level of 91%, close to the ideal synaptic case (96%). The combination of the Photo-Ferroelectric functionalities and the shown synaptic characteristics put all-VdW ferroelectric/semiconductor heterostructures on the roadmap for novel computing architectures.

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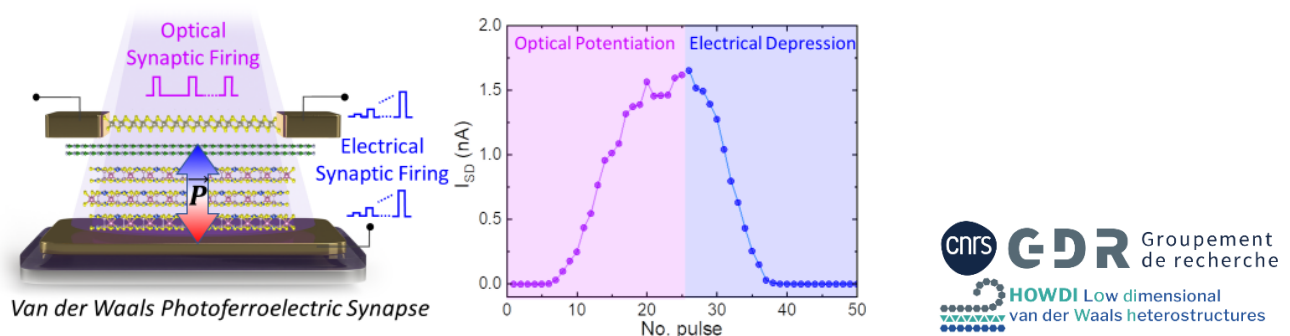


Figure 1: Left: schematic of the device.

Right: Light potentiation/Electrical depression synaptic Plasticity.

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GDR HOWDI 2023 MEETING: GALVANOMAGNETIC EFFECTS IN GRAPHENE: ROLE OF ELECTRON-HOLE PUDDLES AND FERMI VELOCITY RENORMALIZATION

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Graphene Hall sensors (GHS) are very promising devices for industrial applications such as biosensing, position sensing, or data storage reading, but also for fundamental investigations as high lateral resolution magnetometers [1]. In fact, the uncommon electronic properties of graphene, such as its extremely high carrier mobility, its one atomic thickness, and its low carrier density, allow to build micrometer-sized sensors [2-4] that can operate over a wide range of magnetic field and temperature with a sensitivity overpassing the best Hall sensors based on standard semiconductors [3]. The trend of continually pushing sensor performance requires a deep understanding of the physics behind the sensor. In the case of GHS, the physics of Hall Effect cannot be accurately captured by the so-called two-channel model. Hence, we develop a model of galvanomagnetic effects based on Boltzmann formalism that goes beyond and which considers, among other geometry effects, electron-hole puddle formation, diffusion current, bias current influence, energy-dependent scatterers, as well as the formation of highly conducting edge channels [5]. All these ingredients put together allow our model to accurately reproduce our experiments conducted on GHS based on CVD graphene or based on exfoliated graphene encapsulated in boron nitride (hBN). In particular, its main successes are to explain the bias current influence on the amplitudes and shapes of the longitudinal resistance R_{xx} and the magnetic field sensitivity $S_I = R_{xy}/B$ (Figure 1) as well as to explain the rich behaviour (linear and sublinear behaviour) of the magnetoresistance (Figure 2), especially close to the charge neutrality point [6]. Finally, as our model allows us to distinguish the thermal doping from the one caused by the electrostatic environment, intentional or unintentional, it allows us to reveal that to explain the highest recorded S_I in hBN encapsulated graphene [2], a Fermi velocity renormalization has to be considered due to the high permittivity environment [6].

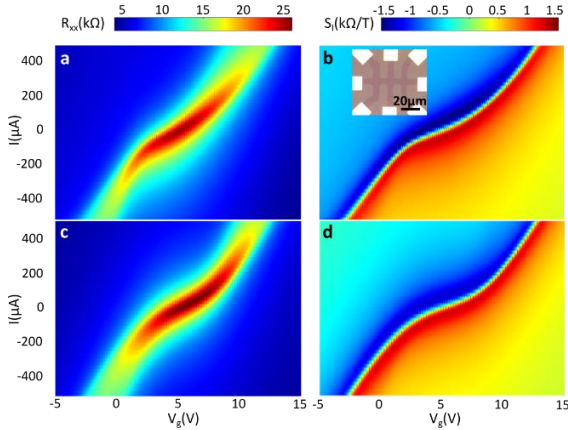


Figure 1: **a, b**, Experiments on CVD graphene (inset: device optical image) performed at 200 K and 1 T. **c, d**, Simulation. **a, c** R_{xx} and **b, d**, S_I as function of gate voltage and current.

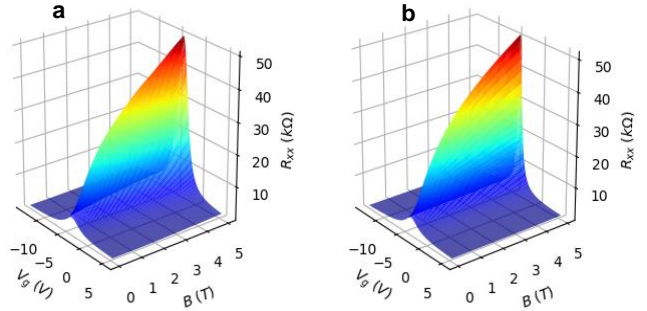


Figure 2: R_{xx} as a function of gate voltage and magnetic field performed with a bias current of 1 μ A at 300 K. **a** Experiments, **b** Simulation.

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GDR HOWDI 2023 MEETING: PROXIMITY-INDUCED ANOMALOUS HALL EFFECT IN GRAPHENE USING TOPOTACTIC GROWTH OF EUO

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Graphene has unique electronic and mechanical properties. The carrier concentration in graphene can be controlled by the gate voltage and it has long spin flip lengths due to weak spin-orbit interaction. It has emerged as a potential candidate in exploring the exciting field of spintronic but is non magnetic. Several ways have been followed in order to achieve a ferromagnetic graphene among which the proximity-induced ferromagnetism appears as a promising method. When kept in proximity to a ferromagnetic material like EuO a large spin polarization has been theoretically predicted [1] opening the way to various interesting phenomenon and new spintronic device concepts [2]. In this work we describe the experimental efforts which includes the growth of magnetic Europium Oxide thin film by an original Molecular Beam Epitaxy method, and their structural and magnetic characterizations. Finally, we present transport measurements revealing Anomalous Hall effect in Graphene in proximity with EuO thin film. Two types of magnetic order are observed where a transition occurs from a ferromagnetic (FM) behaviour to a superparamagnetic (SPM) like behaviour when increasing the temperature. Surprisingly, a large SPM signal survives up to room temperature which could make possible new spintronic applications in graphene.

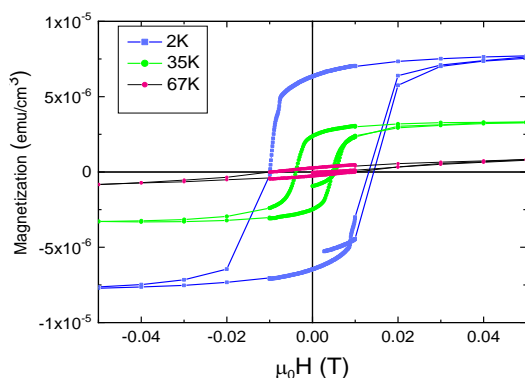


Figure 1: Squid measurements showing a ferromagnetic signal in graphene/EuO heterostructure

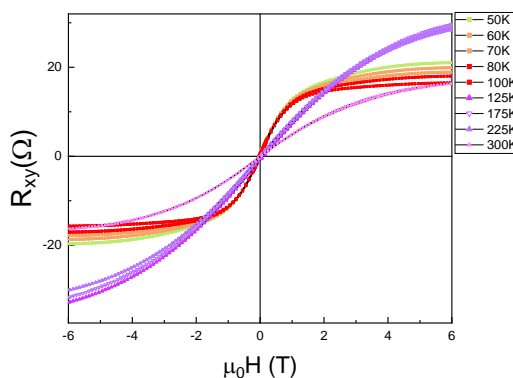


Figure 2: Magneto transport measurements revealing AHE in graphene in proximity to EuO thin films

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Tuesday, 13:30-15:10

Spin properties

TUTORIAL ON SPINTRONICS WITH 2D MATERIALS

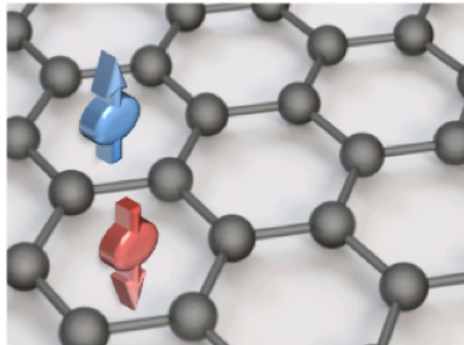
J. Peiro, H. Wei, F. Brunnett, V. Zatzko, M. Piquemal-Banci, R. Galceran, M. Galbiati, F. Godel, A. Vecchiola, C. Carretero, S. Collin, M.-B. Martin, B. Dlubak and
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Spintronics is a paradigm focusing on spin as a unifying information vector : from quantum information to non-volatile data storage. Beyond the first generation data storage revolution, and next generation fast and ultra-low-power non volatile devices such as the new STT-MRAM, it aims at providing complex spin processing architectures (logic gates, spin FET, etc) for a powerful beyond CMOS solution. The discovery of graphene and 2Ds has opened novel exciting opportunities in terms of functionalities and performances for spintronics devices.

In this tutorial, we will introduce key transport concepts for spintronics with 2D materials and provide examples of experimental results, revealing the promising potential impact of 2D materials for spintronics (from early graphene and h-BN to TMDs, etc.). After a brief introduction to spintronics, we will first address why spintronics originally became interested in 2D materials. Indeed, while spin/magnetism was praised for information storage, a longstanding paradox was that spin information could not be transported easily. Despite two decades of intense efforts, efficient spin transport remained elusive. We will highlight the stringent physics conditions that apply to spin transport channels and review initial results, demonstrating that 2D materials have the potential for unprecedented, highly efficient spin information transport, leading to large spin signals and macroscopic spin diffusion lengths.

We will then discuss new developments and explore unexpected opportunities for 2D materials in spintronics, particularly in MRAM, even with single layers, ranging from ferromagnet passivation and use in wet/ambient low-cost processes such as ALD to anisotropy and extreme spin-filtering. In this context, we will emphasize almost perfect band structure spin-filtering and spin proximity/hybridization effects, well beyond conventional inorganic spintronic materials. We will show how this unveils new physics while serving as a key enabler for the advent of envisioned beyond-CMOS spin-based logic architectures.



In collaboration with :

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CORRUGATION INDUCED SPIN RELAXATION IN GRAPHENE

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Controlling spin relaxation rate is important to design devices intended to be applied in spintronics. Since spin injection and detection was demonstrated, graphene has been considered to be applied for spintronic devices. One reason is its low spin-orbit coupling, that allows spin to travel further while can be modified via proximity effect with other materials (such as TMDs).

However, studies report spin relaxation times orders of magnitude lower than predicted by theory. In the other hand, atomic disorder in graphene have been predicted by Guinea et al. [2] to possibly have a deep impact in spin orbit interaction. Here we develop a KPM (Kernel Polynomial Method) real space approach [1] combined with Molecular dynamics relaxations to deal with such real space deformation and study them to estimate the contribution of corrugation to the spin dynamics of a corrugated graphene sample in a wide range of gate voltages and make a discussion based on the main spin relaxation processes known.

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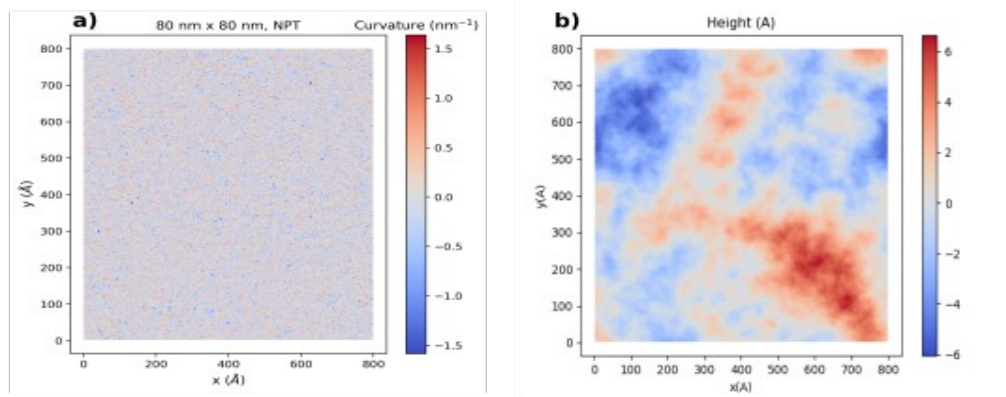


Figure 1: Characterization of the MD relaxed sample both in curvature and Height

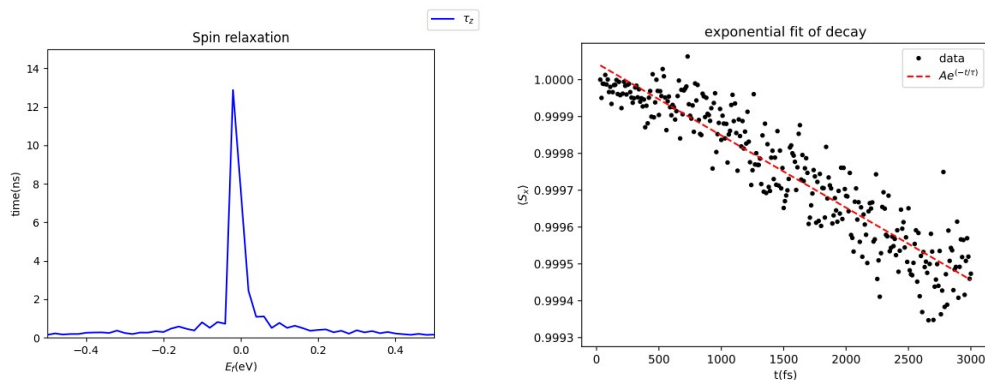


Figure 2: Spin relaxation times computed for the graphene sample (right) and spin relaxation variation with gate voltage (left)

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ARTIFICIAL GRAPHENE SPIN POLARIZED ELECTRODE FOR MAGNETIC TUNNEL JUNCTIONS

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2D materials offer the ability to expose their electronic structure to manipulations by a proximity effect. This could be harnessed to craft properties of 2D interfaces and van der Waals heterostructures in devices and quantum materials.[1,2] We explore the possibility to create an artificial spin polarized electrode from graphene through proximity interaction with a ferromagnetic insulator to be used in a magnetic tunnel junction (MTJ). Ferromagnetic insulator/graphene artificial electrodes were fabricated and integrated in MTJs based on spin analyzers.[3] Evidence of the emergence of spin polarization in proximitized graphene layers was observed through the occurrence of tunnel magnetoresistance. We deduced a spin dependent splitting of graphene's Dirac band structure (~ 15 meV) induced by the proximity effect, potentially leading to full spin polarization and opening the way to gating.[4] The extracted spin signals illustrate the potential of 2D quantum materials based on proximity effects to craft spintronics functionalities, from vertical MTJs memory cells to logic circuits.

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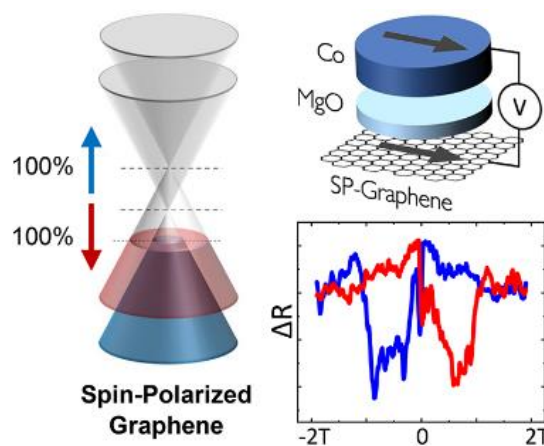


Figure 1: (Left) Exchange-induced spin splitting of the graphene Dirac cones by proximity effect. (Upper right) Device concept of magnetic tunnel junction with magnetized graphene as spin polarizer. (Lower right) Typical spin signal recorder on one of our devices.

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Tuesday, 16:30-17:40

Material growth & fonctionnalization

Growth of selfstanding h-BN crystals: hunting for crystal defects and contamination

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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 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 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) and electrical properties are explored. BNNSs exfoliated from these crystals have been used to fabricate metal-hBN-metal capacitor devices to measure the dielectric constant and the breakdown electric field of hBN, which were found to be 3.136 and 0.64 V.nm^{-1} respectively [3], *i.e* very close to the theoretical values. 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 WSe_2 and 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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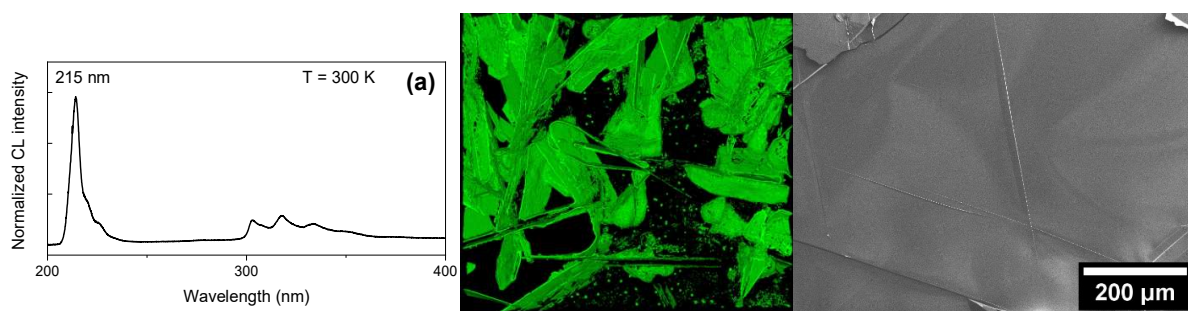


Figure 1: (a) Cathodoluminescence measurement of a PDC hBN crystal [2]; (b) 3D extracted view of entangled crystals inside the as-obtained ingot from X-ray tomography; (c) low magnification SEM view of the crystal surface

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

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Chemical vapor deposition (CVD) is beneficial for large scale high-quality 2D materials. However, most of the reported CVD graphene (Gr) films are inevitably polycrystalline with grain boundaries (GB) limiting graphene quality. Indeed, the GB is a defect line consisting of a series of pentagon, heptagon, and hexagon rings formed at the stitching region between two Gr domains with different orientations (Fig 1a). The electron transport between these domains can hence be affected by scattering at the GB reducing carrier mobility and degrading the overall performance of the graphene device. While the early studies have been focused on the understanding of graphene growth, this has now shifted to the challenge of totally removing Gr defects *via* catalyst engineering. The alignment of Gr domains on the substrate could be improved if monocrystalline Cu(111) is used for graphene growth (Fig 1b). Indeed, single-crystal copper has distinctive properties owing to the absence of GB and strong anisotropy thereby improving Gr orientation. Nevertheless, commercial single-crystal copper is yet small and very expensive. In this presentation, inductive heating is proposed to produce centimeter-scale single crystal Cu(111) by applying a controlled thermal gradient to a commercial polycrystalline copper substrate. Prior to graphene growth, 25 μm thick, 1.35 \times 5 cm² 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. After oxidation of the substrate at 200 $^{\circ}\text{C}$ for 5 min, we can see the color difference with a polycrystalline witness (Fig 1d). Consequently, graphene was synthesized using inductive heating protocol described in details in our previous work [2]. From the optical microscopy image (Fig 1e), 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. The current Cu(111) single crystal synthesis was limited only by the size of the reactor i.e. 1.35 \times 30 cm². The same concept is also applied to CVD h-BN growth on Cu(111) from ammonia borane.

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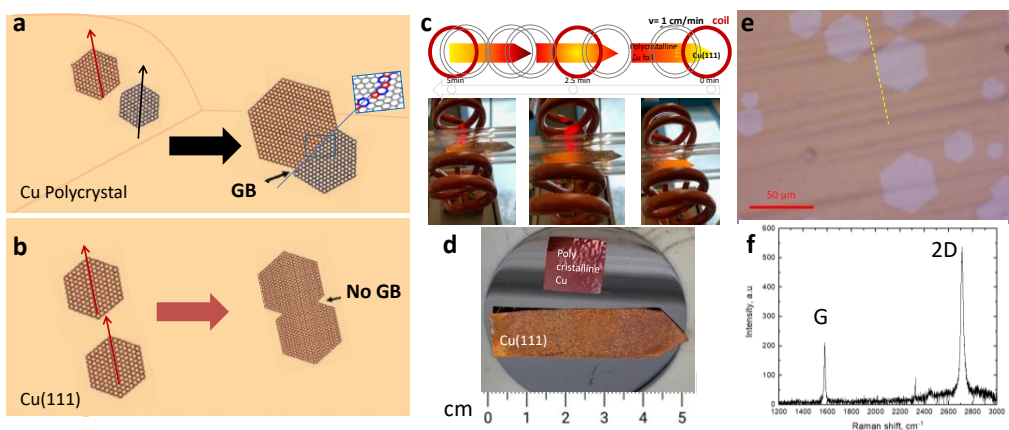


Figure 1: **a,b** Effect of Cu crystallinity on Gr grain boundaries (GB); **c** Inductive heating synthesis of Cu(111); **d** Color change after oxidation of polycrystalline and Cu(111) foils; **e** Optical image of oriented graphene domains on Cu(111); **f** Raman spectra obtained with 473 nm laser excitation on copper foil.

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SIMULATING EPITAXIAL GROWTH OF 2D Pnictogens: FROM PHASE TRANSFORMATIONS TO TOPOLOGIZATION

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Elemental two-dimensional (2D) layers of P, As, Sb, and Bi are stable semiconductors and thus attractive for various device applications and as components in van der Waals (vdW) heterostructure design. Their tunable electronic, optical, catalytic, and electrochemical properties offer wide potential for technologies ranging from drug delivery to transistors.

Due to the possibility to form hybridized and unhybridized bonds and electron lone pairs, the 2D pnictogens are able to adopt a large number of allotropic forms. Much effort has been made in growing ultrathin sheets by means of epitaxial growth techniques, and single layer phases of these four elements have been prepared on surfaces by thermal evaporation and annealing. An intriguing alternative strategy for controlling growth is to induce a transition from one allotrope to another [1,2].

In this talk I will outline, using first principles DFT calculations, the thermodynamic conditions that are necessary to drive epitaxial growth of these materials and demonstrate the feasibility of thermally inducing allotropic phase transformations. Simulations will be supported by STM and ARPES measurements carried out in ISM-CNR for the case of antimonene on bismuth selenide [3]. As an application of the process, I will discuss our results in the context of observing a topological proximity effect in the Sb/Bi₂Se₃ vdW heterostructure [4,5].

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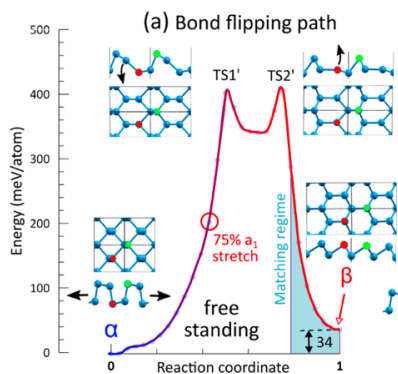


Figure 1: Simulated transformation path between two allotropic phases of antimonene

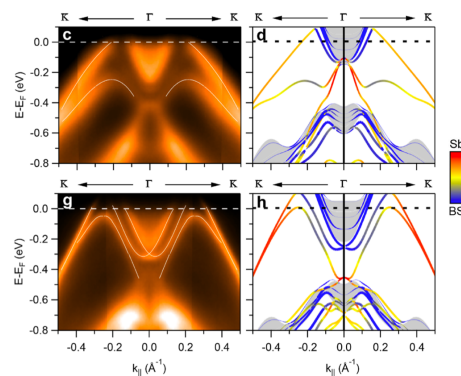


Figure 2: ARPES and band structures of the antimonene/Bi₂Se₃ vdW heterostructure

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Wednesday, 8:40-10:00

Thermal properties

THERMAL ROUTING IN NANOPATTERNED MoS₂

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Layered materials, such as MoS₂ and SnSe₂, are considered as promising materials for next-generation electronics and thermoelectric applications [1-3]. They exhibit relatively high thermal conductivity (κ) [3,4] and, consequently, low thermoelectric figure of merit (ZT) values are expected potentially limiting their prospects for thermoelectric devices. To obtain a better thermoelectric ZT value, patterning of phononic crystals in these materials was carried out to reduce their in-plane κ . To vary the thermal conductivity free-standing MoS₂ layers were patterned defining a phononic crystal by focused ion beam lithography with 30 keV Ga⁺ (see Figure 1.a) [5]. The TEM image in figure 1.b shows an amorphous MoS₂ region formed at the edges around the patterned holes of about 10 nm width. The reduction of the κ of the patterned MoS₂ was systematically studied by two-laser Raman thermometry and simulated by equilibrium and non-equilibrium Molecular Dynamics (MD). We demonstrated that the level of porosity to reduce by the same percentage the κ of layered materials could be much smaller than the porosity needed in other materials such as silicon and silicon carbide. This confirms that layered materials are more sensitive to nanostructuring than silicon and silicon carbide nanomembranes. The impact of thickness and temperature in both pristine and patterned MoS₂ is studied experimentally and the results were validated by MD simulations, elucidating the dominant scattering mechanisms for either pristine or patterned membranes, namely Umklapp phonon-phonon scattering and boundary scattering.

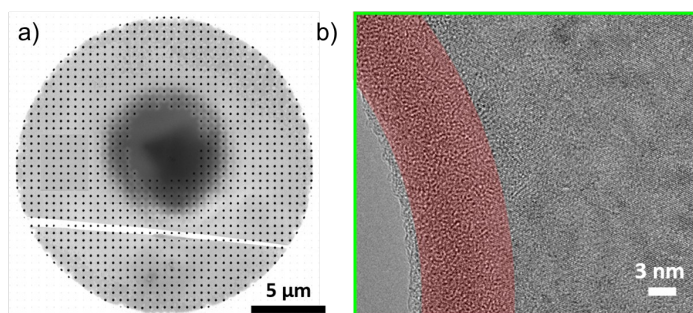


Figure 1: Phonon engineering by patterning MoS₂. a) SEM image of the phononic crystal fabricated on a free-standing 4.5 nm thick (6 layers) MoS₂ membrane. b) TEM image of the amorphous MoS₂ formed at the hole edges caused by the FIB-lithography.

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GDR HOWDI 2023 MEETING:

HEAT TRANSPORT IN HBN

Cléophanie Brochard-Richard¹, Chen Wei¹, Anis Chiout¹, Aymen Mahmoudi¹, Fabrice Oehler¹, Abdelkarim Ouerghi¹, Federico Panciera¹ and Julien Chaste¹

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2D materials have new and intriguing properties, including their thermal properties. Like 3D materials, there is a wide variety of 2D materials with all ranges of thermal conductivity that can be simply assembled on top of each other [1]. Moreover, the thermal conductivity is extremely anisotropic in these materials. It has been demonstrated in the same 2D heterostructures ratios of 3 orders of magnitude between vertical and in-plane thermal conductivity. Moreover, the interest from a fundamental point of view is the appearance at room temperature of a particular regime of phonon scattering, which allows to describe the heat transport as a hydrodynamic flow [2]. Thanks to these characteristics, it is interesting to study their thermal properties. Here, we focus on the thermal conductivity of suspended h-BN. It is an interesting material because it has a very high thermal conductivity but is electrically insulating. Nevertheless, it is difficult to heat it with a laser because of its low absorbance. To overcome this problem, we heated by Joule effect through a cantilever and we calibrate the heat flow through the 2D materials using a second bridge and a temperature mapping. The thermal mapping by means of Raman measurement allows us to have a perfect calibration of our sample temperature, making of this configuration a unique measurement. We were able to extract a thermal conductivity of isotropic h-BN superior to $2000 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$.

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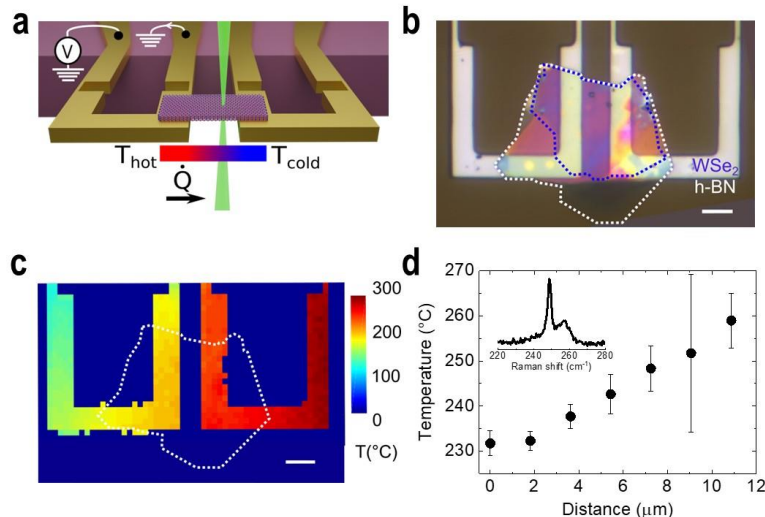


Figure 1: a) b) Schematic sketch (a) and optical image (b) of the device structure with a suspended hBN between two silicon heaters.) c) Temperature map of Si when 6 V are applied on the right electrode. d) Gradient of temperature of WSe₂ along a line from the cold electrode to the hot one (inset: Raman spectrum of WSe₂) All scales bar : 10 microns

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THERMAL BOUNDARY RESISTANCE AT THE CARBON NANOTUBES WATER INTERFACE

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The comprehensive understanding of the thermal boundary resistance (TBR) at the interface between CNTs and water is crucial for a rational design of CNT-based devices operating in the frame of nano-thermics and nano-mechanics. For instance, the TBR plays a key role in the generation of acoustic waves in water [1]. For this reason, the value of the TBR at CNT/liquid is a compelling scientific question. Furthermore, the TBR value is largely influenced by the adopted retrieval method. Here, we investigate the topic both theoretically and experimentally. On the theoretical side, we employ molecular dynamics simulations (MD) to predict the behavior of water at the solid/liquid interface in single-walled CNTs [2]. We inspect the spontaneous filling of water inside the CNT for different surface hydrophilicity and define an energy threshold parameter describing the effects of the Van der Waals forces acting on water molecules (Figure 1). Then, we investigate the dependence of the TBR on surface hydrophilicity via approach-to-equilibrium molecular dynamics (AEMD).

On the experimental side, we investigate thermal exchanges among multi-walled CNTs and water via ultrafast optical transient absorption spectroscopy. Specifically, we measure the cooling dynamics of photo-excited CNTs to quantitatively determine the TBR. A pump laser pulse impulsively heats the sample, and a time-delayed probe pulse allows following the variation of the sample optical absorption over time induced by CNT cooling to equilibrium in the pico to nanosecond timescale. Experimental time-resolved traces are then rationalized via a full opto-thermal model [3], accounting both for the thermal dynamics of the CNT and for the liquid environment and their influence on the CNT optical absorption. The model is solved by a finite element method (FEM), with the TBR serving as the only fitting parameter (Figure 2). The combination of computational (MD, FEM) and experimental (ultrafast optical transient absorption) techniques allows to investigate different sizes of CNTs (single or multi-walled) and to determine the role of the CNT surface, of the liquid composition and of the interface in the thermal exchange process.

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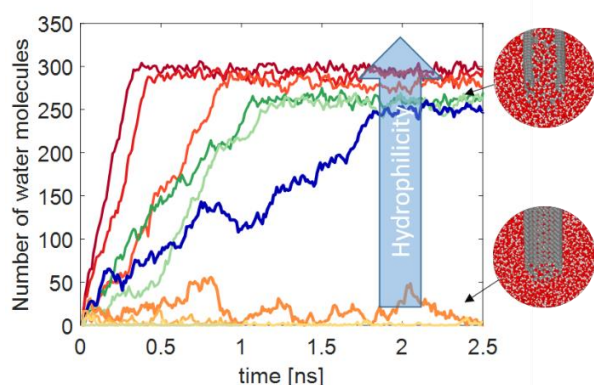


Figure 1. Number of water molecules spontaneously entering a single walled CNT. Each curve corresponds to a different level of hydrophilicity of the solid surface.

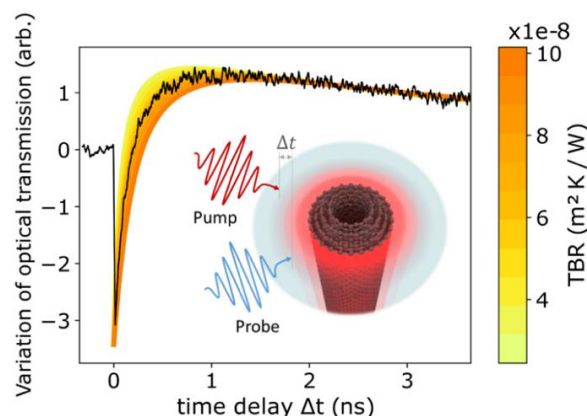


Figure 2. Experimental transient absorption signal of multi-wall CNTs in water (black) and its fits with the opto-thermal finite element model (colors). In the inset, a pictorial representation of the time-delayed pump and probe technique.

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THERMAL CONDUCTIVITY OF NANOPERFORATED GRAPHENE MONOLAYERS: AN ATOMISTIC STUDY

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Graphene, a two-dimensional (2D) material composed of carbon atoms arranged in a hexagonal lattice, has attracted tremendous attention due to its exceptional mechanical, electrical, and thermal properties. However, there is still a lack of consensus in the literature regarding the exact value of its thermal conductivity (κ). Both experimentally and computationally, there is a clear discrepancy in the literature, as some studies report ultrahigh (~ 5000 W/mK), while others find significantly lower κ (~ 100 W/mK) [1]. This could be a direct consequence of the fact that thermal transport in graphene is not accurately described by macroscopic diffusive laws; evidence of phonon ballistic and hydrodynamic transport has been theoretically predicted [2]. Significant scientific interest in tuning the thermal properties of 2D materials has been expressed lately via nanostructuring and chemical functionalization [3]. This of course requires a good understanding of the underlying mechanisms of thermal transport at the nanoscale and, for theoretical/computational studies, also an understanding of the effects of computational parameters and modeling limitations on the final calculated value.

Here, we investigate computationally the effect of nanoporation on the thermal conductivity of monolayer graphene through Nonequilibrium Molecular Dynamics. Towards this goal, we first examine and discuss the effects of the different computational artifacts on κ , ranging from the Boundary Conditions, the type of the thermostats, to more physical parameters such as the very definition of the thermal conductivity, the thermal gradient, the heat flux etc. After the study of the effects of the computational parameters, graphene samples with varying porosity levels were created by varying pore diameters, neck distances between pores, as well as pore size dispersion and spatial distribution of the pores. The effective thermal conductivity of these samples is compared with that of pristine graphene. Our results show that even the least perturbation from the pristine configuration leads to a dramatic reduction of κ , consistent with previous experimental and computational studies. We also observe that the reduction in κ is more significant for smaller neck distances, larger pore sizes and higher porosities. Overall, this study suggests that κ can be controlled by porosity engineering, while it also provides some deeper understanding of the mechanisms governing the effect of nanoarchitecturing on the thermal properties of graphene. These findings can offer significant insights into the impact of perforation on design and optimization strategies on graphene-based thermal management and energy conversion devices.

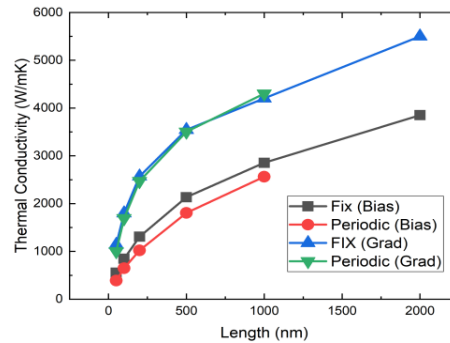


Figure: Thermal Conductivity of pristine graphene with respect to system length, for different simulation conditions. Fix and periodic boundary conditions, and different definition of the temperature gradient.

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Wednesday, 10:30-12:00

Boron Nitride

HEXAGONAL BORON NITRIDE: UNDERSTANDING AND TAILORING ITS UNIQUE ELECTRONIC AND PHONONIC PROPERTIES

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Hexagonal boron nitride (hBN) is a key compound in the field of 2D materials research. It has been shown to have unique physical properties that make it suitable for a wide range of applications, from quantum technologies to thermal management applications and deep UV optoelectronics[1, 2]. It exhibits strong thickness-dependent second order non-linearities. By modifying its defects, it can become a single-photon emitter at room temperature and, finally, even indirectly, its wide band gap provides a very high internal quantum efficiency for deep UV emitters and detectors. All these features derive from its highly anisotropic crystal structure and polar chemical bonding, which result in a peculiar electronic band structure, phonon dispersion, strong electron-phonon coupling and huge excitonic effects. In this talk, starting from the description of its constituent elements, I will describe the reasons for its unique properties and highlight recent discoveries, from thermal-radiative to optical response, from the monolayer to the bulk limit, suggesting then possible ways to further exploit its enormous potential[3, 4, 5, 6, 7].

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GDR HOWDI 2023 MEETING: FIRST-PRINCIPLES STUDY OF LUMINESCENCE IN HEXAGONAL BORON NITRIDE SINGLE LAYER: EXCITON-PHONON COUPLING AND THE ROLE OF SUBSTRATE

P. Lechiffart¹ F. Paleari², D. Sangalli³ and C. Attaccalite^{1,4}

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Hexagonal boron nitride (hBN) is a wide band gap material with both strong excitonic light emission in the ultraviolet and strong exciton-phonon coupling. Recent luminescence experiments performed on the synthesized monolayer form (m-hBN) present emission spectra that differ from one another, with some suggesting a coexistence between phonon-assisted and direct emission channels [1-3]. Motivated by these results, we investigated the optical response of (m-hBN) using a new ab initio approach that takes into account the effects of atomic vibrations on the luminescence spectra. We construct the dynamical exciton-phonon self-energy [4], then use it to perturbatively correct the optical response functions and test this approach on bulk hBN as a benchmark. Within our approach we are able to estimate the renormalisation of the direct peak induced by phonon-assisted transitions, and this allows us to accurately describe spectra where both processes are present. As the experiments were performed with different substrates, we also investigate the effect of a graphite substrate on the photoluminescence spectrum.

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MACHINE LEARNING ASSISTED CALCULATION OF PHONON PROPERTIES IN LAYERED HBN

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The calculation of finite temperature properties of solids is a topic under heavy discussion in recent years. There are mainly three predominant approaches to the problem: harmonic theory [1], effective harmonic models (e.g. the sSCHA [2] or sTDEP [3,4]) which renormalize the phonons to account for temperature dependent effects using stochastic sampling, and *ab initio* molecular dynamics (aiMD) simulations ([5]) which samples the classical distributions exactly. The latter two overcome the clear faults of the first in dealing with anharmonicity, resulting in the correct prediction of quantities like thermal expansion and the shift of the potential energy surface minima.

These approaches all do, however, suffer from the same problem of needing large amounts of DFT calculations in order to obtain converged results. This is especially the case for aiMD, where some systems reach prohibitive calculation times to obtain relevant properties.

In this work we show how taking advantage of Machine Learning (ML) assisted canonical sampling (MLACS) and interatomic potentials (MLIP) [6] as a general accelerating method allows for the usage of long propagation time MD and TDEP as an easy approach for predicting accurate temperature dependent quantities. We exemplify this with the cases of monolayer and bilayer hexagonal boron-nitride (hBN) by calculating the temperature evolution of their phonon band-structures, Raman shifts and thermal conductivities.

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IMPROVED STABILITY AND MECHANICAL PROPERTIES OF AMORPHOUS BORON NITRIDE UPON CARBON AND HYDROGEN CONTAMINATION

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Miniaturization of interconnects is a crucial step to fasten the response of the device and improve its performance of logic and memory devices in electronic circuits. Recently grown amorphous boron nitride seems to be a suitable candidate for these applications due to its low dielectric constant, high thermal and chemical stability, as well as being a great metal diffusion layer. Additionally, it is more suitable for large-area deposition compared to its crystalline counterpart since it can be grown relatively lower temperature, which opens new integration opportunities with 2D materials into flexible devices for nanoelectronics and spintronics applications [1, 2, 3]. The uniqueness of amorphous materials derives from the inherent imperfect structure, which can be controlled at fabrication level, represents the key ingredient for specific target applications. In this respect, new fabrication strategies to modify the structural properties and a systematic theoretical characterization of the impact of the structural properties on thermal stability and mechanical properties are urgent. In this talk, using Artificial Intelligence-based approach, I will present our theoretical investigation of thermal and mechanical properties of aBN as a function of varying external parameters such as temperature, quenching rate, presence of unwanted or dopant atoms using molecular dynamics. Using machine learning technique, we ensure the reliability of calculations of properties by first describing the atomic interactions more accurately, introducing two Gaussian Approximation Potentials (for aBN:C and aBN:H) which are trained on a large dataset of atomic structures which generated by ab-initio calculations [4, 5]. We found that then incorporation of both C and H atoms causes a significant change in structural properties of aBN, which is strongly reflected in the resulting the thermal stability and mechanical properties of the compounds [5, 6]. We mention the challenge of studying dielectric properties of those materials in the context of ultralow dielectric constant and interconnect technologies [1,3].

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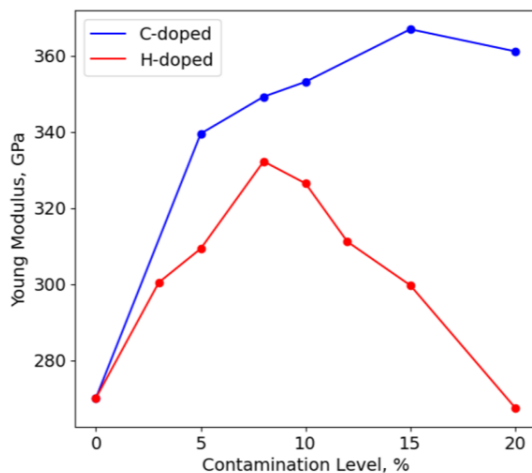


Figure 1: Thermal stability of aBN samples with varying amount of C and H.

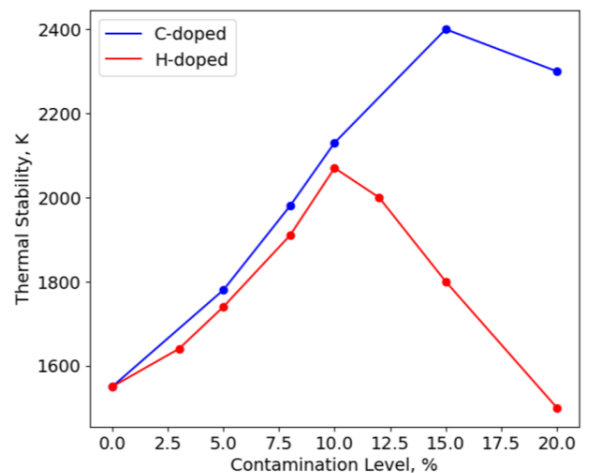


Figure 2: Young's modulus of aBN samples with varying amount of C and H.

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Wednesday, 14:00-15:30

Characterization & Structure

MAGNONS AND PHONONS IN LAYERED ANTIFERROMAGNET FePS₃

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²Laboratoire National des Champs Magnétiques Intenses, LNCMI-EMFL, CNRS UPR3228, Univ. Grenoble Alpes, Univ. Toulouse, Univ. Toulouse 3, INSTA-T, Grenoble and Toulouse, F-38042, FRANCE

Following the isolation of graphene and the remarkable successes in the study of atomically thin layers of semiconducting transition metal dichalcogenides, the exploration of other layered materials, commonly referred to as two-dimensional (2D) materials, has been of a particular interest. Recently re-visited magnetic semiconducting materials, broaden the landscape of these 2D materials, providing new platforms to study the fundamental magnetic ordering in low dimensions. These layered compounds with weak interlayer van der Waals (vdW) interactions exhibit a large variety of magnetic phases and have attracted great research interest with the promise of developing novel spintronic devices with new functionalities [1,2].

A unique material belonging to the transition metal phosphorus group is a semiconducting antiferromagnet FePS₃. Experiments with inelastic neutron scattering show that the Fe²⁺ spins are aligned along the direction perpendicular to the layers plane and its transition temperature (T_N) is 120 K [3]. Its optical and magnetic properties have attracted much attention due to its characteristic magnon-gap excitation that appears at a significantly high frequency of a few terahertz.

By means of magneto-optical spectroscopy techniques, we have explored the response of the collinear antiferromagnet FePS₃ and revealed the interaction between the magnon and selective phonon modes in this material [4]. The hybrid magnon-phonon modes are detected by Raman experiments, but also couple directly to light, leading to the pronounced resonances in FIR transmission spectra. In addition, the FIR magneto-optical studies uncover a novel magnetic excitation – a single-ion 4-magnon bound state – that can be explained by a full reversal of a single magnetic moment of the Fe²⁺ ion [5].

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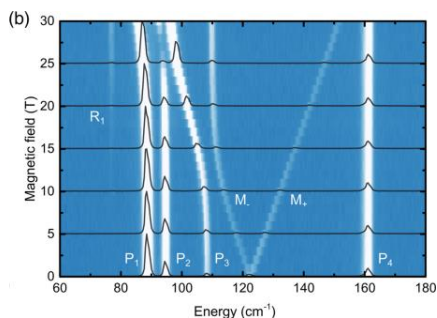


Figure 1: False-color map of the evolution of the low-temperature magneto-Raman scattering response of FePS₃ with an applied magnetic field oriented perpendicular to the plane of the layers.

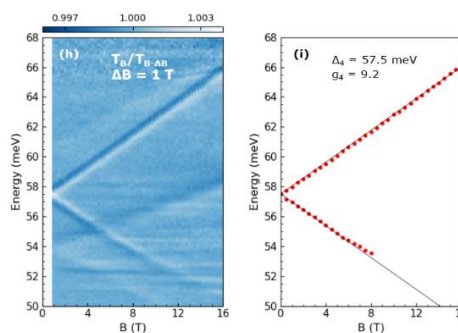


Figure 2: Magneto-transmission false-color map evolution of magnon excitation and its extracted position as a function of applied magnetic field.

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GDR HOWDI 2023 MEETING: FLAT BAND AND LIFSCHITZ TRANSITION IN LONG-RANGE- ORDERED SUPERGRAPHENE BY ERBIUM INTERCALATION

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We report the observation of a heavily electron-doped graphene up to the Lifshitz transition obtained solely by the intercalation of Erbium atoms [1]. A new long range ordered hexagonal supergraphene has been observed by Scanning Tunneling Microscopy (STM) Fig. 1(a). The ARPES measurements show a strong linear dispersion around K points with a shift of Dirac point energy by about 1.72 eV below the Fermi level Fig. 1(b) (which is the highest doping level ever reported so far) and a wide flat band around the M point Fig. 1(c). The measured Fermi surface indicates that the Lifshitz transition has been reached with an electron density of $5.1 \pm 0.8 \times 10^{14} \text{ cm}^{-2}$ Fig. 1(d). XPS measurements show that the Er atoms are free standing in between the graphene layer and the substrate and keep their metallic character. On the basis of Tight-Binding calculations we propose a theoretical model where diluted ordered Erbium atoms act as impurities under the graphene and induce a local-density-of-states perturbation, as for a kekulé order, which is usually observed for a Fermi level around the Dirac point [2]. We also discuss the possible effects of a spin-orbit coupling on the topology of the Fermi surface and the flattening of the band around M at Lifshitz transition.

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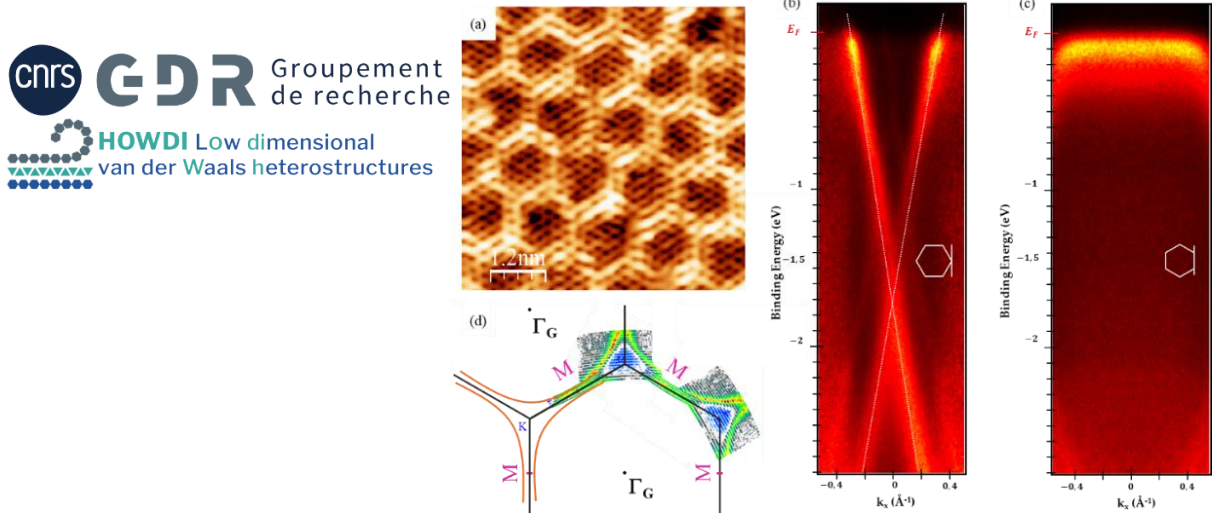


Figure 1: (a) Topographic STM image of the $(5.75 \times 5.75) R19^\circ\text{-G}$ superstructure, $6 \times 6 \text{ nm}^2$. ARPES measurements of the dispersion band around K point in (b) and around M point in (c). (d) Fermi surface of the system.

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DETECTION OF NEGATIVE CHARGE INDUCED BY SINGLE ATOM V DOPANT IN 2D WSe₂ USING 4D-STEM

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Structural anomalies in 2D materials have been known as the key to locally modify the electrical, optical and magnetic properties. In order to tailor the material properties and to explore their functionalities, the ability to survey the local electric properties together with their structural configuration at the atomic scale is essential. Today, low-voltage Scanning Transmission Electron Microscopy (STEM) stands out as one of the most powerful techniques for structural and chemical analysis of 2D materials at atomic scale by Z-contrast imaging as well as EDX and EELS spectroscopies. Recently, a new imaging technique called Differential Phase Contrast – Center of Mass (DPC-CoM) sensitive to local electrostatic field was demonstrated in STEM [1-2]. Analyzing the deviation of the transmitted beam position gives access to the local electric field in a sample with atomic resolution, and to the electrostatic potential and the charge density through Poisson's equation [3]. However, the lack of quantitative understanding and interpretation of DPC-CoM images are the main reason that this imaging mode is not yet routinely used for the study of 2D materials.

In this work, we explore the use of 4D-STEM: DPC-CoM for the atomic scale mapping of local electrostatic field and potential around a single atom V dopant in WSe₂/graphene heterostructure. The quantitative analysis is achieved by comparing the experimentally obtained E-field and potential maps to the DFT-based multislice STEM image simulations [4] taking into account the influence of important microscope parameters such as: convergence angle, defocus and aberrations. Finally, a negative charge around V dopants is detected as a drop in the electrostatic potential maps. These results proved that 4D-STEM can be used for detecting the single dopant charge states in 2D materials [5].

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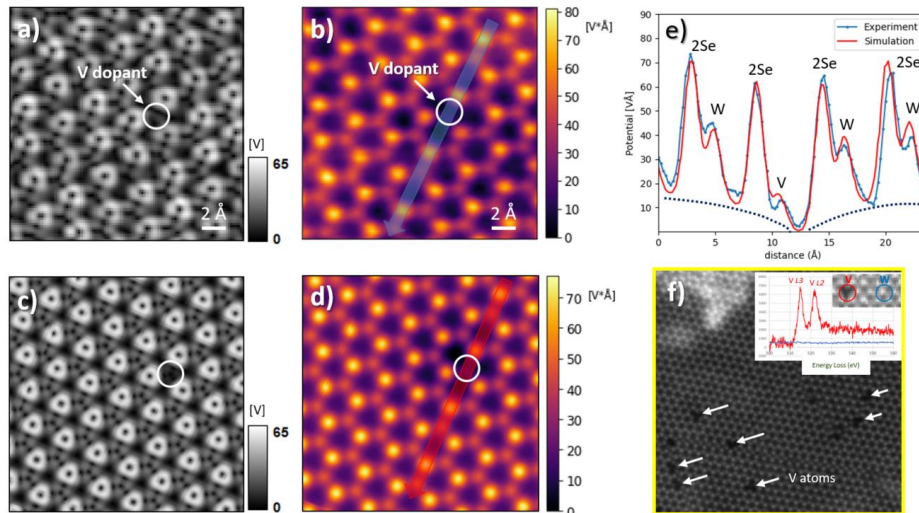


Figure 1: a)–b) Experimental projected E-field and potential around V dopant; c)–d) Simulated projected E-field magnitude and potential around charged V dopant; e) potential line profile comparison between experiment and the simulation; f) HAADF image of MBE grown V-doped WSe₂ and the corresponding EELS spectrum (inset)

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DIRECT IMAGING OF BAND STRUCTURE FOR CVD GROWN RHOMBOHEDRAL-STACKED BILAYER WSe₂ USING NANOSPOT ANGLE-RESOLVED PHOTOEMISSION

Aymen Mahmoudi¹, Meryem Bouaziz¹, Nathan Ullberg², Geoffroy Kremer¹, Pavel Dudin³, José Avila³, Mathieu Silly³, Vincent Derycke², Marco Pala¹, Iann C. Gerber⁴, Julien Chaste¹, Fabrice Oehler¹, Abdelkarim Ouerghi¹

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Twisted layers of atomically thin two-dimensional materials support a broad range of novel quantum materials with engineered optical and transport properties^{1,2}. Transition metal dichalcogenides (TMDs) in the rhombohedral (3R i.e. 0° twist) crystal phase have been the focus of significant research interest in optical applications due to their particular broken inversion symmetry. Here, we report experimental and theoretical study of WSe₂ homo-bilayers obtained in stable 3R configuration by chemical vapor synthesis^{3,4,5}. We investigate the electronic and structural properties of these 3R WSe₂ bilayers with 3R stacking using micro-Raman spectroscopy, angle-resolved photoemission nano-spectroscopy measurements (nano-ARPES) and Density Functional Theory (DFT) calculations. Our results demonstrate that WSe₂ bilayers with 3R crystal phase (AB stacking) show a significant spin-orbit splitting estimated to 550 ± 20 meV. We derived experimentally effective hole masses of 0.48 me and 0.73 me at K point for upper and lower bands, respectively. Our work opens up new perspectives for the development of optoelectronic and spintronic devices based on 3R TMD homo-bilayers.

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Figure 1: Optical image of CVD-grown WSe₂ bilayer flakes

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Wednesday, 16:00-17:20

Nanotubes & Heterostructures

FABRICATION OF 1D VAN DER WAALS HETEROSTRUCTURES BY DEPOSITION OF ATOMIC LAYERS OF BORON NITRIDE ON CARBON NANOTUBES

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The isolation of graphene has sparked great interest in 2D materials and the possibility of stacking 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 the connection of two different materials to combine their intrinsic properties and/or create new ones. Interest in this coupling is currently extending beyond 2D materials, with one-dimensional (1D) VdW heterostructures that consist of a 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 over the initial ones. In particular, hexagonal boron nitride (hBN) is of great interest because it is isostructural to graphene with a large band gap, excellent thermal stability, and photoluminescence intensity in the visible or UV spectral regions; thus, coaxial stacking of hBN on carbon nanotubes (CNTs) can enrich the optoelectronic properties of the initial structures [1]. The fabrication of these high-quality hBN/CNT heterostructures requires a synthesis approach capable of precisely controlling the epitaxial deposition on substrates at the atomic scale. Based on self-limiting gas-surface reactions, atomic layer deposition (ALD) has proven to be ideally suited for the fabrication of functional hetero-nanostructures, such as carbon nanotube-based materials [2].

Here, a two-step ALD process of hBN is used to fabricate hBN/CNT heterostructures based on polymer-derived ceramic chemistry [3]. Briefly, a polyborazine preceramic layer is successfully deposited on single- or multi-walled CNTs in the first ALD step and then annealed at high temperature in the second step to convert the polyborazine into crystalline hBN. The resulting BN-coated CNTs are extensively studied using advanced characterization techniques. Specifically, high-resolution transmission electron microscopy shows the fabrication of highly crystalline hBN/CNT heterostructures and electron energy loss spectroscopy allows to observe conformal and homogeneous coating of hBN layers on single and multi-walled CNTs. The influence of ALD parameters and post-annealing treatment on the growth of BN (thickness and number of layers, homogeneity) and its 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 the successful fabrication of 1D VdW heterostructures consisting of single-walled carbon nanotubes covered with a few layers of hBN. Raman and photoluminescence spectroscopies are performed to evaluate the structural and optical properties of the obtained heterostructures.

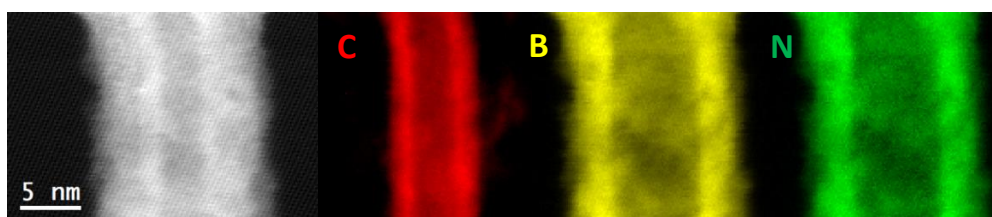


Figure 1: Scanning TEM image of BN coated multi-wall CNT and its corresponding C (red), B (yellow) and N (green) elemental EELS mapping

References

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ELECTRONIC STRUCTURE INVESTIGATION OF ENDOHEDRAL METALLOFULLERENES (EMFS)

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For the purpose of creating single-molecule junctions, which can convert a temperature difference ΔT into a voltage ΔV via the Seebeck effect, it is of interest to screen molecules for their potential to deliver high values of the Seebeck coefficient $S = -\Delta V/\Delta T$. Here we demonstrate that insight into molecular-scale thermoelectricity can be obtained by examining the widths and extreme values of Seebeck histograms. Using a combination of experimental scanning-tunnelling-microscopy-based transport measurements and density-functional-theory-based transport calculations, we study the electrical conductance and Seebeck coefficient of three endohedral metallofullerenes (EMFs) $\text{Sc}_3\text{N}@C_{80}$, $\text{Sc}_3\text{C}_2@C_{80}$, and $\text{Er}_3\text{N}@C_{80}$, which based on their structures, are selected to exhibit different degrees of charge inhomogeneity and geometrical disorder within a junction. We demonstrate that standard deviations in the Seebeck coefficient σ_S of EMF-based junctions are correlated with the geometric quantity σ and the charge inhomogeneity σ_q . We benchmark these molecules against C_{60} and demonstrate that both σ_q, σ_S are the largest for $\text{Sc}_3\text{C}_2@C_{80}$, both are the smallest for C_{60} and for the other EMFs, they follow the order $\text{Sc}_3\text{C}_2@C_{80} > \text{Sc}_3\text{N}@C_{80} > \text{Er}_3\text{N}@C_{80} > C_{60}$. A large value of σ_S is a sign that a molecule can exhibit a wide range of Seebeck coefficients and if orientations corresponding to high values can be selected and controlled, then the molecule has the potential to exhibit high-performance thermoelectricity. For the EMFs studied here, large values of σ_S are associated with distributions of Seebeck coefficients containing both positive and negative signs, which reveals that all these EMFs are bi-thermoelectric materials.

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Figure 1: Conference logo.

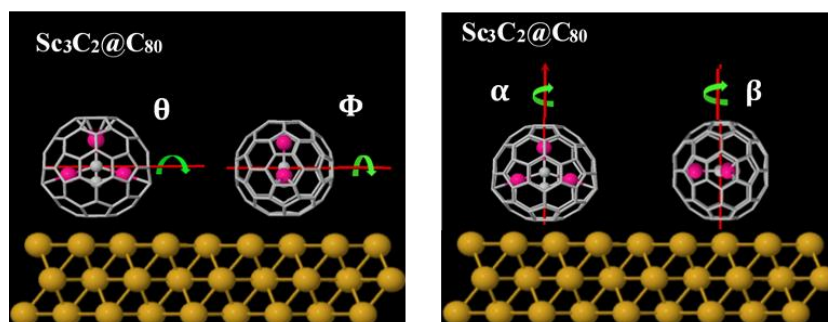


Figure 2: Illustration of the four rotation axes: θ and Φ are horizontal axes, α and β are vertical axes. This Figure shows how the axes pass through the I_h - C_{80} cage + metallic moiety.

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TMDs FUNCTIONALIZED-SWCNTs HETEROSTRUCTURED MATERIALS FOR SENSING APPLICATIONS

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Recent years have witnessed extensive efforts focused on search for multidimensional nanostructures containing and synergistically combining both one-dimensional (1D) and two-dimensional (2D) nanostructures. Individual 1D and 2D nanostructures exhibit outstanding electrical properties, due to their large specific surface areas, and their configuration that provides oriented electronic transport pathway and reduces the electrical resistance. 2D structures as Transition Metal Dichalcogenides (TMDs) have received considerable attention due to their specific chemical and physical properties [1]. TMDs are defined with the MX_2 formula where M is a transition metal (Mo, W, etc.) and X is a chalcogen (S, Se, etc.). They consist of hexagonally stacked three atomic layers of X-M-X covalently bonded and weak van der Waals bound (vdW) out of planes interactions of individual X-M-X layers [2]. TMDs, such as WS_2 and MoS_2 , have chemical and physical properties depending on their numbers of layers, i.e. with direct and indirect band gaps. TMDs have been proven to also exhibit some limitations in terms of their electrical properties, such as limited carrier mobility, and high contact resistance [3]. To overcome this challenge, hybrid TMDs@SWCNTs were fabricated in order to test the synergy between the two materials and to achieve new functions and physical properties. Such heterostructures can be of particular high interest in gas sensors applications where the interaction of gas molecules with the materials leads to changes in their electrical properties. The high surface area and the porosity of the CNTs can enhance the gas adsorption and sensitivity of the material whilst the TMDs, on the other hand, can provide selectivity towards specific gases due to their unique electronic properties [1].

In the present work, high-quality WS_2 @SWCNTs and MoS_2 @SWCNTs were fabricated using a bottom-up approach. First, the SWCNTs were synthesized via a chemical vapor deposition (CVD) method on a quartz substrate where the characteristics of the SWCNTs, i.e., diameter, density, and length are controlled by controlling the catalyst and CNT growth conditions. Next, mono and bilayer WS_2 and MoS_2 nanoflakes with diameters ranging between 10-20 nm were directly synthesized on the walls of the CNTs using homemade molecular beam evaporation/epitaxy (MBE) system. The characterization of the hybrid materials was carried using different in-situ surface analysis techniques as TEM, XPS, EELS, UPS, AES. It has been proven by different spectroscopy techniques that Nanoflakes (WS_2 and MoS_2) with a trigonal prismatic crystal structure, noted 2H, have grown on the walls of the SWCNTs. These hybrid materials were used to fabricate high-performance relative humidity sensors. An opposite electrical response towards humidity is obtained for the two types of heterostructures, highlighting the opposite intrinsic properties of TMD@SWCNTs-based devices. The sensors are easy to produce and exhibit high sensitivity, making them suitable for applications in different environments.

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ELECTRONIC STRUCTURE OF CARBYNE ENCAPSULATED INSIDE DOUBLE-WALLED CARBON NANOTUBES

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An infinitely long linear carbon chain (LCC) or carbyne, consisting of a single file of sp^1 -hybridized carbon atoms, represents the truly 1D allotrope of carbon. Ultra-long LCCs have only recently started to become accessible experimentally thanks to their synthesis inside carbon nanotubes (CNTs)¹, which protect their structure while at the same time modifying their electronic and optical properties². In this study, wavelength-dependent resonant Raman spectroscopy is employed to investigate the excited states of ultralong LCCs encapsulated inside double-walled CNTs³. In addition to the optical gap, the resonance Raman profile shows three additional resonances which are assigned to a vibronic series of a different excited electronic state. These observations are corroborated with DFT calculations on LCCs with up to 100 carbon atoms, which predict the existence of two optically allowed electronic states separated by an energy of 0.14–0.22 eV in the limit of an infinite chain, in agreement with the experimental results. Furthermore, among these two excited states, the one with highest energy is also characterized by the largest electron-vibration couplings, which explains the corresponding vibronic series of overtones.

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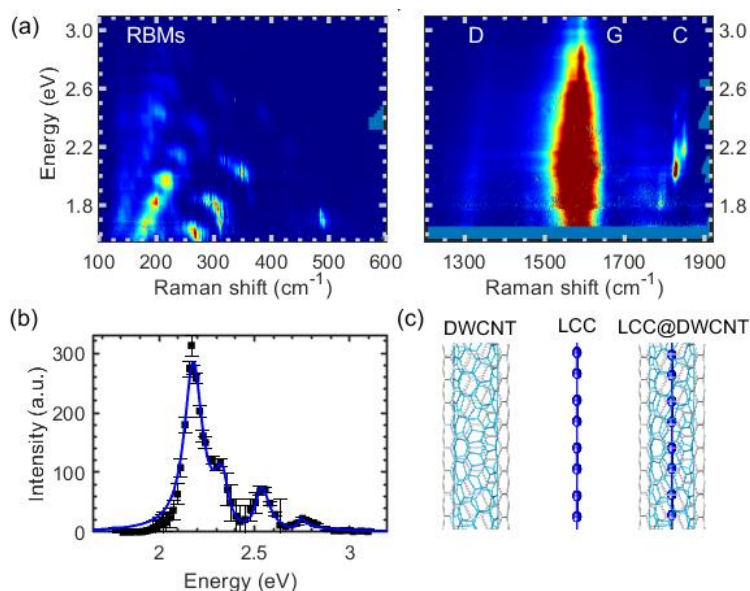


Figure 1: a) Wavelength-dependent resonant Raman map of LCC encapsulated inside DWCNT. b) Example of resonance Raman profile of the LCC Raman mode showing four resonances as a function of laser excitation energy. c) Representation of a double walled CNT, a LCC and of a LCC encapsulated inside a double walled CNT.

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Thursday, 8:30-10:00

Optics 1: Original Systems

ULTRAFAST EXCITON DYNAMICS IN COLLOIDAL 2D PEROVSKITE NANOPATELETS

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Using femtosecond transient absorption (fs-TA), we investigate the hot exciton relaxation dynamics in strongly confined lead iodide perovskite nanoplatelets (NPLs). The large quantum and dielectric confinement leads to discrete excitonic transitions and strong carrier-induced Stark features in the TA spectra. This prevents the use of conventional relaxation analysis methods [1] extracting the carrier temperature or measuring the buildup of the band-edge bleaching. Instead, we show that the TA spectral lineshape near the band-edge reflects the state of the system, which evolution in time can be used to probe the exciton cooling dynamics (Figure 1). The ultrafast hot exciton relaxation in one- to three- monolayer-thick NPLs confirms the absence of intrinsic phonon bottleneck. Indeed, the measured exciton cooling time surprisingly decreases for thinner NPLs. However, excitation fluence-dependent measurements reveal a hot phonon bottleneck effect, with a delayed relaxation when increasing the exciton density. This hot phonon bottleneck effect is found to be independent of the nature of the internal cations (organic versus inorganic), in contrast with 3D perovskites [2]. However, it is strongly affected by the ligands and/or sample surface state. Together, these results suggest a role of the surface ligands in the cooling process in these ultrathin colloidal 2D nanostructures [3].

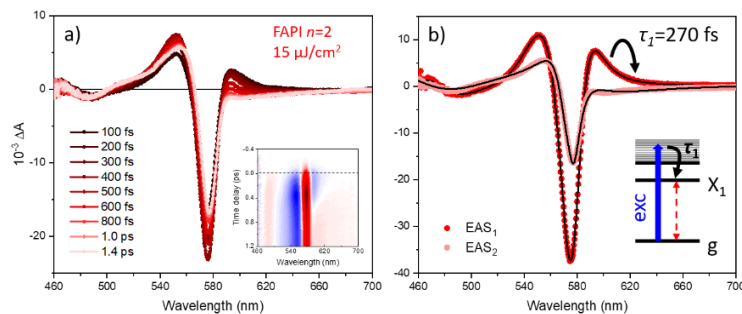


Figure 1: a) TA spectra of formamidinium lead iodide NPLs of 2 monolayers (FAPbI₂ n=2) excited at low fluence at 400 nm. Inset: full TA map. b) Corresponding evolution associated spectra (EAS, red and pink dots) obtained with global analysis using a sequential kinetic model with two components. The rate $k_1=1/\tau_1$ characterize the cooling process. The EAS were fitted (in black) by modeling the change of the absorption in terms of amplitude, center energy and line width. Inset: schematics of the cooling process to the band-edge after high-energy excitation in the continuum of states.

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OPTICAL PROPERTIES OF SINGLE NANOGRAPHENES

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Recent years have shown an increasing number of studies focused on new light emitters for various applications and in particular for quantum technologies. In this context, nanographenes have great assets since bottom-up chemistry allows a total control on the structure, which opens the way to wide customization of their optical, and spin properties [1–3]. The full benefit from these opportunities needs addressing nanographene intrinsic photophysical properties. To do so, single molecule photoluminescence experiment is a powerful tool [4].

Here, we will focus on small nanographenes where electrons are confined in the three dimensions of space, the so-called graphene quantum dots (GQDs). We will show that our degree of control on the structure allows us to address both the influence of the size and of the symmetry of the GQD on its properties: emission wavelength, polarization selection rules, oscillator strength... We will report on experiments performed at the single molecule level and from room to cryogenic temperatures. We will show that the experimental results are well predicted by extensive DFT/TDDFT calculations combined with molecular dynamics simulations. [5-7].

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TWO-PHOTON INTERFERENCE FROM A QUANTUM EMITTER IN hBN

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In the context of photonic quantum information science, hexagonal boron nitride (hBN) has emerged as a very promising material. The two-dimensional character of hBN renders it attractive for the realisation of compact heterostructures and integrated photonic devices. Moreover, this wide-gap material has been shown to host single-photon emitters (SPEs) with appealing optical properties in the red and near infrared regions [1]. However, the deep defects initially observed in hBN suffer from the wide distribution of their emission wavelength and, in most cases, a random spatial location [2,3]. These limitations hinder the scalability of the system for applications.

Recently, a new family of quantum emitters has been observed in hBN – a class of blue-emitting colour centres that have appealing properties [4,5,6]. We demonstrated deterministic positioning (fig. 1,2) of these SPEs with reproducible emission wavelengths (fig. 3), based on irradiation with an electron beam [5,7].

Here, we investigate two-photon interference between consecutively emitted photons based on the Hong-Ou-Mandel effect. We use coherent photons from the zero-phonon-line that are obtained under non-resonant excitation. This measurement leads to a sizeable degree of indistinguishability of 0.56 ± 0.11 in a 3 ns time window, after accounting for imperfect emitter purity (fig. 4) [8]. The dependence of the HOM visibility on the width of the post-selection time window allows us to estimate the dephasing time of the emitter to be ~ 1.7 ns. This is the first observation of photon indistinguishability from a 2D material quantum emitter and opens the way to the use of these SPEs for quantum information applications.

Our results suggest new avenues towards top-down realisation of integrated quantum optical devices based on indistinguishable single photon sources in hBN.

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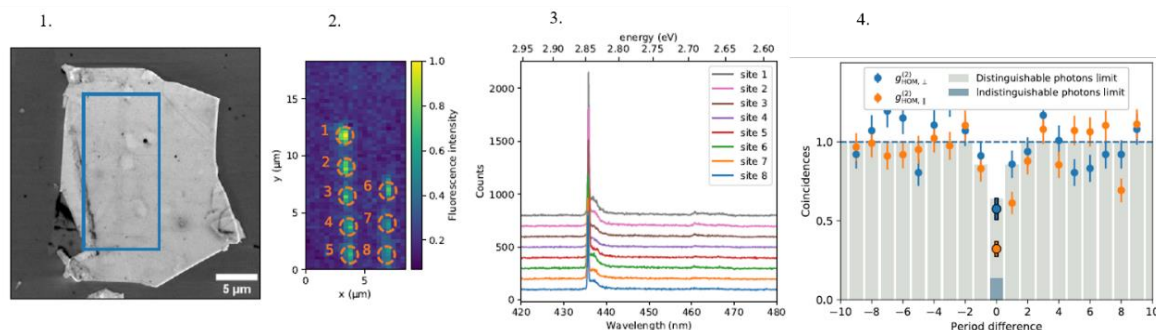


Figure 1. hBN flake with eight irradiation sites. Figure 2. Corresponding confocal map.

Figure 3. Corresponding spectra, displaying reduced statistical dispersion of the emission wavelength.

Figure 4. Photon correlations with a signature of Hong-Ou-Mandel effect between consecutive photons.

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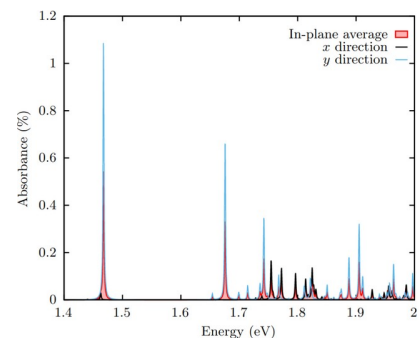
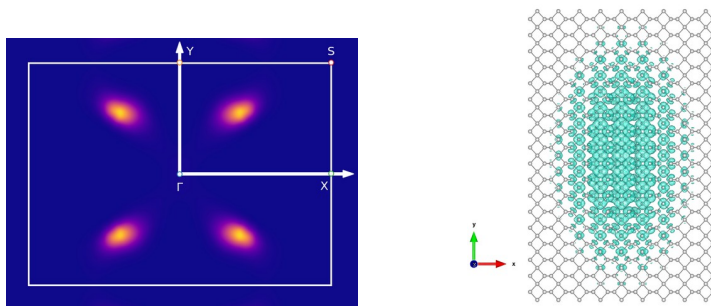
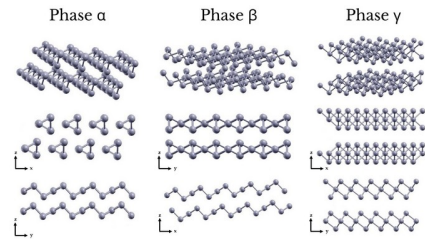
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Tellurene is an emerging 2D anisotropic semiconductor, with fascinating electronic and optical properties that differ dramatically from its bulk counterpart, which has come to us owing to its unique chained structures. Tellurene is the 2D form of Tellurium and it was proposed by theoretical calculations – and then verified by experiments – in 2017 [1]. In this work, we investigate the electronic and optical properties of three different allotropic forms of few-layer Tellurene by means of ab initio calculations based on Density Functional Theory (DFT) and Many-Body Perturbation Theory (MBPT), using the Quantum ESPRESSO suite [2] and the YAMBO code [3]. Following our previous work [4], we focus our attention on the most stable and interesting β - and γ -phase – concerning the monolayer (1L) configuration –, also including bilayer (2L) α -phase, since 1L α -phase is unstable and can be transformed into β -phase without barriers. These three very diverse structures are semiconductors with both direct (γ) and indirect (α , β) electronic (quasiparticle) bandgap, ranging from about 1 to 2 eV. Each system shows its characteristic optical fingerprint and absorbs light mainly in the far-infrared range, showing very high photon absorptions for in-plane light polarization, superior to that of other previously studied 2D materials. Moreover, due to their orthorhombic crystal structure and very peculiar chemical bonding, α - and β -phase exhibit strong optical anisotropy which is hardly to be found in the 2D world. Lastly, we propose a comparison of the (GW) bands alignments with that of different 2D materials for possible type-2 heterostructures involving Tellurene.

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Thursday, 10:00-12:00

Optics 2: Heterostuctures

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 micro-spectroscopies 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.

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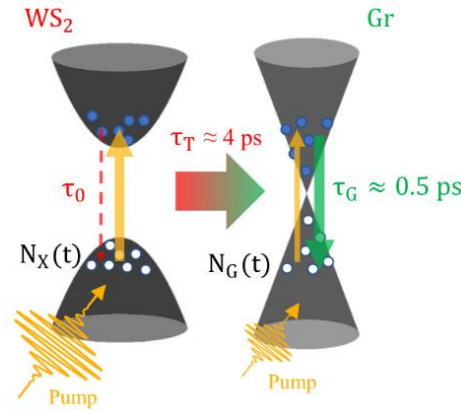


Figure 1: Modeling energy transfer in a WS_2 -Gr heterostructure. The pump pulse can generate an exciton population in WS_2 or populate the electronic states of Gr with e - h pairs. These latter decay with a timescale τ_G . In contrast, the excitons in bare WS_2 have a long lifetime τ_0 . Exciton decay is strongly accelerated in WS_2 -Gr due to energy transfer to Gr with a characteristic time τ_T

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ABSORPTION AND EMISSION IN TWISTED VAN DER WAALS HETEROSTRUCTURES FROM FIRST-PRINCIPLES

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8-12 May 2023

Van der Waals (VdW) heterostructures of two-dimensional transition metal dichalcogenides (TMDs) allow researchers to explore a plethora of phenomena related to the elegant interplay of charge, spin, and moiré superlattice with many-body effects [1][2]. Optoelectronic devices based on these materials require the ability to control their optical properties via various degrees of freedom (a charge, (pseudo)spin, valley, twist angle, strain, . . .). From a theoretical point of view, the *ab initio*-MBPT framework based on the GW-BSE method [4] is the optimal tool to obtain a detailed microscopic description of the optical properties of the system of interest. The information on the mentioned degrees of freedom is stored in the eigenstate of the many-body Hamiltonian. The interaction between the layers strongly influences the magnitude and character of the optical transitions. Here we show that structural properties, such as geometrical relaxation are crucial to achieve both qualitative and quantitative accurate prediction of the band structure and absorption spectra. As recently shown by our group [5], the relative positions of the valley in the band structure of TMDs are sensible to the in-plane and out-of-plane strain of the unit cell and the overall position of the atoms.

In this project, we explain how the optical properties change with the twist angle, considering twisted MoSe₂/WSe₂ as a representative of this class of systems. To date, most of the work on twisted TMDs has been done on small angles [3]. However, experiments [6] have recently proposed that a higher angle configuration of this system shows interesting physical properties such as missing quenching of the emission channel from the WSe₂ layer and a transition from type II to a type I band alignment. This effect can be attributed to the modulation of the moiré potential that enters the simulation via a proper relaxation of the ground state geometry. In order to compare on equal footing the deduction obtained from experiments via the time-resolved photoluminescence (TRPL) technique, we analyze not only the absorption spectra computed within the GW-BSE scheme but we also the photoluminescence (PL) spectra, as recently implemented by us in the Yambo code[7][8].

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TOWARDS A MICROSCOPIC UNDERSTANDING OF PHOTOLUMINESCENCE QUENCHING IN MONOLAYER MOSE₂/N-LAYER GRAPHENE HETEROSTRUCTURES

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The van der Waals heterostructure consisting of transition metal dichalcogenide (TMD) and graphene is an interesting system as it provides an opportunity to understand the microscopic charge and energy transfer processes occurring at two-dimensional semiconductor-metal heterointerfaces. For this purpose, photoluminescence (PL) and Raman spectroscopy are frequently used. The coupling between graphene and TMD gives rise to intriguing effects such as the neutralization of the TMD and the quenching of its PL [1,2]. Whether the PL quenching occurs through short-range charge tunneling or longer-range dipole-dipole interactions still remains unclear [1].

Here, the heterostructure of monolayer MoSe₂ covering thin graphene of different thicknesses is studied to reveal details about transfer mechanisms, exciton dynamics and their dependence upon incident laser energy and thickness of graphene. The changes in photoluminescence of MoSe₂ with respect to thickness of graphene attached to it (Fig. 1) indicates that the interaction between MoSe₂ and graphene is of short range (~1nm) as the quenching factor saturates when graphene gets thicker than 3 layers (Fig. 2).

As an outlook, we will introduce our ongoing study to control the light emission in MoSe₂/graphene heterostructures by controlling their charge carrier density over a broad range of hole and electron doping. The ionic glass LaF₃ is used to achieve strong doping in monolayer graphene by applying a voltage across it and the Raman modes are used to quantify the charge doping, which can be as high as 1 eV above the Dirac point of graphene [3,4]. Preliminary results in charge-tunable MoSe₂/graphene layers will also be introduced.

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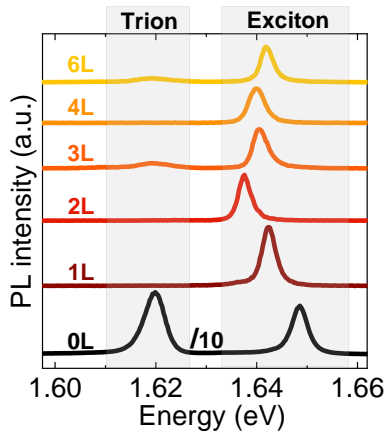


Figure 1: Photoluminescence of monolayer MoSe₂ coupled with a given nL (n number of layers of graphene). Data recorded at T=16 K under laser illumination at 633 nm with power of 30 μW. The spectra are vertically offset for clarity.

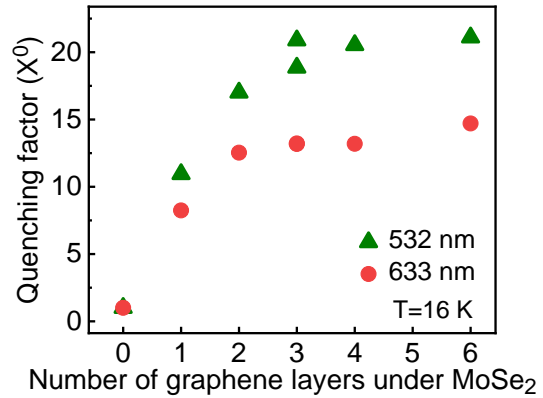


Figure 2: Quenching factor of exciton (intensity of exciton in MoSe₂/intensity of exciton in MoSe₂ coupled to graphene) with respect to number of graphene layers for incident laser wavelengths of 532 nm and 633 nm.

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EXCITON SPECTROSCOPY AND UNIDIRECTIONAL TRANSPORT IN MOSE₂-WSE₂ LATERAL HETEROSTRUCTURES

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Here we perform optical spectroscopy at $T = 4$ K and 300 K in CVD grown MoSe₂-WSe₂ lateral heterostructures that are transferred from the growth substrate and are encapsulated in hBN. We reveal a high-quality lateral junction by optical spectroscopy and study the excitonic transport induced by the type2 junction. Our experiments give access to the excitonic structures at cryogenic temperatures, with neutral exciton transition linewidth of the order of 5 meV. Tip-enhanced, sub-wavelength optical spectroscopy mapping (spatial resolution 40 nm) shows the high quality of the heterojunction which acts as an excitonic diode resulting in unidirectional exciton transfer from WSe₂ to MoSe₂. This is confirmed by a simple diffusion model where the exciton energy difference between the two materials acts as an effective field over a distance of a few nm.

In more details, photoluminescence (PL), reflectance contrast and Raman spectroscopy reveal considerably narrowed optical transition linewidth similar to high quality exfoliated monolayers. In high-resolution transmission electron microscopy (HRTEM) we find junctions with a typical extent of 3 nm for the covalently bonded MoSe₂-WSe₂. In PL imaging experiments we find effective excitonic diffusion length that are longer for WSe₂ than for MoSe₂ at low $T=4$ K, whereas at 300 K this trend is reversed.

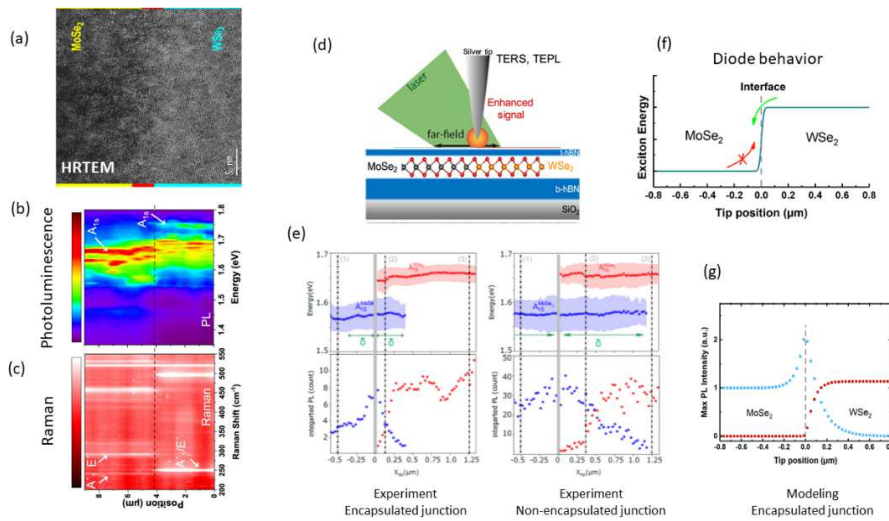
Further study compares lateral junction with or without top hbN. Near field PL (tip-enhanced PL) evidences longer diffusion length on non-encapsulated junction. Far field spatio-temporal PL indicates a variation of transport properties (lifetime and diffusion coefficient) with generated excitons density. The modulation of the latter can be controlled by varying the top hbN thickness in the near-field approach.

In conclusion, we have performed detailed spectroscopic studies on CVD grown lateral MoSe₂-WSe₂ heterostructures. Near field optical study using tip-enhanced experiments shows the important role of the heterojunction, as we show that an excitonic current can only flow from WSe₂ to MoSe₂ and not the other way. This highlights the high structural quality of the heterojunction that can be regarded as an efficient excitonic diode. A possible control of the excitonic density might further give an extra knob to control the excitonic transport.

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Thursday, 14:00-15:40

Strong correlation & topology

MAGNETIC FIELD DRIVEN QUANTUM PHASES IN MAGIC ANGLE TWISTED BILAYER GRAPHENE

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The recent discovery of magic angle twisted bilayer graphene (MATBG), in which two sheets of monolayer graphene are precisely stacked to a specific angle, has opened a plethora of grand new opportunities in the field of topology, superconductivity, and other strongly correlated effect. In twisted van der Waals materials, lattice mismatch can generate moiré patterns, which act as an additional periodicity that has a length scale order of magnitude larger than the underlying atomic lattice scale. For MATBG with a small twist angle close to $\theta = 1.1^\circ$, the electronic bands are flattened by the periodic potential of the moiré bands and isolated from higher-energy dispersive bands. These flat electronic bands in MATBG have recently emerged as a rich platform to explore strong correlations. However, the phases of MATBG in a magnetic field and what they reveal about the zero-field phase diagram remain relatively uncharted. We report a rich sequence of wedge-like regions of quantized Hall conductance with Chern numbers $C = \pm 1, \pm 2, \pm 3$ and ± 4 , which nucleate from integer fillings of the moiré unit cell $\nu = \pm 3, \pm 2, \pm 1$ and 0, respectively. The exact sequence and correspondence of the Chern numbers and filling factors suggest that these states are directly driven by electronic interactions, which specifically break the time-reversal symmetry in the system. The analysis of Landau-level crossings from higher energy bands enables a parameter-free comparison to a newly derived ‘magic series’ of level crossings in a magnetic field and provides constraints on the parameters of the Bistritzer–MacDonald MATBG Hamiltonian [1]. Additionally, we studied the detailed magnetotransport behaviour of the Hofstadter spectrum of MATBG. We observed the re-entrance of insulating states at $\nu = +2, \pm 3$ of the moiré unit cell of MATBG upon applying an external magnetic field close to the full flux quantum $\Phi/\Phi_0 = 1$ of the superlattice unit cell ($B = 25\theta^2$ T) and interaction-driven Fermi-surface reconstructions at other fillings, which are identified by new sets of Landau levels originating from these. These experimental observations are supplemented by theoretical work that predicts a new set of eight well-isolated flat bands at Φ_0 , of comparable band width, but with different topology than in zero field [2].

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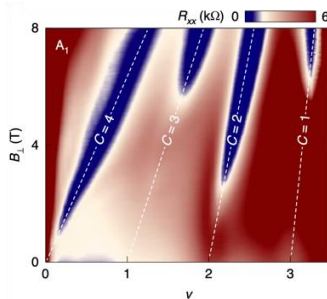


Figure 1: Color plot of R_{xx} as a function of B and ν showing the Chern insulators.

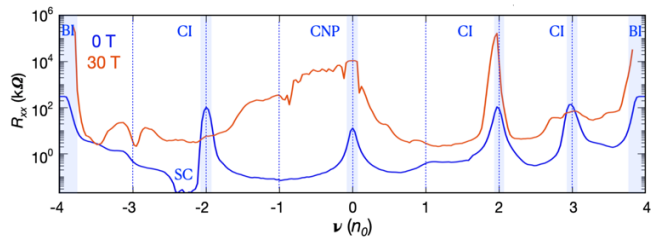


Figure 2: Re-entrant correlated peaks at different integer fillings at $B = 0$ T and $B = 30$ T.

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THE ROLE OF THE BERRY CURVATURE ON INTERACTING ELECTRONS IN 2D CRYSTALS

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The Berry curvature, a quantum-geometric property encoded in the Bloch wave functions, has long been discarded in band structure calculations. Indeed the latter are mainly concerned with spectral properties of electrons in matter, such as the energy bands and the density of states relevant for spectroscopy and transport, while the Berry curvature does not seem to have a spectral effect. In this talk, I will show that this is indeed not the case and that the Berry curvature has indeed to be taken into account in order to describe correctly the spectral properties of 2D electronic materials. To unveil the Berry curvature, electric fields beyond those given by the periodic lattice potential need to be taken into account, and this is naturally the case if electronic interactions are considered [1,2]. I will show that the Berry curvature plays a role in the correct description of excitonic spectra in 2D transition-metal dichalcogenides in the vicinity of the K points [1]. Furthermore, the Berry curvature equally affects the formation of Cooper pairs in such materials and generically lowers the pairing interaction [3].

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GDR HOWDI 2023 MEETING:

ELECTRONIC AND MAGNETIC PROPERTIES IN TWISTED BILAYER GRAPHENE AND MoS_2

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The moiré pattern of the magic-angle twisted bilayers graphene and twisted bilayer MoS_2 leads to localization of the low energy electrons in the AA-stacking regions, reflected by very flat bands at low energy [1,2]. This reduction of the kinetic energy enhances the importance of interactions and thus renders the bilayer systems much more susceptible to correlation effects, as show experimentally by the discovery of correlated insulators and superconductivity [3]. Despite numerous theoretical and experimental studies, the understanding of this new electronic localization is still incomplete. The rotation angle is of course a key parameter, but we have also shown that a small expansion or contraction of one layer with respect to the other (“*heterostrain*”) can strongly modify the electronic structure of flat bands [4].

Here we present theoretical study of the electronic structure and quantum transport properties of electronic flat bands, considering as well as possible the structural parameters that condition them (rotation angle, bias voltage [5], heterostrain and/or local defects [6]). We also investigate the magnetic instabilities using a combination of real-space Hartree-Fock and mean-field theories, starting from a tight-binding description of the non-interacting bilayer systems to which we add a local Hubbard interaction U in order to model the Coulomb repulsion between electron [7]. At half filling, localized magnetic states emerge for values of the Coulomb interaction U that is significantly smaller than what would be required to render an isolated layer antiferromagnetic. We also show how heterostrain strongly modifies the magnetization and the local magnetic order for realistic values of U .

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SUPERCONDUCTIVITY AND THE NORMAL STATE'S BAND GEOMETRY: A HIDDEN INFLUENCE

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Superconductivity has, since 1911, become a pillar and a flagship of condensed matter physics. The main paradigm is given by BCS theory [1] which, in its standard form, consists of quasiparticles in a single, partially filled band, pairing and thus condensating in a single collective dissipationless state. This single band approximation has its limits. Indeed, since the 1980s, physicists have come to realize that in a multiband setting, even adiabatic, each band will carry an influence of the other bands in the form of two geometric quantities, namely the Berry curvature and the quantum metric [2]. These quantities form what we call band/quantum geometry. In the context of superconductivity, this means that even if a single band is involved in the Cooper pairing, it will carry a band geometry if the normal state has more than one band. Its influence on the superconducting state is the subject of this talk. On one side, we study the influence of the normal state's Berry curvature on BCS theory in the context of two-dimensional massive Dirac fermions [3]. We find that it generally lowers the critical temperature, in a quantifiable way. On another side, we apply a theory developed recently [4] to the (111) LAO/STO interface. We find an influence of the normal state's quantum metric on the superconducting state, and particularly the associated dome [5].

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Friday, 9:10-11:30

Applications & devices

ARTIFICIAL NEURAL NETWORKS ACCELERATION BASED ON MONOLAYER MoS_2

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The rise of machine learning applications [1,2] in the past years requires the development of specialized hardware to meet the energy constraints of edge devices [3]. As a solution, in-memory computing architectures have been gaining attention to target this issue by performing the required machine learning operations in the physical layer of memory devices which avoids the von-Neumann bottleneck of traditional computers [4]. Although its promising performances, this technology does not possess a material platform that meets all its requirements. Two-dimensional materials have been demonstrating outstanding electrical performances which could make them a promising candidate to target this type of application. Here, we show a layer of artificial-neural network accelerator based on monolayer MoS_2 . Fig. 1a shows the illustration of a floating-gate field-effect transistor (FGFET) array that can perform hardware dot-product multiplication. Fig. 1b shows the characterization of one of these memory devices, showing a substantial memory window created by charges in the trapping layer. To demonstrate the application of this array for artificial-neural network acceleration, we apply these devices for classifying noise numbers of a 7-segment display in Fig. 1c. Fig. 1d shows the perceptron-layer created for targeting this problem and the feature maps transferred to the memories after *ex-situ* training of this network. Fig. 1e shows the output signals used for the classification of the perceptron layer, obtaining a maximum of 91.5% experimental accuracy [5].

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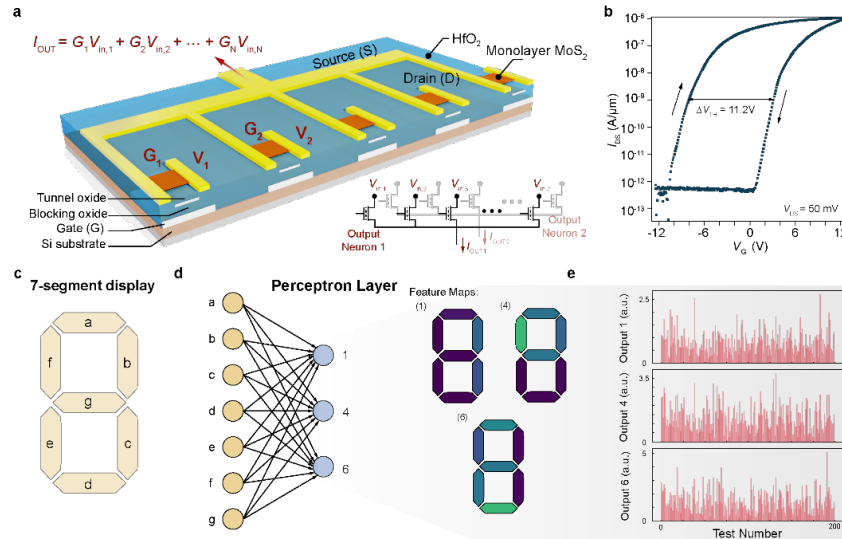


Figure 1: Perceptron layer based on monolayer MoS_2 . (a) 3D schematic representation of the MoS_2 memory device array and the corresponding circuit schematic for the multiplication-accumulation operation. (b) I_{DS} as a function of V_G for constant drain-source voltage, $V_{DS} = 50$ mV. (c) Representation of a seven-segment display. (d) One-layer perceptron network for seven-segment figure classification and feature maps (e) Sample of inference operations after different test signals are sent to the input layer and measured in one of the neurons.

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STRAINTRONICS IN BALLISTIC TWO-DIMENSIONAL LATERAL JUNCTION TRANSISTOR

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In the context of advanced nanoelectronics, two-dimensional semiconductors such as transition metal dichalcogenides (TMDs) are gaining considerable interest due to their ultimate thinness, clean surface and high carrier mobility. Those characteristics would enable device miniaturization at the atomic scale, while improving electrostatic control and suppressing short channel effects significantly [1].

The engineering prospects offered by those materials are further enlarged by the recent realization of atomically sharp TMD-based lateral junctions, whose electronic properties are governed by strain effects directly arising from the constituents lattice mismatch. In essence, deformation can be designed in a controllable manner through the type of substrate, the supercell dimension or the growth process [2].

On this basis, tunnel field-effect transistors FETs based on TMDs lateral junctions were found to be ideal for ultra-low power consumption devices owing to the presence of misfit strain [3]. Conversely, the opportunities opened by the application of extrinsic strain in those systems remain yet to be explored.

In this work, *ab initio* simulations are employed to investigate the transport properties under external deformation of a FET constructed from a MoS₂/WSe₂/MoS₂ junction (see Fig.1). Charge density is modulated in this central region by the top gate voltage, modeled here as an electric potential added to the Hamiltonian. Assuming a rigid shift of the band structure, thermionic current is computed in the ballistic regime using the Landauer formula for a drain-source voltage of 0.1 V, using first-principles simulations as implemented in OpenMX [4].

Owing to the change in band offset, large current modulation is reported in Fig.2, illustrating the importance of strain on the p-n junction characteristics. The exponential dependence of transport mechanisms on strain is understood through a semi-empirical model based on quantum tunneling. This strong modulation contrasts with the moderate gain theoretically predicted in homogeneous MX₂ n-type FETs. Lastly, the device operation is demonstrated for both local and global deformations, even for ultra-short channels, suggesting potential applications for ultra-thin body straintronics [5].

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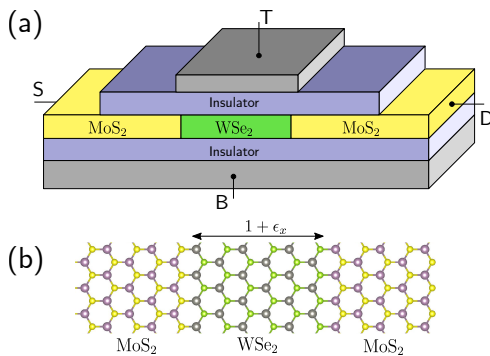


Figure 1: The lateral junction based FET, (a) composed of top (T) and back (B) gates, source (S), drain (D) and a MoS₂/WSe₂/MoS₂ channel, (b) where WSe₂ is strained by $(1 + \epsilon_x)$ along the transport axis.

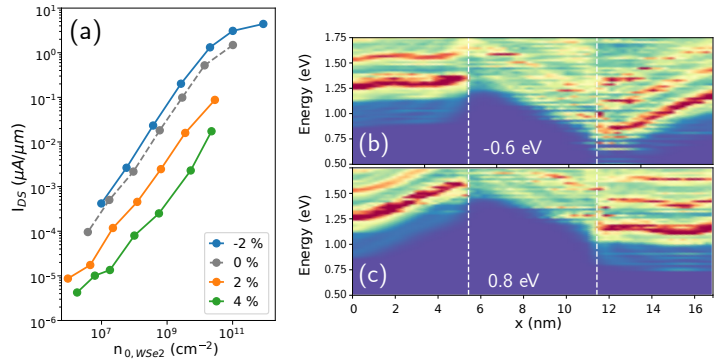


Figure 2: Transport properties of a lateral junction based FET. (a) Transfer characteristics for a channel composed of a 5.8 nm long central strip of WSe₂ for an applied bias of 0.1 V. The corresponding local density of states is provided when $\epsilon_x = 4\%$ at an electrostatic potential of (b) -0.6 eV and (c) 0.8 eV, respectively.

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TMD ENGINEERING OF 2D-MAGNETIC TUNNEL JUNCTIONS – FROM BARRIERS TO ELECTRODES

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Spin-based electronics has already revolutionized data storage and readout technologies. Nowadays it targets a variety of new architectures like embedded MRAMs, spin logics or neuromorphic computing, which makes it one of the most promising post-CMOS approaches. Meanwhile, 2D materials and their combination in heterostructures have opened novel exciting opportunities in terms of functionalities and performances for spintronics devices. The broad family of 2D materials offers many possibilities to engineer the properties of layered stacks and devices in particular via interfacial exchange and proximity effects. One very attractive topic is the field of MTJs based on 2D materials (2D-MTJs). [1] Being able to control the physical behaviour of the MTJ is of crucial interest, in order to improve their functionality and efficiency. From major influence hereby are electrodes and the tunnel barrier, in terms of interfaces and band alignments. Recent work utilised 2D materials to enhance barriers and their performance. Graphene has proved its strong potential as a barrier for MTJs with evidence for spin-filtering through band structure or strong hybridization effects (i.e. spinterface) achieving a record spin polarization of up to -98%. In parallel, advances within the broad Transition Metal Dichalcogenides family of 2D semiconductors and 2D ferromagnets have opened new possibilities to tailor spintronics properties further. As an example, we will show how TMDs could be integrated into a hybrid spin-valves 2D-MTJs and show layer-dependent spin filtering effects. We can show that the spin polarisation can be reversed depending on the number of layers. The layer thickness largely influences the band structure and thus allows control over the open spin channels for vertical electron transport. We will also discuss how to reach one step further with the large scale integration of these materials into tailored 2D heterostructures. For this we developed 2D ferromagnets based on $\text{Fe}_{3+x}\text{GeTe}_2$ which can act as a spin source. We will show that they can be grown in large scale using Pulsed laser deposition (PLD) and reach Curie Temperatures (T_c) above room temperature (RT) while being integrated with other TMDs. We will highlight how these PLD grown ferromagnetic 2D layers could further reinforce the 2D materials family's potential for 2D-MTJs and how they open the way for the design of in-situ full 2D MTJ fabricated devices with artificial properties. [2,3]

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Electrical monitoring of organic crystal phase transition using MoS₂ field effect transistor

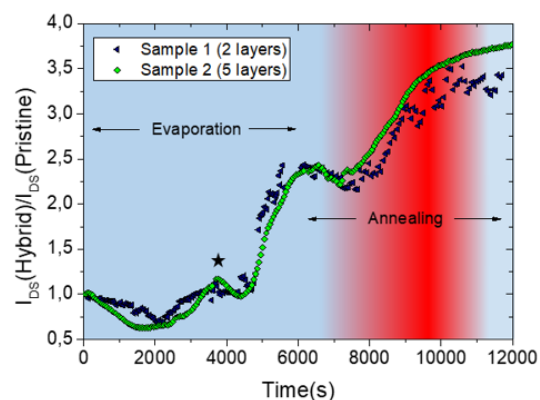
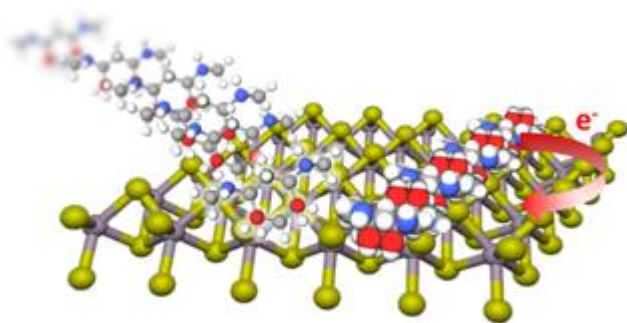
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Hybrid van der Waals heterostructures made of 2D materials and organic molecules exploit the high sensitivity of 2D materials to all interfacial modifications and the inherent versatility of the organic compounds [1-3]. In this study, we are interested in the quinoïdal zwitterion/MoS₂ hybrid system in which organic crystals are grown by epitaxy on the MoS₂ surface and can reorganize in other forms after thermal annealing [4]. By means of field effect transistor measurements and atomic force microscopy, we demonstrate that the charge transfer between organic molecules and 2D materials strongly depends on the conformation of the molecular film. This work shows the great sensibility of MoS₂ transistors for sensing molecular events occurring at the nanoscale providing a new experimental tool in addition to the usual microscopies and spectroscopies techniques.



Left : Schematic representation of charge transfer from Quinoïdal Zwitterion to MoS₂ monolayer.

Right : Curve of the evolution of the current in the transistors over the time.

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GRAPHENE FOR TERAHERTZ RADIATION DETECTION AND BEYOND

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Graphene has several advantages as a material for detectors of terahertz radiations. These include but are not limited to relatively high mobility, tunability of properties by electrostatic gating and geometric control of the band structure. Graphene has also been proved to support long-living plasma excitations that significantly enhance the range of optoelectronic applications of graphene in terahertz and mid-infrared range.

In this talk I will present several graphene-based detector configurations and show how plasma waves in the graphene channel affect their photoresponse. In particular I will discuss plasmon resonance in a 6-micron long channel formed by a boron-nitride (BN) incapsulated double-layer graphene. I will show that the observed features can be used for analysis of the single-particle spectrum.

Nex I will discuss how plasmonic effects can be unveiled in devices based on graphene grown on a metallic surface by chemical vapor deposition (CVD) and transferred onto a dielectric substrate. Until recently it was generally believed that such graphene has too small mobility for any observable plasmonic effect. Nevertheless, our recent works prove that it is not the case [2, 3]. The data I will present in this talk is interpreted as a fingerprint of plasmon interference inside graphene channel with a length of few microns.

Finally I will report on how tunneling in graphene channel can give rise to strong enhancement of the terahertz detector photo response [4].

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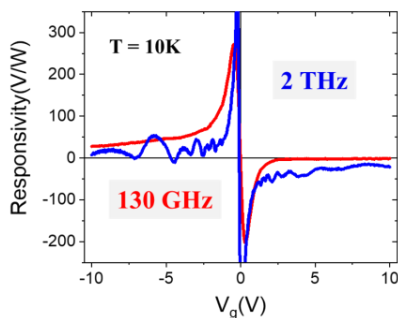


Figure 1: Illustration of plasmonic resonance effect on the photo response of a by-layer graphene based field-effect transistor [1].

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Poster List

AB-INITIO STUDY OF THE EFFECTS OF Pb INTERCALATION IN GRAPHENE/SiC HETEROSTRUCTURES

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Graphene has paved the way to a widespread interest in two dimensional materials. Due to its peculiar electronic, mechanical, and electron-transport properties it is regarded as a promising material for nanoelectronic and spintronic applications. Many efforts have thus been made to find proper substrates and efficient processes for high quality graphene growth, and SiC has been found to be one of the leading solutions. However, the absence of a tunable band gap in graphene is a crucial barrier for nanoelectronics applications. Moreover, the strong covalent interactions with the SiC in graphene/SiC heterostructures results in a high electron doping in graphene, which affects the charge carrier mobility [1]. Finding an efficient way to open a band gap and decouple graphene from the substrates is thus essential. A solution to overcome these obstacles, which has attracted much interest in recent years, is the intercalation of atomic species into the graphene/substrate interface. In fact, two key factors in the opening and tuning a band gap in graphene are the symmetry breaking of the sublattice and the presence of strong spin-orbit (SO) interaction. Intercalated metals have become promising to engineer a large band gap in graphene via spin-orbit coupling. Several species have been found to be able to intercalate in the graphene layer like H, Au, Pt, Li, Na, F, Mn, Si, Ge. Among them, intercalation of heavy atoms like Pb with large SO coupling was used to modify the energy spectra and density of states of graphene in order to make it equivalent to the energy levels of a 2D electron gas in a constant magnetic field [2][3]. It has been experimentally observed that twisted Plumbene is able to open a gap of 30 meV at the Fermi energy [4]. Moreover, it has been found that intercalating atoms under epitaxial graphene can efficiently decouple it from the substrate. The aim of this work is to investigate, via DFT calculations, the intercalation of a 2D plumbene layer in graphene on a SiC substrate. Calculation of DOS and band structure projection onto atomic states highlight the effect of Pb intercalation in altering the dispersion of the states near the Dirac cones due to energy levels hybridization. Analysis of the vacuum level, work function as well as investigation of charge transfer in the designed Van der Waals heterostructure, before and after intercalation, are included in this study. Starting from the choice of a proper coincidence lattice, calculations also reveal, after the intercalation, the formation of a disordered Pb monolayer covalently bonded to the SiC substrate.

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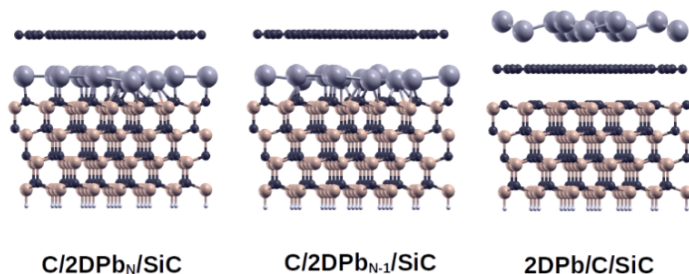


Figure 1: Crystal structures of graphene/plumbene bilayer on SiC(000-1) before and after Pb intercalation

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GDR HOWDI 2023 MEETING: ACTIVATION OF A QUANTUM EMITTER IN A hBN WAVEGUIDE FOR INTEGRATED QUANTUM PHOTONICS

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We created single-photon sources that are directly integrated into a monolithic hBN (hexagonal Boron Nitride) waveguide. Such structure would be the starting point for designing a nanophotonic circuit.

Single-photon emitters in hexagonal boron nitride are promising candidates for applications in integrated quantum nanophotonics. One requirement for creating quantum photonic circuits is to find a way to couple a quantum emitter to the guided mode of a photonic waveguide. Several structures have already been developed, including hybrid integration of a quantum dot on a silicon waveguide [1], or etching of a monolithic waveguide around previously created color centers [2].

Here we propose a protocol that starts with the fabrication of the waveguide by performing electron beam lithography on an exfoliated hBN flake. Then we integrate a quantum emitter within the waveguide by electron irradiation. Indeed this technique enables position-controlled activation of defects that emit single photons at 436 nm [3,4]. Previous studies on these color centers have shown that they display high and stable count rates, good single-photon purity and coherence properties that allow indistinguishability between the emitted photons [5,6].

After irradiation the waveguides are studied with a confocal microscope at room temperature. The emitters are spotted along the waveguide and their photophysical properties are determined using usual photon-counting techniques. The excitation path is then separated from the collection path, so that the photoluminescence that couples to the guided mode can be collected at one end of the waveguide. The second-order auto-correlation histograms reveal a good preservation of the source's antibunching when the photons couple to the waveguide.

Extending and building from this prototype would enable to design integrated quantum photonic circuits in the frame of applied quantum information science.

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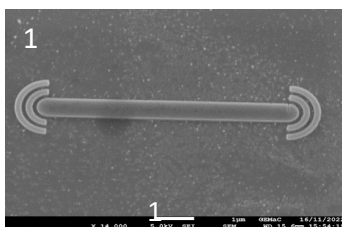


Figure 1: SEM image of a hBN waveguide.

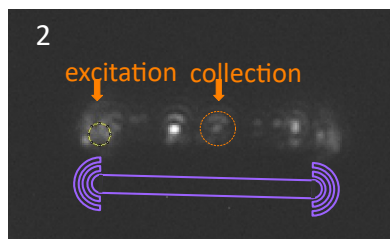


Figure 2: CCD image showing the emitters along the waveguide (white spots) when they are excited by a 405nm laser passing through the waveguide.

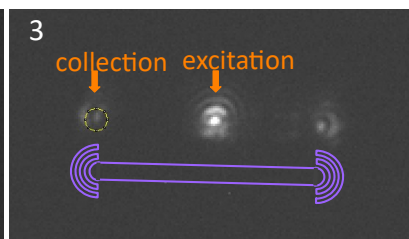


Figure 3: CCD image showing the photoluminescence of one single-photon emitter that is directly excited. The photons that coupled to the guided mode appear at both ends of the waveguide.

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ANHARMONICITY OF THE CURRENT-PHASE RELATION IN GRAPHENE JOSEPHSON JUNCTIONS FOR PARITY-PROTECTED SUPERCONDUCTING QUBITS.

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Errors are currently the limiting factor preventing the opening of a widespread quantum computing era. Quantum errors corrections scheme enable the mitigation of this issue but require to realize a single logical Qubit a very large number of physical Qubits. Since this number increases dramatically with the error rate of the single Qubit, focusing on enhancing the base performance of Qubits is a promising strategy towards fault tolerant quantum computing. We investigate the anharmonicity of the current phase relation (CPR) in Josephson junctions (JJ) in which graphene is the intermediate medium between two superconductor electrodes. We isolate the non-first order harmonics of the CPR using a DC SQUID in the frustrated regime. Such device will be later included in a topologically protected Qubit architecture meant to prevent transition between the first excited and ground states and hence enhance the relaxation time T_1 .

We fabricate gate tunable h-BN encapsulated graphene JJs. Thanks to the high transparency of the graphene JJ ($T > 0.8$), the CPR exhibits a significant deviation from the usual harmonic CPR $I(\varphi) = I_c \sin(\varphi)$ due to the presence of higher order harmonics [1] (Figure 1). By using two graphene JJs arranged in a SQUID, we can use an external magnetic field to set the system in a “frustrated” regime where odd terms of the two junctions CPR cancel themselves out, resulting in a π periodic CPR (Figure 1). A key feature of the graphene JJs is here its tunability with gate voltage that enables the realization of identical JJs necessary for maximal efficiency.

As phase and charge are conjugate variables in superconducting Qubits, vanishing odd terms in the CPR prevents the tunneling of a single Cooper pair, as well as all odd numbers of Cooper pairs, which results in tunneling events being mainly tunneling of pairs of Cooper pairs. From this property, a transmon Qubit based on this graphene JJ SQUID has a ground and first excited states with opposite parities in charge basis (Figure 2). Such pair of states are then parity protected against single Cooper pair scattering operators, which suppresses dominant recombination channels responsible for the limitation of the Qubit relaxation time T_1 [2].

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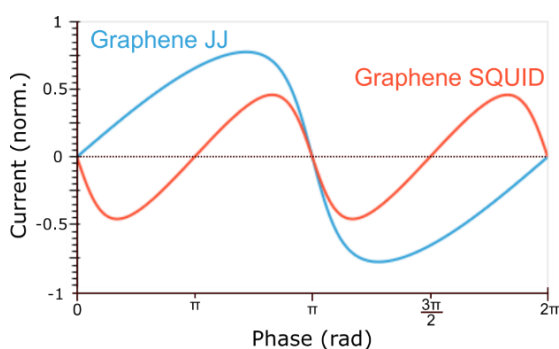


Figure 1: Current-phase relation for a single graphene JJ and for a symmetric graphene JJ SQUID in the frustrated regime. Analytical formulas are plotted here. Experimental realization will be discussed at the workshop.

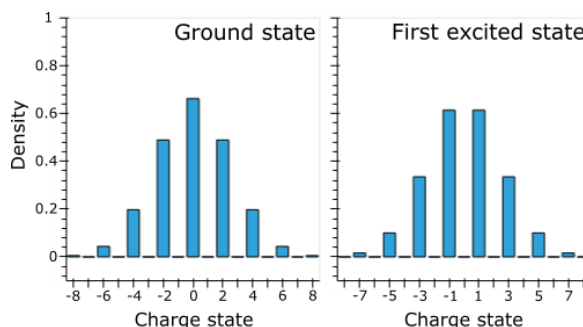


Figure 2: Representation in charge basis of the ground and first excited states of a transmon Qubit based on a graphene JJ SQUID in the frustrated regime.

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COMPARISON BETWEEN MgO AND Al₂O₃ BARRIERS IN GRAPHENE-BASED HETEROSTRUCTURES FOR SPINTRONICS

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Due to its unique physical properties and ultimate thickness, monolayer graphene (Gr) has been widely used in nanoelectronics. The importance of this material for both fundamental spintronics and future applications was quickly realized after the first unambiguous demonstration of spin transport in graphene at room temperature [1]. Thanks to its weak spin-orbit coupling and large spin diffusion length, the Gr has been the subject of research in a number of applications, such as magnetic junctions with or without a tunnel barrier. However, in addition to the wavy surface of the Gr, the deposition of a metallic layer on it causes defects or even amorphisation of the Gr layer [2]. Controlling the quality of the Gr/ferromagnetic material (FM) interface, which directly affects the magnetic properties of the basic units of spintronic devices, is a major challenge, and few works in the literature have been reported for the effect of intercalating an insulating barrier between the Gr and the FM on the dynamic magnetic properties of these units. Here we report on a comparative study on the effects of two barriers MgO and Al₂O₃ on structural and magnetic properties of SiO₂/Gr/Barrier/CoFeB (CFB)/Ta structures (Figure 1.a), which are compared with those of control samples (without Gr layer). In our work, a monolayer of high quality Gr was synthesized by inductive heating CVD, while MgO and Al₂O₃ were deposited by molecular beam epitaxy and atomic layer deposition, respectively. Characterization by Raman spectroscopy showed that MgO induces more defects in the Gr than Al₂O₃, confirmed by the increase in intensity of defect peak (D) of Gr/MgO/CFB Raman spectrum, but without reaching the amorphisation stage (Figure 1.b). Our results are consistent with the literature [2]. The static magnetic properties were characterized by using the Magneto-Optical Kerr effect (MOKE). While no difference is observed for the control samples (inset fig 1.c), the Gr/MgO/CFB system showed high coercivity compared to Gr/Al₂O₃/CFB system, as shown in Figure 1.c. This indicates that the system has more heterogeneities in the presence of MgO barrier. Dynamic magnetic properties were also investigated. Ferromagnetic Resonance (FMR) results showed that the Gr/MgO/CFB structure exhibits different resonance modes, which is not the case for Al₂O₃ barrier (Figure 2.a); this result is another indication of the heterogeneity of the MgO based system. Brillouin light scattering (BLS) characterizations showed that the good quality of the Gr/Al₂O₃/CFB led to an increase in the perpendicular magnetic anisotropy (Figure 2.b), illustrated by lower frequencies, which is a key property for spintronic devices. This study provides a good understanding of the magnetic behavior of graphene-based heterostructures intercalated with two different insulating barriers.

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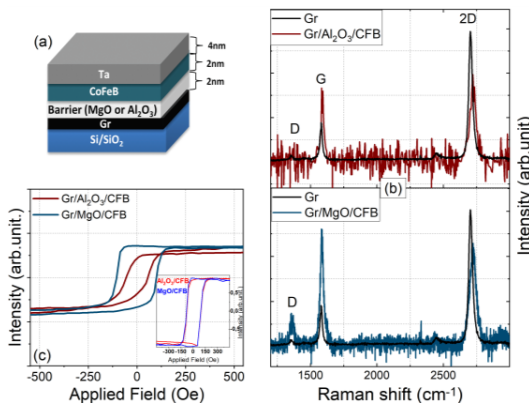


Figure 1: a. samples structure, b. Raman spectra, c. MOKE cycles. The inset of (c) is the controls MOKE cycles.

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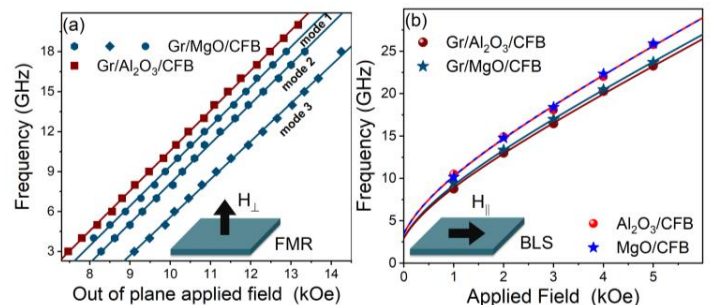


Figure 2: Dynamic characterizations: a. FMR results, b. BLS results

DYNAMICAL SCREENING OF REMOTE ELECTRON-PHONON SCATTERING IN BN-ENCAPSULATED GRAPHENE

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BN-encapsulation leads to some of the highest mobilities in graphene devices, even approaching the ideal, intrinsic limit in the high doping regime. At low doping, however, electron scattering seems to increase with respect to intrinsic models based on density-functional theory (DFT) calculations. In that case, remote electron-phonon scattering from the BN encapsulator may play a role. We investigate this mechanism using DFT-based seminumerical models. The phonons of BN inducing remote couplings to electrons in graphene are identified, and the interaction is quantified as a function of the number of layers. The main challenge is the prohibitive cost of full DFT calculations on the whole heterostructure. To avoid it, the bare electron-phonon interactions originating from each layer is extracted from DFT[1] and then screened with the dielectric response from the heterostructure computed within a semi-analytical model[2]. BN's LO phonons couple remotely via the well-known Fröhlich interaction. BN's ZO phonon also couple remotely. In fact, they only couple remotely, because the associated perturbation is odd with respect to the plane of the BN layer, implying a vanishing intralayer coupling. The dynamic electronic response of graphene is accounted for in the form of standard electronic screening, as well as the coupling between graphene's plasmons and BN's phonons. While strongly screened most of the time, remote couplings with BN lead to a significant increase of resistivity at low doping, when scattering momenta and energies are around and above graphene's plasmons dispersion.

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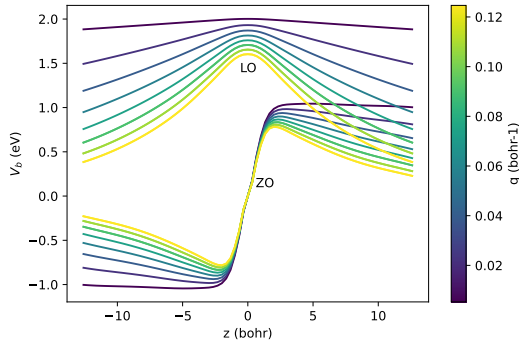


Figure 1: Perturbing potentials associated to the LO and ZO phonons of a single layer of BN in the x-y plane at $z=0$.

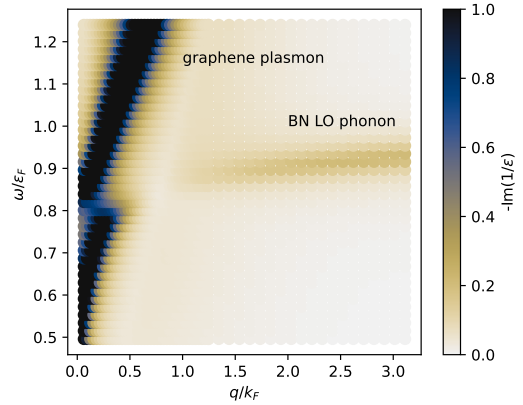


Figure 2: Plasmon-LO phonon coupled modes in the graphene/5-BN heterostructure, revealed by the imaginary part of the inverse dielectric function.

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GDR HOWDI 2023 MEETING: ENCAPSULATION OF DICYANODISTYRYLBENZENE IN SINGLE- WALL CARBON NANOTUBES

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Single-walled carbon nanotubes (SWCNTs) are known for their unique optical and electronic properties. Moreover, their nanometric size, combined with their hollow core, allows quasi-one-dimensional confinement of molecules¹.

In this work, we study the encapsulation of dicyanodistyrylbenzene, an organic dye known to present fluorescence enhancement in solid state. This aggregation-induced enhanced emission (AIEE) is due the formation of specific staking state of the molecule². The idea of this project is to use SWCNTs as a template to access various staking state of the BDCS, driven by the diameter of the SWCNT, to study the new resulting luminescence. We first synthesize the dicyanodistyrylbenzene that we encapsulate in SWCNT using classical infiltration in the liquid phase. A first indication of the success of the encapsulation was obtained by UV-VIS absorption, where a shift in the optical transition of the SWCNTs and the dye was observed (Fig.1).

Furthermore, the encapsulation of the dye in SWCNTs should result in the photosensitization of SWCNTs by an energy transfer bringing added value in the field of photoconversion and by extension for applications in the field of photovoltaics.

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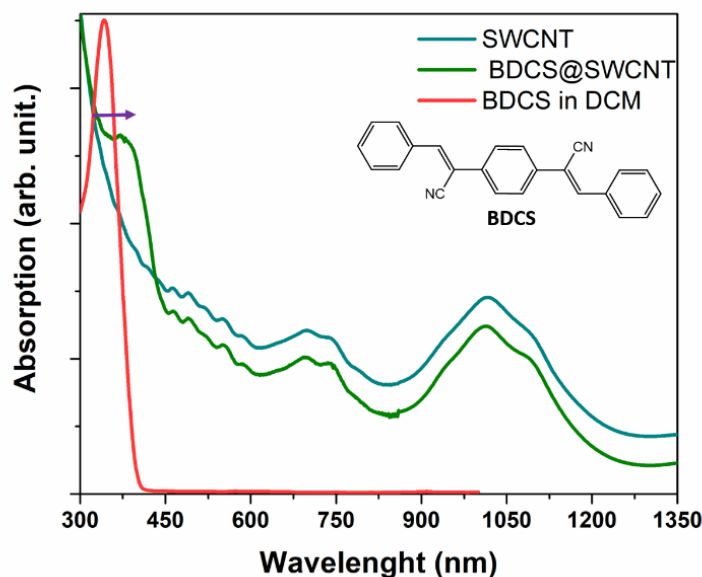


Figure 1 : Absorption spectra of the BDCS in solution (red), BDCS encapsulated in SWCNT (green) and of water filled SWCNT (blue) as a reference.

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GDR HOWDI 2023 MEETING: EXCITONS IN DISORDERED BORON NITRIDE

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Hexagonal Boron Nitride (hBN) is a two-dimensional material well known for its very strong excitonic effects. More recently, *amorphous* Boron Nitride (aBN) has attracted strong attention as an ultralow dielectric constant material, with potential for next generation interconnects [1]. Because of this ultralow dielectric constant, one can expect bound electron-hole pairs – excitons – to also play a significant role in the optical activity of this system, and therefore in its characterization.

There is thus presently a need for methods to compute excitonic properties of large disordered systems while explicitly taking their atomic geometry into account; and to investigate the complex interplay between disorder-induced localization, Coulomb interaction and screening effects. Using BN as a prototypical material, we start from an electronic tight-binding (TB) model for a disordered BN system and perturbatively map the Bethe-Salpeter equation onto an effective TB Hamiltonian for localized electron-hole pairs [2]. We are then able to extract relevant properties for large systems at a low computational cost by means of linear scaling techniques (KPM, recursion...) [3, 4].

As a proof of concept for this approach, we discuss the optical absorption of single layer hBN in the presence of Anderson (onsite) disorder (fig. 1), as well as a simple toy model of geometrically disordered BN based on aBN structures obtained through molecular dynamics [5].

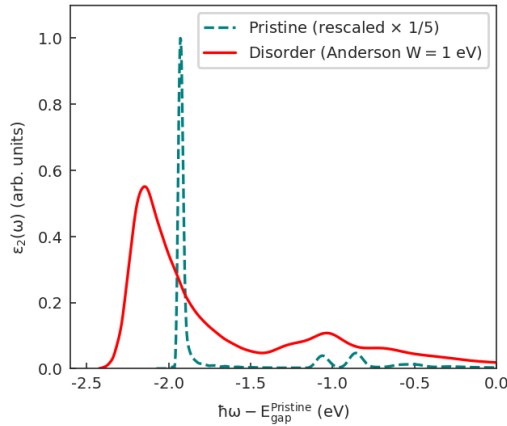


Figure 1: approximation of the absorption spectrum of single-layer hexagonal Boron Nitride in the presence of Anderson disorder (without exchange interaction).

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EXPERIMENTAL PROGRESS IN HYDROGENATION AND FLUORINATION OF MONOLAYER GRAPHENE AND CHARACTERIZATION BY RAMAN SPECTROSCOPY

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Two-dimensional (2D) in-plane sp^2/sp^3 -C heterostructures based on graphene would be a significant improvement in building high carrier mobility 2D devices for applications in nanoelectronics [1] or biology. Theoretical studies had already demonstrated that hydrogenation or fluorination of monolayer graphene (1LG) allows sp^2 to sp^3 conversion of carbon atoms hybridization in graphene giving birth to a new 2D material named graphane. DFT calculations of electronic band structure have shown that graphane is an insulator with a direct energy gap [2]. Recently, with the collaboration of PUCMM, and Clermont university, we obtained important results in the hydrogenation and fluorination of 1LG. Different experimental conditions were tested on 1LG samples deposited on SiO_2 using mechanical exfoliation of highly oriented pyrolytic graphite (HOPG). A thin layer of polymethyl methacrylate (PMMA) was spin-coated onto the samples and patterned by electron beam lithography in order to get samples partially covered by the resist. Low-temperature hydrogenation and fluorination were performed with different thermodynamic conditions and Raman spectroscopy at 2.33 eV was used to characterize the 1LG flakes at different points. For both hydrogenation and fluorination, we observed significant differences in Raman spectra between covered and uncovered 1LG areas. The covered areas remained unchanged while the uncovered ones showed the D and D' bands arising from point defects in graphene. The calculated intensity ratios $I(D)/I(D')$ for these two bands reach values up to 17.2 for hydrogenated samples and 12.8 for fluorinated ones. These values are large enough to conclude that point defects in hydrogenated and fluorinated samples are not vacancies but sp^3 -C defects [3], which was confirmed by releasing of hetero-atoms at moderate temperature (loss of the D band) contrary to vacancies where no change is observed.

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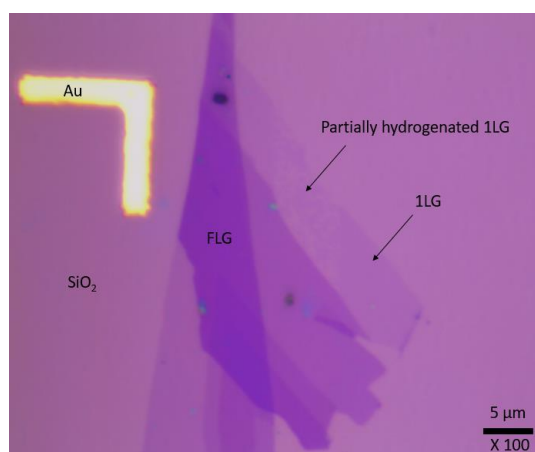


Figure 1: Optical image of a 1LG flake with a partially hydrogenated area.

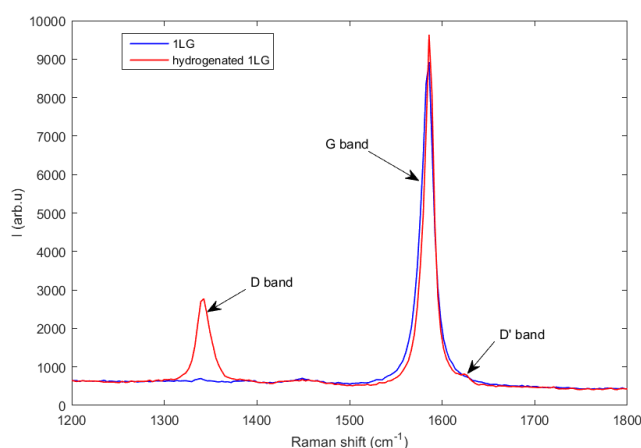


Figure 2: Raman spectrum of a 1LG hydrogenated area (red) and 1LG non-hydrogenated area (blue).

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GROWTH MECHANISMS AND HYDROGENATION OF GRAPHENE USING PROPANE/HYDROGEN CVD ON SiC

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Propane/hydrogen CVD growth of graphene on SiC, studied since 2010 [1], consists simply to grow graphene from propane in a hydrogen/argon atmosphere. The presence of hydrogen in the gas phase promotes Si excess on the surface, hence making impossible graphene growth without propane flow [2]. This makes propane/hydrogen CVD very different from silicon sublimation where graphene grows from a carbon excess on SiC. Graphene films are mainly grown in a propane/hydrogen/argon gas mixture at high temperature (1550°C) near atmospheric pressure, conditions allowing to grow uniform n-doped monolayers on 2'' SiC wafers. Graphene films prepared in such conditions have been widely used for applications in electrical metrology [3] or as a substrate for van der Waals epitaxy of nitrides [4] or 2D materials [5]. Though, a complete growth study for these specific growth conditions was still missing. Our contribution will present first elements of this study and discuss the growth and hydrogenation mechanisms occurring both during growth step and cooling down.

A first set of samples, consisting in graphene films grown with different hydrogen/argon ratio, allows to observe the formation of different graphene structures and interfaces with SiC, from disordered multilayer graphene on a hydrogenated interface to monolayer graphene on a buffer layer (see AFM in Fig. 1.a-d). In order to study the different steps of graphene formation, we have grown samples with different growth time in conditions leading to the formation of a buffer layer interface (see AFM in Fig. 1.e-f). Surprisingly, incomplete graphene layers presented hydrogenated interfaces (revealed by wrinkles in Fig. 1.f), suggesting hydrogenation of the interface during cooling down. This led us to optimize the cooling down to minimize changes in graphene interface during this last step. The new set of graphene samples with different growth time and optimized cooling down allows to observe the different steps of graphene formation, leading to a better understanding of growth. In addition, the optimized cooling down allows to improve the quality of graphene films grown on 2'' wafers.

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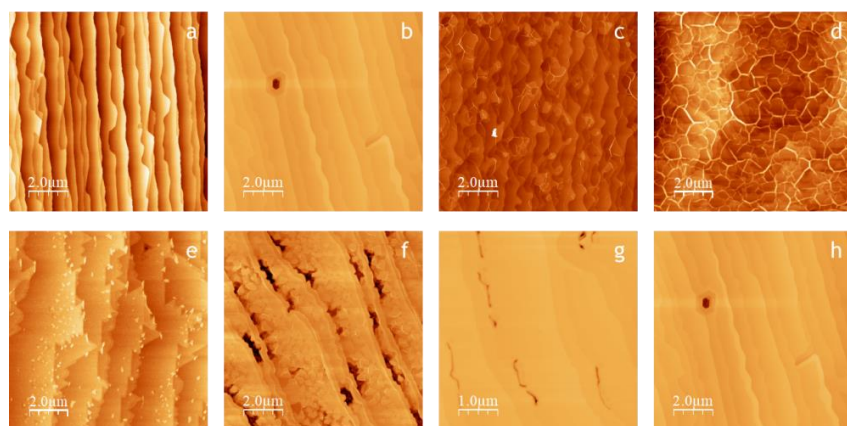


Figure 1: AFM images on sample grown for 15 minutes with increasing hydrogen/argon ratio (a-d), and with different growth time (e-f).

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GROWTH OF 1T'-WTe₂ THIN FILMS BY MOLECULAR BEAM EPITAXY

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Transition metal dichalcogenides (TMDCs) have garnered significant interest due to their unique properties and potential for various applications in electronics, photonics, and energy. Typically, TMDCs are obtained through mechanical or chemical exfoliation of bulk crystals into thin atomic layers. However, growth of these materials through molecular beam epitaxy (MBE) offers significant advantages, including the production of high-quality films and precise control over layer thickness, making it more suitable for industrial applications.

Among TMDCs, WTe₂ is the only one for which the 1T' phase is most energetically favored. Monolayer TMDCs with this phase have been theoretically predicted to be quantum spin Hall insulators^[1], which are promising materials for spintronic applications. WTe₂ has also been experimentally demonstrated as ferroelectric for 2 and 3 layers^[2].

In this study, growth of 1T'-WTe₂ thin films by molecular beam epitaxy was achieved on a graphene substrate. A band structure similar to the literature^[3] of monolayer 1T'-WTe₂ was measured by ARPES (Figure 1), highlighting the good quality of the film.

Several growth conditions were explored in order to improve the film quality. We show that by reducing the nucleation density, island size can be increased (Figure 2.a). We achieved a mean island size of 125nm so far (Figure 2.b), which is up to one order of magnitude larger than results reported in the literature for MBE growth of WTe₂^{[4][5][6]}. Large islands are important to improve transport properties because large density of grain boundaries can act as scattering centers for carrier transport, reducing the mobility of grown films^[7].

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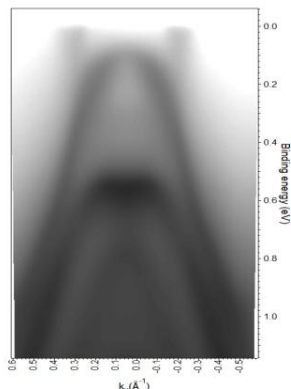


Figure 2: Monolayer 1T'-WTe₂ band structure measured by ARPES.

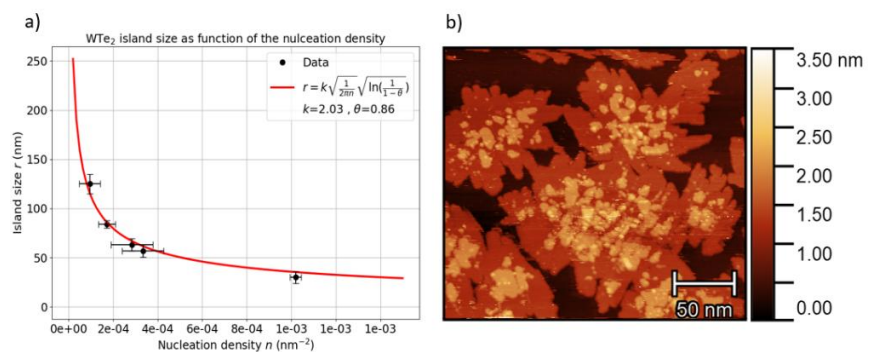


Figure 1: a) WTe₂ island size as function of the nucleation density b) STM image of WTe₂ islands grown by MBE.

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GROWTH OF MONOLAYER MoS_2 FLAKES BY MBE ON GAN

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Since the discovery of two-dimensional (2D) graphene monolayer and its exceptional physical properties, research on 2D materials has generated a lot of interest. Among these 2D materials, molybdenum disulfide (MoS_2) has attracted enormous attention in the last ten years due to its unique electronic and optical properties and also tunable depending on the number of layers [1].

Synthesis of these 2D materials can be carried out either by exfoliation or by epitaxy. Exfoliation technique is difficult to reproduce on a large scale and difficult to industrialize. Our work focused on molecular beam epitaxy (MBE), a conventional method used to grow semiconductor materials on wafer-scale. This growth technique has advantages such as precise control of composition, purity and layer thickness. In this study, we investigated the growth of MoS_2 on a gallium nitride (GaN) surface by MBE. GaN is a semiconductor material widely used in optoelectronics and electronics, moreover its compatibility (hexagonal structure and close lattice parameter) with MoS_2 has many advantages for the development of new devices. The MoS_2 growth was carried out at temperature around 700°C in a sulfur-rich environment using an electron beam evaporator for the evaporation of Molybdenum (Mo) and a reflection high energy electron diffraction (RHEED) system for in-situ monitoring. Growth parameters such as temperature and deposition time have been optimized to obtain high quality films.

Atomic force microscopy (AFM) was used to characterize morphology and height. Figure 1, shows triangular-shaped domains of MoS_2 with an average side length of 100 nm and a height of approximately one monolayer (~ 0.7 nm). Mainly 2 orientations of domains (0° and 60°) are observed in the plane of the GaN surface. Raman spectrum (figure 2) shows the characteristic peaks of MoS_2 at 383 cm^{-1} (E_{2g}), 405 cm^{-1} (A_{1g}). The results demonstrate that MBE is a promising technique to produce high-quality MoS_2 domains on GaN substrates with controlled shape and coverage. The study contributes to a better understanding of the mechanism of MoS_2 growth by MBE and opens opportunities for the development of electronic and optoelectronic devices based on MoS_2 .

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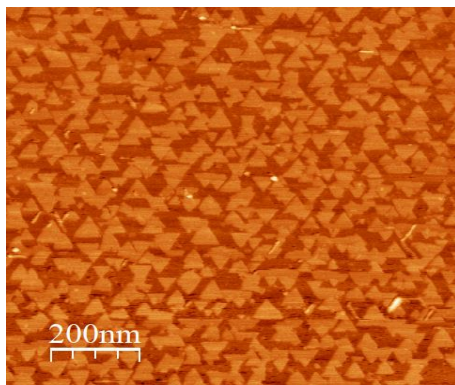


Figure 1: $1 \times 1 \mu\text{m}^2$ AFM image showing MoS_2 flakes grown on GaN surface

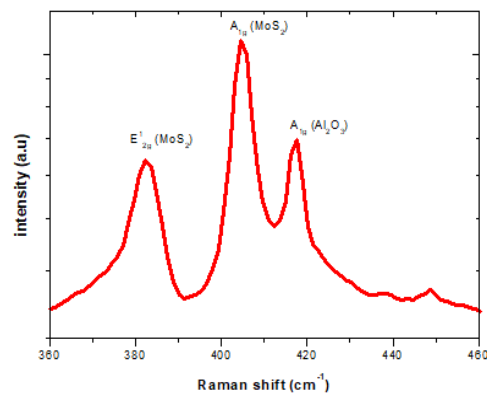


Figure 2: Raman spectrum characteristic of A_{1g} (at 405 cm^{-1}) and E_{2g} (at 383 cm^{-1}) vibrations of MoS_2 and substrate (sapphire at 417 cm^{-1})

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IMPACT OF SHELL THICKNESS IN 2D CDSE/CDS CORE/SHELL NPLS FOR HIGH PERFORMANCE PHOTODETECTOR APPLICATIONS

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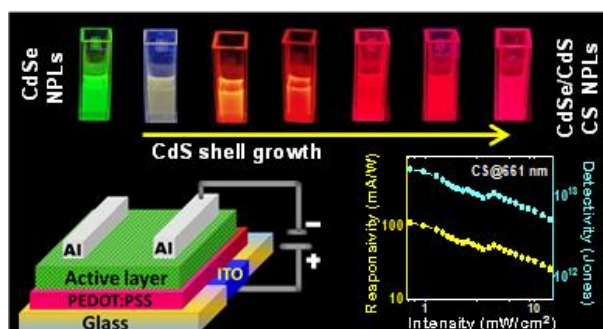
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The rapid development of photonics technologies in our everyday life, there is a high demand for high performance photodetectors for applications in biosensors, optical communication, and thermal imaging etc.¹ Therefore, a well-defined, cost-effective, high quality, and stable photodetector fabricated with solution processed nanostructures is very much needed. Colloidal two-dimensional (2D) CdSe nanoplatelets (NPLs) have drawn a surge of research interest for promising optoelectronic applications such as LEDs, laser diodes, solar cells, photoconductors, and photodetectors.²⁻⁴ The optical properties and stability of these CdSe NPLs could be enhanced by overcoating it with wider band gap shell materials.⁵ 2D CdSe/CdS core/shell NPLs has been successfully synthesized by high temperature colloidal hot injection method. Rietveld analysis of XRD patterns suggests the coexistence of zinc-blende and wurtzite polymorph in ~5:3 ratio in the CdSe/CdS NPLs. TEM images reveal the total thickness of ~3.8 nm in CdSe/CdS NPLs over the core thickness of ~1.2 nm. The tuning of emission from green to red and ~12 times enhancement of PL decay time are achieved by controlling the reaction growth time. The carrier dynamics of CS NPLs depends largely on the shell thickness due to their quasi type-II band alignment, where the electrons get delocalized in the CdS shell, and the holes remain localized in the CdSe core. Femtosecond transient absorption spectroscopy reveals slower bleach recovery dynamics after shelling indicating effective separation of charge carriers in core/shell NPLs and it is very much beneficial for photodetector applications. The photodetector devices fabricated with CdSe/CdS core/shell exhibit high photocurrent (~60 μ A), fast photoresponse of ~100 ms with a responsivity of ~113 mA/W and a very high detectivity value of ~2.1 \times 10¹³ Jones in the visible region. This study provides insight into structural and carrier relaxation dynamics of CdSe/CdS core/shell NPLs for designing high-performance photodetectors.

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Scheme 1. Schematic presentation of the red shift of photoluminescence of core/shell NPLs with increasing shell thickness and the high photodetector performance of the CdSe/CdS core/shell NPLs.

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MOLECULAR BEAM EPITAXY OF TASE₂ ON GAP(111)B

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Transition-Metal Dichalcogenides (TMDCs) consist in layers of 3 covalently-bound atomic planes made of a transition metal between two chalcogens (S, Se or Te), connected by van der Waals forces. Thanks to the large number of atom combinations and layer-stacking sequences they provide a large variety of properties while their two-dimensional structure offers the possibility of growing high-quality heterostructures regardless of the lattice mismatch [1]. Among them, metallic TaSe₂ has attracted significant attention because it exhibits Charge Density Wave (CDW) and superconductivity, but very few attempts have been reported to grow TaSe₂ by Molecular Beam Epitaxy (MBE). Especially among III-V semiconductors, only growth on AlN and GaAs have been demonstrated [2, 3]. In this study, we investigated TaSe₂ growth on GaP, a substrate that provides a higher temperature stability than GaAs and a small lattice mismatch with Si.

GaP(111)B substrates are deoxidized and Se-terminated before TaSe₂ growth by Molecular Beam Epitaxy (MBE). The layers are characterized *in-situ* by Reflection High Energy Electron Diffraction (RHEED) and X-ray Photoelectron Spectroscopy (XPS), and *ex-situ* by Atomic Force Microscopy (AFM) and Scanning Tunneling Microscopy (STM) in ultrahigh vacuum (UHV). For this latter, a protective Se cap layer is deposited after growth and desorbed under UHV prior to STM experiments. The effect of substrate temperature, growth rate and Se:Ta ratio have been studied.

Despite the RHEED pattern shows diffuse streaks indicating a poor crystallinity at low temperature and spots interpreted as surface roughness at intermediate temperature, it is significantly improved after a short annealing leading to thin streaks. Since the octahedrally coordinated 1T phase of TaSe₂ exhibits a CDW at ambient temperature, it results in a splitting of the Ta4f energy band that is clearly observed in XPS and enables an easy phase determination. Similarly to what was reported on graphene [4], a temperature selective growth of 1T and 1H polytypes is obtained in monolayer (1ML) TaSe₂. By contrast the polytypes with hexagonal coordination (stacking of 1H layers) are consistently found in multilayer TaSe₂.

AFM images on 1ML 1T-TaSe₂ show a rather uniform surface coverage whereas Low Energy Electron Diffraction (LEED) and STM images reveal a moiré caused by the lattice difference between GaP and TaSe₂. The characteristic CDW of 1T-TaSe₂ has been observed by STM and Scanning Tunneling Spectroscopy (STS) confirms that the 1T-TaSe₂ 1ML grown on GaP is a Mott insulator at low temperature.

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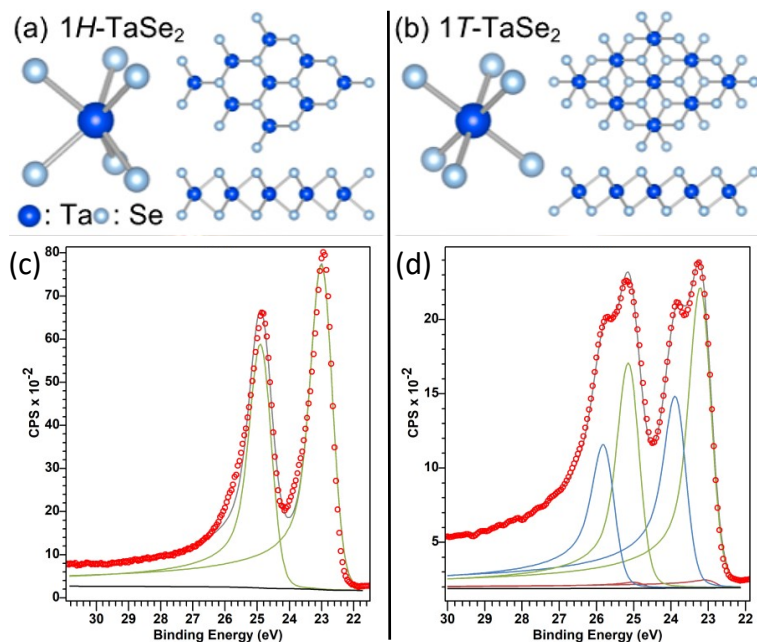


Figure 1: (a) and (b) TaSe₂ polytypes [4], (c) and (d) respective XPS spectra of Ta4f lines.

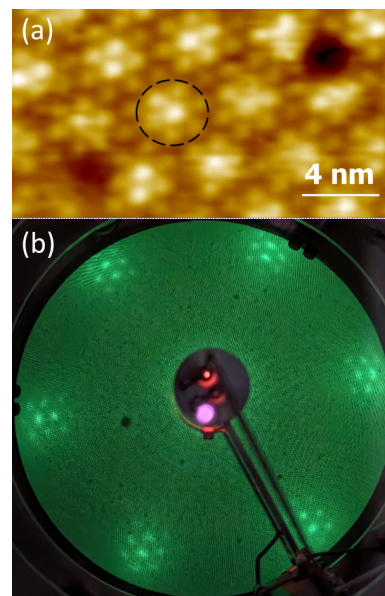


Figure 2: (a) STM image of a monolayer 1T-TaSe₂ on GaP(111)B presenting both CDW (dots) and moiré (circled pattern), (b) LEED pattern with moiré.

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NANOGRAPHENES IN LAYERED HETEROSTRUCTURES

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Nanographenes such as graphene nanoribbons (GNRs) and graphene quantum dots (GQDs) have a great potential for a wide range of applications including optoelectronic devices or quantum sensing. In particular, one of their assets is their synthesis by bottom-up chemistry that allows a total control on their structure, opening the way to the customization of their electronic properties [1–3]. In particular, we recently investigated the intrinsic properties of such objects embedded in a polymer matrix used to stabilize their emission properties [4-7]. In order to go a step further, the inclusion of GQDs in real devices is mandatory. In this direction, their coupling with other materials in heterostructures is a way that has to be explored.

In this poster, we will present our preliminary results on the coupling of nanographenes with different materials (h-BN, TMDCs, perovskite...). The properties of nanographenes are investigated by optical experiments down to the single molecule level.

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OPTICAL PROPERTIES OF SINGLE ELONGATED GRAPHENE QUANTUM DOTS

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Since its discovery in 2004, graphene proved to be a 2D material with interesting properties in many fields. However, being a semi-metal, it has a zero band gap. Thanks to their low dimensionality, resulting in confinement in two directions of space, graphene quantum dots (GQDs) have a non-zero gap which gives them advantageous properties similar to semi-conductor. Moreover, it's possible to control the dimensionality of GDQ during their synthesis, therefore modifying the size of the band gap. The study of the optical and electrical properties of these objects suggests many applications in the field of optoelectronic, bio-imaging, or again in quantum computing.

Recently, we reported the synthesis of a new class of very soluble elongated graphene quantum dots [1]. In this poster, a spectroscopic study of these new GQDs at the individual scale is reported. The goal is a better understanding of the link between the optical properties and the structure. The L-C₉₆tBu₈ in a polystyrene matrix was studied in microphotoluminescence at room temperature. A statistical study of the central wavelength of emission as well as the dynamics of photons emission was performed. The stability of the emitters according to several parameters was also studied.

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SCANNING TUNNELING MICROSCOPE STUDY OF THE VAN DER WAALS FERROMAGNET CrCl_3

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CrCl_3 is a van der Waals material particularly interesting for its magnetic properties. In each layer, the Cr atoms are coordinated in an octahedral configuration to the neighboring Cl atoms (Cr-Cl bonds are off-plane and the Cr atoms form a honeycomb lattice). The Cr atoms are coupled ferromagnetically via super-exchange and their magnetic moments lie in-plane. Its magnetic properties have been extensively studied in the bulk form [1], it is a weak ferromagnet with a Curie temperature of 17 K. Recently, X-ray Magnetic Circular Dichroism was employed to show that it remains ferromagnetic down to the monolayer, with a Curie temperature very close to the one of the bulk material [2]. Motivated by these findings we have investigated the CrCl_3 monolayer on the Au (111) surface. In this communication I will show our Scanning Tunneling Microscopy (STM) investigation.

CrCl_3 was deposited by molecular beam epitaxy on the Au (111) surface, where it forms large monolayer islands of a width of several hundreds of nanometers. Our STM study shows that the lattice parameters of CrCl_3 are close to the ones of the free layer, indicating a weak structural interaction with the Au substrate. Upon cooling the sample to 4 K, we observed the appearance of a superstructure with a period of about 6 nm. One can see in *Figure 1* that the superstructure displays dislocations with a Burgers vector of 2. We found that the superstructure originates from a peculiar kind of moiré effect between the CrCl_3 monolayer and the Au substrate: a second order moiré. This effect has previously been reported only for systems with a large rotation between the two layers [3] and leads to some interesting properties, amongst them the fact that an edge dislocation with $B=1$ in the CrCl_3 crystalline lattice is transformed in a $B=2$ dislocation of the moiré super-lattice.

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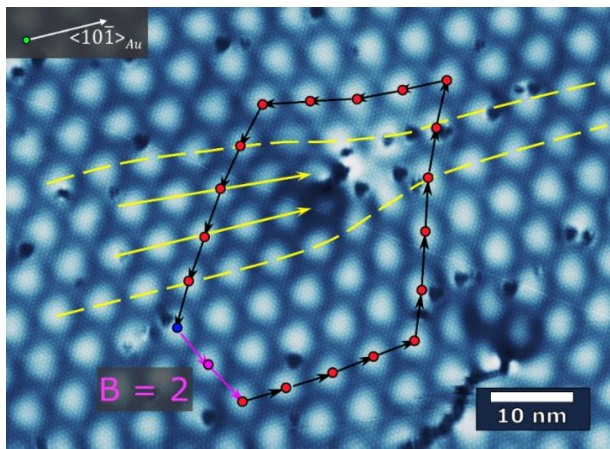


Figure 1: STM constant current topography of CrCl_3 monolayer island on Au.

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SPIN FILTERING IN 2D BASED MAGNETIC TUNNEL JUNCTIONS

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In this talk we first discuss an emerging physical picture of spin-filtering in multilayered graphene-ferromagnet systems supported by *ab initio* calculations and we compare it with experimental data. This picture involves spin filtering effects of arising from (i) graphene-FM hybridization, (ii) graphene k-point selection at the interface and (iii) “graphite” bulk band structure purification. These effects are shown to be either cooperating or competing. These results on graphene-FM systems are then compared predictions regarding other 2D based magnetic tunnel junctions (MTJs). Overall, this study unveils paths to better harness the potential of 2D based MTJs.

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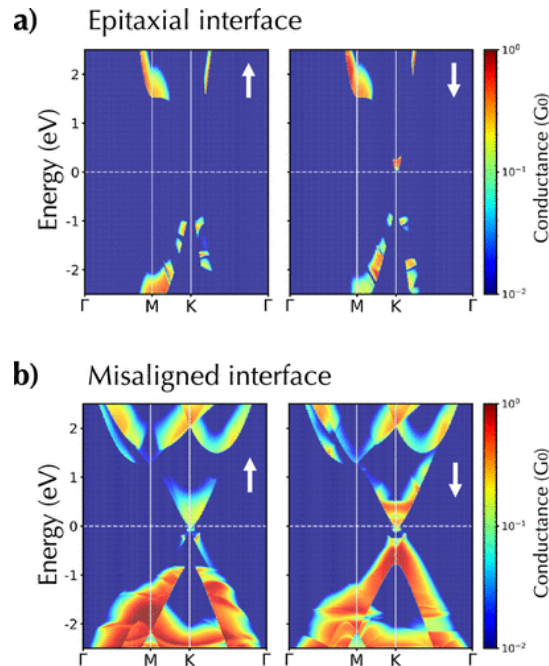


Figure 1: Electronic transmission across (a) the epitaxial and (b) the misaligned Ni/MLGr interfaces. Transmission coefficients are depicted in units of the quantum of conductance (G_0) along the conventional high symmetry k-path in the plane parallel to the interface.

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GDR HOWDI 2023 MEETING: SPINTRONICS WITH BLACK PHOSPHORUS

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Spintronics is a paradigm focusing on spin as the information vector in fast and ultra-low-power non-volatile devices such as the new spin-transfer-torque Magnetic Random Access Memory (MRAM). Beyond its widely distributed applications, spintronics aims at providing more complex architectures and a powerful beyond CMOS solution from storage to quantum information. The recent discovery of graphene, and other 2D materials such as hexagonal boron nitride (h-BN) or dichalcogenides (WS₂...), has opened novel exciting opportunities in terms of functionalities and performances for spintronics devices [1]. Typically, graphene has shown a strong versatility by providing both highly efficient spin information transport properties [2] and potential for strong spin filtering in 2D-MTJs [1]. However, the lack of a gap has led to extensive research to find a semiconducting sibling of graphene that would display its good properties in addition to a gap.

In this direction, Black phosphorus (BP) has attracted an explosive interest since 2014 as it displays major properties for (opto-)electronic devices: (a) high hole and electron mobilities in thin layers exfoliated BP (about 3000 cm²/Vs) and (b) high ON/OFF current ratio (about 10⁵) in a transistor configuration with ambipolar characteristics. Additionally, the bandgap of BP is predicted to be widely tunable in relation to the number of stacked layers and remains direct from the bulk to the monolayer. Thanks to the natural low spin-orbit coupling of phosphorus, BP is expected to present highly efficient spin information transport, similarly to graphene [2] but with the addition of a band gap. This difference with graphene is fundamental for the implementation of spin manipulation schemes and the experimental realization of a spin gate.

However, the key issue for BP devices has been the handling of its degradation under atmospheric conditions. While the mechanism has been well understood [3] this still remains a clear problem for applications. We will present a recently developed in-situ approach to circumvent the issue of degradation under atmospheric conditions [4]. By passivating the BP without exposing it to air we achieve protection down to the monolayer with 1 nm Al₂O₃. We will further discuss how this passivation layer can play the role of the tunnel barrier required for efficient spin injection [2,4] and provide a high potential path for spintronics applications from vertical to lateral devices. In addition, we will talk about the demonstration of BP integration into Co/BP/Co spin valves showing large spin signals. We will discuss a novel selective spin-split transport mechanism as supported by first-principle theoretical investigation. This illustrates the potential of BP for spin injection/detection, strongly supporting BP's vision as an outstanding platform for spintronics.

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Split-gate Ferroelectric Field-effect Transistor based on $WSe_2/CuInP_2S_6$ Heterostructures for memory and photovoltaic applications

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The development of two-dimensional (2D) materials has opened up new possibilities for designing and implementing innovative devices. Recently, 2D ferroelectric van der Waals materials (vdW) have attracted interest¹ due to their intrinsic ultrathin ferroelectric behavior. Moreover, they offer an unprecedented ease of processing with other materials, and unique interfaces free of dangling bonds. This opens the doors for exploring uncharted ferroelectric properties and devices concepts, not accessible with traditional ferroelectrics thin films.²

The Ferroelectric Field Effect Transistor (FeFETs)³ is a key building-block for non-volatile memory and neuromorphic computing. In this study, we present a novel split-gate architecture for a 2D FeFET based on $WSe_2/hBN/CuInP_2S_6$ heterostructures (**Figure 1a**). The two $CuInP_2S_6$ ferroelectric gates provide switchable and non-volatile polarizations, used to alleviate the doping profile along the WSe_2 semiconducting channel.

The strong polarization of $CuInP_2S_6$ enables to exhibit the ambipolar behavior of WSe_2 (**Figure 1b**). The FeFET demonstrate excellent performance as nonvolatile memory, including a high on/off ratio ($>10^5$) and long data retention ($>10^4$ s). The split-gate architecture enables to encode remanent and reconfigurable p-n junction with an excellent rectification ratio. This allows us to achieve the implementation of non-volatile XOR logic gates through a single-active channel, which is a key building-block of next generation neuromorphic computing scheme.

Finally, we address the optoelectronic properties of our device. Here, we demonstrate that our device can operate both in phototransistor and photovoltaic modes. While forming the p-n junction, we take advantage of the built-in electric field to assist charge dissociation. This unlocks photovoltaic functionality, that demonstrates large open circuit voltage (**Figure 1c**) and close-circuit photovoltaic current.

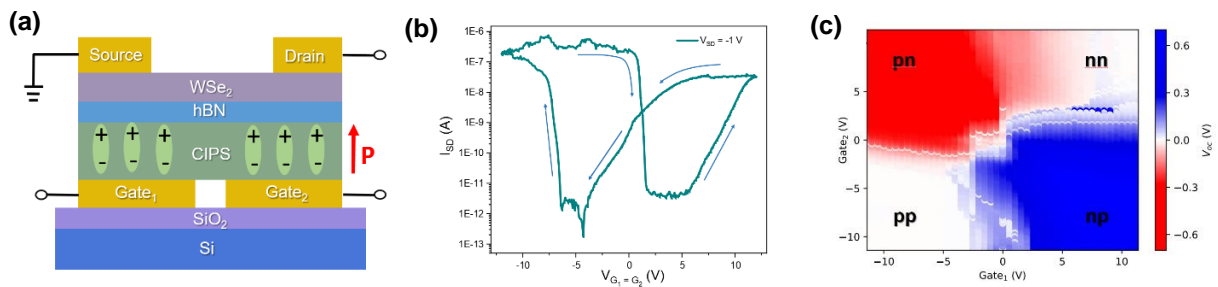


Figure 1: (a) Schematic of a split-gate FeFET based on a $WSe_2/hBN/CIPS$ heterostructure.

(b) $I_{SD}-V_G$ transfer characteristics. (c) Photovoltaic map representation of reconfigurable transistor.

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STRAINTRONICS IN 2D SEMICONDUCTORS

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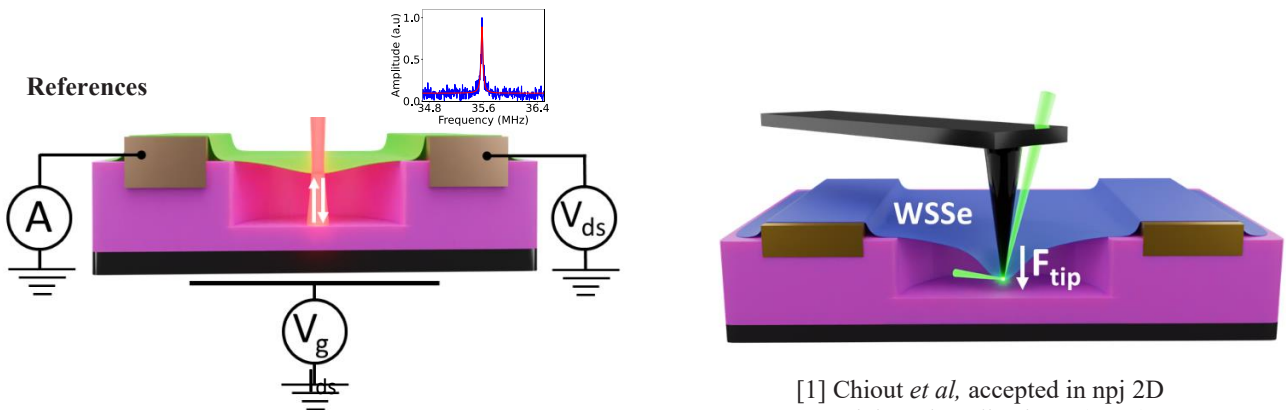
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Two-dimensional transition metal dichalcogenides (TMDs) have been investigated for applications in optomechanics and optoelectronics thanks to their properties (thickness, high Young modulus, very low mass and direct bandgap in monolayers). The control over strain is at the heart of many new applications in these fields. In order to highlight the interest of this topic, we achieve strong strain tuning in suspended 2D materials via thermal expansion and tip indentation.

First, we propose a new scheme to tune efficiently the mechanical vibration of 2D suspended membrane using Joule heating. This electrothermal tuning of the vibration of MoS₂ nanoresonator is much more efficient than previous reports. The thermal dilatation slightly changes the intrinsic strain and modify the resonant frequency using the nano-opto-elctro-mechanical platform (NOEM) shown in Figure 1. Considering these properties, we extract the thermal conductivity and demonstrate a good temperature sensitivity¹.

To go beyond this high strain tuning regime, we also apply a local force on the membrane with an AFM tip indentation. We observe a very strong tuning of the optical bandgap. Then, we investigated locally the properties of our suspended membrane of WS_{1.3}Se_{0.7} under non-uniform strain exploiting the tip enhanced photoluminescence (TEPL) under the AFM tip shown in Figure 2. This non-uniform strain, obtained in this system, leads to the diffusion of the excitons² and the conversion of excitons to trions³.

The strain engineering drives many properties of the 2D materials and generate many experimental outcomes.



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←
MoS₂

Figure 1: NOEM platform using electrical actuation and optical detection. Inset: resonant frequency of MoS₂ membrane

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SULFUR / SILICON NANOSTRUCTURED ELECTRODES FOR A RECHARGEABLE BATTERY

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Lithium-ion battery is the most mature and most used technology in the market today. The optimization of the storage properties of batteries requires the search for new materials offering specific capacities superior to current materials. Incorporation of nanomaterials with high specific capacities has proven to be an effective method to improve the electrochemical performance of the lithium-ion battery.

The present work explores a promising and original approach for the implementation and development of a new bottom-up technique for hierarchical hybrid nanostructured electrodes based on vertically aligned carbon nanotubes (VACNTs) decorated with nanoparticles (NPs), i.e. NPs@VACNTs. The non-metallic lithium battery is composed of S@VACNTs as a positive electrode and Si@VACNTs as a negative electrode.

This battery provides a theoretical energy of 1940 Wh kg⁻¹, which is five times more than the theoretical energy of existing lithium-ion batteries based on LiCoO₂ and graphite (~ 364 Wh kg⁻¹). Moreover, the nanostructured design of the two electrodes overcomes the problems associated with the use of sulfur compounds and silicon in lithium-ion batteries, including poor electrical conductivity and large volumetric variations. [1-2]

This work benefited from the support of EDF in the framework of the research and teaching Chair «Sustainable energies» at Ecole Polytechnique.

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Swinging Crystal Edges of Growing Carbon Nanotubes

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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. These stochastic switches call into question the possibility of chirality selection based on growth kinetics. A simple model, supported by Kinetic Monte Carlo and Molecular Dynamics simulations, 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.

GDR HOWDI 2023 MEETING:

SYNTHESIS AND PROPERTIES OF “BOTTOM-UP” GRAPHENE QUANTUM DOTS (GQD)

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Despite its outstanding electronic, optical and mechanical properties, the use of graphene for real-world applications is severely limited because of its semi-metallic character. It is well known that when a material is reduced to nanoscale dimensions, the electronic confinement induces original size-dependent properties. For the last decade, a great attention has been paid to the size reduction of graphene using conventional “top-down” approaches (lithography and etching, thermal treatments and oxidation of bulk materials) to fabricate graphene quantum dots (GQDs)^[1] or graphene nanoribbons (GNRs).^[2] However, the “top-down” approaches do not allow a sufficient control of the structure of the material and of the oxidation state of the edges, which drastically affect the properties. In order to truly control, with the required level of precision, the morphology and the composition of the materials and of its edges, the bottom-up approach is the relevant way to proceed.^[3, 4]

Here, I'll present the “bottom-up” synthesis of graphene quantum dots and the first investigation of the photoluminescence (PL) properties of at the single molecular-scale. The GQDs exhibited emission of single photons at room temperature with high brightness and purity.^[5-7] Beyond this first demonstration, our interest deals with the study of the structure-property relationship in GQDs and how the size, the symmetry of the particles will permit to tune the emission properties and finally be able to perform reverse engineering to design GQD with tailor-made properties.^[8]

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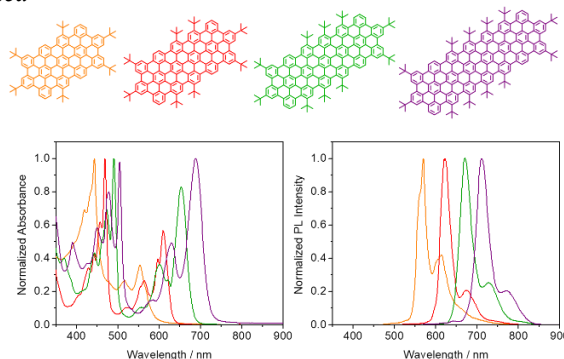


Figure 1: Structure, absorption and photoluminescence spectra of rod-shaped graphene quantum dots.

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ULTRAFAST OPTICAL SPECTROSCOPY OF GRAPHENE QUANTUM DOTS

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Graphene quantum dots (GQDs), big polycyclic aromatic hydrocarbon molecules with ~100 carbon atoms, have a great potential for a wide range of applications including quantum sensing. One of their assets is the total control on their structure allowed by their synthesis by bottom-up chemistry. This allows the customization of their electronic properties [1–3]. In our group, we recently investigated the intrinsic properties of several geometries of GQDs down to the single molecule [4-7]. In this poster, we will present preliminary results on the femtosecond transient absorption (fs-TA) spectroscopy of C114-tBu₁₀ rod-shaped GQDs. Population dynamics are probed using transition-selected excitation above the bandgap with fluence-dependent measurements while different polarization configurations were used in order to probe the relative transition dipole orientation.

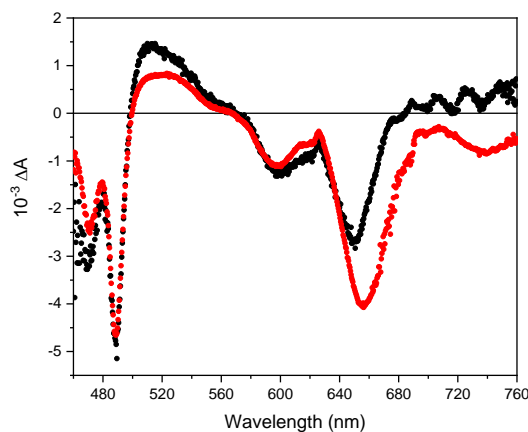


Figure 1: Typical TA spectrum of C114-tBu₁₀ G-QDs following excitation at 400 nm (black). Within about 265 fs, the TA spectrum evolves in lineshape and amplitude toward the red spectrum. We attribute this dynamics to the hot excited state relaxation.

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WETTING 2D MATERIALS AT THE MICROSCALE

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2D materials, with their atomically-flat dangling-bond-free surface and their tunable interface properties, correspond to model systems for experimental studies in nanofluidics, where behaviors of liquids are investigated when confined as films or channels at the nanoscale. In the recent years, original devices based on 2D materials (graphene, MoS₂, hBN...) in geometries such as nanotubes, nanopores drilled membranes or lithographed slits, have been implemented [1]. Yet, complex nanofabrication and limited knowledge on the actual cleanliness and behavior of 2D material surface in devices still hinder their full potential. In particular, an on-going debate remains about their intrinsic properties and the influence of the supporting substrate when the number of layers is reduced, with the so-called wetting transparency and wetting translucency [2-4]. Surface inhomogeneities, including crystalline defects, layer wrinkles, and adsorbed contaminants, are also key elements to consider.

Here we focus on the study of the wetting properties of freshly exfoliated 2D materials, presenting flat and pristine surface, at the micron scale. We introduce an original experimental setup and demonstrate the deposition and study of few-micron-diameter droplets on samples placed in a chamber with saturated humidity environment to prevent evaporation. Micro-controllers and coupled microscopies allow for micron-scale localized deposition and contact angle measurement. We explore the influence on the wetting properties of the 2D materials nature, the number of layers, and the underlying substrate.

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BUILDING SUB- λ ARRAYS OF QUANTUM EMITTERS IN 2D MOSe₂

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Control of single photon emitters, both in terms of energy, decay channels, and position is crucial for integrated quantum nanophotonic targeting applications towards quantum communication and quantum computing. 2D semiconducting crystals (e.g. TMD) enable to deterministically create such quantum emitters [1] using various approaches based on strain [1], defect [2], or electrostatic [3] engineering of the exciton trapping potential. However, to study coherent interactions between QEs and harvest quantum collective effects [4], one needs to create a dense sub-wavelength array of these emitters to enhance dipolar interactions.

Here, we present our strategy to build such sub-wavelength array of quantum emitters in monolayer MoSe₂ which combine large exciton binding energy (unlocking dissociation-free electrically tuning) and local strain engineering using nanopillars to create QEs. We are targeting GaN nanopillar substrate to create QEs in transferred 2D heterostructure. The dry transfer setup is used to transfer the 2D crystals onto the patterned substrate (the array of nanopillars). Furthermore, to avoid crystal contamination and trapped charge influence on the exciton properties during and after the transfer process, the 2D crystal is first encapsulated by other 2D crystals (e.g. hBN) and then transferred onto GaN nanopillars using the dry viscoelastic technique. In addition, we will present recent progress on a fully motorized confocal micro-photoluminescence and micro-absorption setup.

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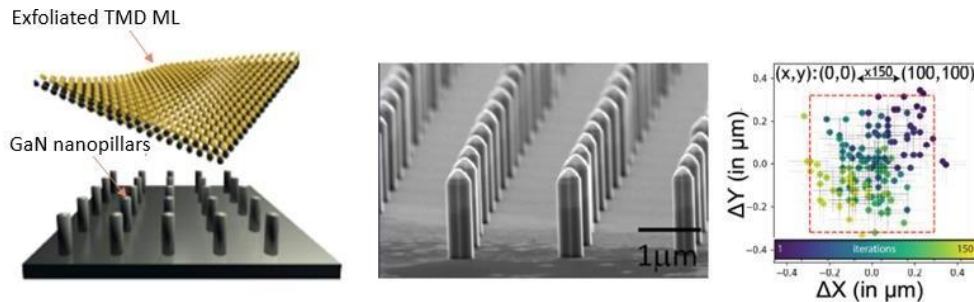


Figure 1: right panel: schematic representation of a TMD monolayer and an array of GaN pillars, middle panel: SEM image of a GaN pillar array grown at CRHEA, left panel: repositioning errors of the motorized translation stage.

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