	Mon. 09	Tue. 10	Wed. 11	Thu. 12	Fri. 13
07:00		Breakfast	Breakfast	Breakfast	Breakfast
08:00		Material growth	Strong correlation and topological effects	Spin transport	Electronic transport
09:00					
10:00		Coffee break	Coffee break	Coffee break	Coffee break
11:00		Functionalization and molecular assembly	Magnetism	VdW optics	Quantum emitters
12:00					Closing
13:00		Lunch	Lunch	Lunch	Lunch
14:00	Arrival - Coffee	Tribute to François Ducastelle	Social event	Nanotubes	Departure
15:00	Opening Nanophotonics				
16:00	Break	Coffee break		Coffee break	
17:00	Spin coupling	Optics of 2D and layered materials	Applications and devices	hBN optics	
18:00	Break Strain engineering	Poster clips I	Poster clips II	General assembly	
19:00					
20:00	Dinner	Dinner	Dinner	Gala dinner	
21:00		Poster session I	Poster session II	Party	
22:00					
23:00					

Program

Monday, May 9, 2022

TIME	EVENT
13:30 - 14:50	Arrival - Coffee
14:50 - 15:00	Opening - Julien Barjon
15:00 - 16:20	Nanophotonics - Jean-Sébastien Lauret
15:00 - 16:00	› QUANTUM OPTICS WITH VAN DER WAALS HETEROSTRUCTURES - *TUTORIAL: Martin Kroner, Swiss Federal Institute of Technology in Zurich - ETHZ*
16:00 - 16:20	› QUANTUM NANOPHOTONICS WITH 2D MATERIALS - *Antoine Réserbat-Plantey, Centre de recherche sur l'hétéroepitaxie et ses applications*
16:20 - 16:40	Break
16:40 - 17:30	Spin coupling - Clément Faugeras
16:40 - 17:10	› STRAIN CONTROL OF CHARGE-, VALLEY-, AND SPIN DEGREES OF FREEDOM IN TMDS - *INVITED: Kirill Bolotin, Freie Universität Berlin*
17:10 - 17:30	› HIGH MAGNETIC FIELD SPIN-VALLEY SPLIT SHUBNIKOV–DE HAAS OSCILLATIONS IN A WSE2 MONOLAYER - *Walter Escoffier, Laboratoire national des champs magnétiques intenses - Toulouse*
17:30 - 17:50	Break
17:50 - 18:40	Strain engineering - Clément Faugeras
17:50 - 18:20	› Strain switching in van der Waals heterostructures by incorporating spin-crossover materials - *INVITED: Carla Boix Constant, Institute of Molecular Science (ICMol), Universitat de València*
18:20 - 18:40	› Electronic transport in corrugated graphene - *Romaine Kerjouan, Laboratoire de Physique de l'ENS - ENS Paris*
19:30 - 21:00	Dinner

Tuesday, May 10, 2022

TIME	EVENT
07:00 - 08:30	Breakfast
08:30 - 10:00	Material growth - Amandine Andrieux
08:30 - 09:00	› BN GROWTH ON NICKEL UNDER ULTRA-HIGH VACUUM CONDITIONS FROM BORAZINE - *INVITED: Dominique Vignaud, Univ. Lille, CNRS, Centrale Lille, Univ. Polytech. Hauts-de-France - IEMN - Institut d'Electronique, de Microélectronique et de Nanotechnologie*
09:00 - 09:20	› Advances in selfstanding hBN crystal synthesis via the PDC route - *Camille Maestre, Laboratoire Multimatériaux et Interfaces, Mateis, Lyon*
09:20 - 09:40	› Conception d'un réacteur CVD chauffé par induction pour la synthèse de nitrure de bore hexagonal - *Wafa Alimi, Laboratoire des Sciences des Procédés et des Matériaux, Villetaneuse*
09:40 - 10:00	› CROISSANCE D'HETEROSTRUCTURES VAN DER WAALS PAR ABLATION LASER PULSE - *Florian Godel, Unité mixte de physique CNRS/Thalès, Palaiseau*
10:00 - 10:30	Coffee break

TIME	EVENT
10:30 - 12:00	Functionalization and molecular assembly - Stéphane Campidelli
10:30 - 11:00	› Novel Non-Benzenoid Graphene Isomers by On-Surface Synthesis - *INVITED: Michael Gottfried, Department of Chemistry, University of Marburg*
11:00 - 11:20	› Synthesis and optical properties of rod-shaped graphene nanoparticles - *Daniel Medina Lopez, Laboratoire Innovation en Chimie des Surfaces et NanoSciences, Gif-sur-Yvette*
11:20 - 11:40	› HYDROGENATION OF GRAPHENES FROM H RADICALS - *Pascal Puech - CEMES, UPR-8011, CNRS, Université de Toulouse, Toulouse*
11:40 - 12:00	› Structure, chemistry and charge density in MBE grown TMDs investigated by 4D-STEM - *Hanako Okuno, Univ. Grenoble Alpes, CEA, IRIG-MEM*
12:30 - 14:00	Lunch
14:30 - 16:10	Tribute to François Ducastelle - Stephan Roche
14:50 - 15:10	› Twisted Bilayers of Hexagonal Boron Nitride - *Sylvain Latil - Institut Rayonnement Matière de Saclay*
15:10 - 15:30	› Influence of bias voltage on the observed Moiré patterns of MoTe2/graphene heterostructure grown by molecular beam epitaxy - *Thanh Trung PHAM - Namur Institute of Structured Matter (NISM), Department of Physics, University of Namur*
15:30 - 15:50	› Unfolding the electronic bands of twisted 2D materials - *Alberto Zobelli - Laboratoire de Physique des Solides*
15:50 - 16:10	› RADIATIVE LIFETIME OF FREE EXCITONS IN HEXAGONAL BORON NITRIDE - *Sébastien ROUX, Groupe d'Etude de la Matière Condensée, UVSQ-CNRS, Versailles & Laboratoire d'Etude des Microstructures (LEM), ONERA, Université Paris-Saclay, CNRS, Châtillon*
16:10 - 16:40	Coffee break
16:40 - 17:40	Optics of 2D and layered materials - Guillaume Cassabois
16:40 - 17:00	› Optical signatures of the strong 3D anisotropy in black phosphorus - *Léonard Schué, Université de Montréal*
17:00 - 17:20	› Semiconducting thin layers of transition metal dichalcogenides under pressure - *Thomas Pelini, LNCMI, CNRS, EMFL, Université Grenoble Alpes*
17:20 - 17:40	› 2D MoS2 capacitors and transistors studied by excitonic reflection microscopy - *Nathan Ullberg, Laboratoire d'Innovation en Chimie des Surfaces et Nanosciences, Université Paris-Saclay, CEA, CNRS, NIMBE, LICSEN, Gif-sur-Yvette*
17:40 - 18:20	Poster clips I
19:30 - 21:00	Dinner
21:00 - 23:00	Poster session I - Poster session I

Wednesday, May 11, 2022

TIME	EVENT
07:00 - 08:30	Breakfast
08:30 - 10:10	Strong correlation and topological effects - Jean-Christophe Charlier
08:30 - 09:30	› A glimpse into the world of topological phases in two dimensions - *TUTORIAL - David Carpentier, Laboratoire de Physique de l'ENS Lyon*

TIME	EVENT
09:30 - 09:50	› METAL-INSULATOR TRANSITION IN ANNEALED MOS2 DEVICES - *Sébastien Nanot, Laboratoire Charles Coulomb, Montpellier*
09:50 - 10:10	› A graphene-based voltage-tunable Josephson parametric amplifier - *Julien Renard, Institut Néel, Grenoble*
10:10 - 10:40	Coffee break
10:40 - 12:10	Magnetism - Kirill Bolotin
10:40 - 11:00	› Qnami ProteusQ: A commercial solution unlocking magnetic field measurments in 2D materials - *Peter Rickhaus - Qnami AG*
11:00 - 11:30	› Scanning Nitrogen-Vacancy Magnetometry of van der Waals Magnets - *INVITED - Märta Tschudin - University of Basel*
11:30 - 11:50	› MAGNETIC ORDERING IN WEAKLY COUPLED VAN DER WAALS SYSTEMS, WITH APPLICATION TO VI3 - *Karel Carva, Charles University Prague*
11:50 - 12:10	› Structural, magnetic and transport properties of van der Waals Cr2Te3 based heterostructures - *Quentin Guillet - CEA, IRIG-Spintec*
12:30 - 14:00	Lunch
14:30 - 17:00	Social event - Visiting
17:30 - 18:30	Applications and devices - Aurélie Pierret
17:30 - 17:50	› A SCALING LAW FOR CHARGE TRANSPORT IN LAYERED 2D MATERIALS AND ITS APPLICATION TO REDUCED GRAPHENE OXIDE - *Haldun Sevincli, İzmir Institute of Technology*
17:50 - 18:10	› 2D SWITCHES FOR RF APPLICATION - *Simon SKRZYPCZAK, Carbon - IEMN*
18:10 - 18:30	› A van der Waals Heterojunction Based on Monolayers of MoS2 and WSe2 for Solar Water Splitting - *Paul Dalla Valle, Institut des Matériaux, de Microélectronique et des Nanosciences de Provence*
18:30 - 19:10	Poster clips II
19:30 - 21:00	Dinner
21:00 - 23:00	Poster session II

Thursday, May 12, 2022

TIME	EVENT
07:00 - 08:30	Breakfast
08:50 - 10:00	Spin transport - Cyrille Barreteau
08:50 - 09:20	› Proximity-induced spin-orbit phenomena in graphene-based devices - *INVITED - Williams Fernando Savero Torres - Néel Institute*
09:20 - 09:40	› Spin Current in van der Waals Ferromagnet Fe3GeTe2 - *Jiaqi Zhou, Université Catholique de Louvain*
09:40 - 10:00	› OPTICAL DETECTION OF LONG ELECTRON SPIN TRANSPORT LENGTHS IN A MONOLAYER SEMICONDUCTOR - *Lei Ren, Université de Toulouse, INSA-CNRS-UPS, LPCNO*

TIME	EVENT
10:00 - 10:30	Coffee break
10:30 - 12:00	VdW optics - Cédric Robert
10:30 - 11:00	› THEORETICAL INVESTIGATIONS OF OPTICAL PROPERTIES OF 2D SEMICONDUCTORS IN VAN DER WAALS HETEROSTRUCTURES - *INVITED: Iann Gerber, Laboratoire de physique et chimie des nano-objets*
11:00 - 11:20	› Interlayer excitons of MoSe2-WSe2 hetero-bilayers - *Lucille Caussou, Institut des NanoSciences de Paris*
11:20 - 11:40	› Dielectric screening in van der Waals materials probed through Raman spectroscopy - *Loïc Moczko, Institut de Physique et Chimie des Matériaux de Strasbourg*
11:40 - 12:00	› AB INITIO STUDY OF GRAPHENE/BN VAN DER WAALS HETEROSTRUCTURE: EFFECT OF ELECTRIC FIELD, TWIST ANGLES AND P-N DOPING ON THE ELECTRONIC PROPERTIES - *Simone Brozzesi, University of Roma Tor Vergata*
12:30 - 14:00	Lunch
14:30 - 16:00	Nanotubes - Annick Loiseau
14:30 - 15:00	› 1D HETEROSTRUCTURES BASED ON NANOTUBE TEMPLATES: CONFINEMENT OF 6T MOLECULES INSIDE BNNT FOR POLARIZED LIGHT EMISSION. - *INVITED - Etienne Gaufrès, Laboratoire Photonique, Numérique et Nanosciences, Université de Bordeaux, Centre National de la Recherche Scientifique*
15:00 - 15:20	› Diameter-dependent single- and double-file stacking of squarylium dyes inside single-wall carbon nanotubes - *Salomé Forel, Nanostructured and Organic Optical and Electronic Materials, University of Antwerp, Laboratoire des Multimatériaux et Interfaces, Université Claude Bernard Lyon 1*
15:20 - 15:40	› SINGLE-WALLED CARBON NANOTUBES CHARGE MANAGEMENT BY CONTROLLED FUNCTIONALIZATION - *Antonio Setaro, Free University Berlin*
15:40 - 16:00	› ULTRAFAST GENERATION OF ACOUSTIC WAVES IN WATER MEDIATED BY A CARBON NANOTUBE - *Fabien Vialla, Institut Lumière Matière*
16:00 - 16:30	Coffee break
16:30 - 18:00	hBN optics - Julien Barjon
16:30 - 17:00	› Optical properties of h-BN: from bulk to monolayer - *INVITED: Christine Elias, Laboratoire Lumière, Matière et Interfaces, Laboratoire Charles Coulomb*
17:00 - 17:20	› Optical characterization of exfoliated monolayer boron nitride by means of hyperspectral microscopy in the deep-UV - *Adrien Rousseau, Laboratoire Charles Coulomb*
17:20 - 17:40	› Exciton-phonon coupling and optical properties in hexagonal-BN - *Claudio Attaccalite, CNRS, Aix-Marseille Université, CINaM*
17:40 - 18:00	› Atomic Scale Mapping of the Electric Field in 1D and 2D BN Nano-Structures By 4D-STEM - *Laura Susana, Laboratoire de Physique des Solides*
18:30 - 19:30	General assembly
19:30 - 21:00	Gala dinner
21:00 - 23:00	Party

Friday, May 13, 2022

TIME	EVENT
07:00 - 08:50	Breakfast
08:50 - 10:20	Electronic transport
08:50 - 09:20	› COHERENT JETTING FROM A GATE-DEFINED CHANNEL IN BILAYER GRAPHENE - *INVITED: Carolin Gold, Laboratory for Solid State Physics, ETH Zürich*
09:20 - 09:40	› Pinch-off resistance and Schwinger effect in hBN-encapsulated GFETs - *Aurélien Schmitt, Laboratoire de physique de l'ENS - ENS Paris*
09:40 - 10:00	› ELECTRONIC WHISPERING-GALLERY RESONANT TRANSPORT IN GRAPHENE P-N JUNCTION - *Viet Hung Nguyen, Institute of Condensed Matter and Nanosciences, Université catholique de Louvain*
10:00 - 10:20	› AB-INITIO SIMULATION OF PHONON-ASSISTED ELECTRON TRANSPORT IN VAN DER WAALS HETEROSTRUCTURES - *Adel M'foukh, Centre de Nanosciences et de Nanotechnologie, CNRS, Université Paris-Saclay*
10:20 - 10:50	Coffee break
10:50 - 12:00	Quantum emitters - Stéphane Berciaud
10:50 - 11:20	› Single photon emitters in hexagonal boron nitride for scalable quantum photonics - *INVITED: Aymeric Delteil, Groupe d'Étude de la Matière Condensée*
11:20 - 11:40	› Optical signals of qubits in defected 2D TMDs - *Pedro Melo, Condensed Matter and Interfaces group, Debye Institute for Nanomaterials Science, Utrecht University*
11:40 - 12:00	› Optical Investigation of C96 Graphene quantum dots - *Thomas Liu, Laboratoire Lumière, Matière et Interfaces*
12:00 - 12:10	Closing - Julien Barjon
12:30 - 14:00	Lunch
14:00 - 15:00	Departure

GDR HOWDI 2022 MEETING: QUANTUM OPTICS WITH VAN DER WAALS HETEROSTRUCTURES

Martin Kroner[1]

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Van-der-Waals materials have attracted a significant attention over the past decade, owing to their interesting optical and electronic properties as well as the versatility of combining different materials into heterostructures exhibiting emergent phenomena. In this tutorial, I will focus on the optical properties of one specific class of van-der-Waals materials: Transition Metal Dichalcogenides (TMD). In the monolayer limit TMDs are semiconductors that exhibit a direct band gap which renders them ideal for optical studies [1]. Due to their almost perfect 2D nature, the low screening of Coulomb interactions leads to the observation of tightly bound excitons, which are strongly coupled to the optical fields. Furthermore, TMD monolayers can easily be doped with electrons or holes by electrical gating [2]. I will discuss optical spectroscopy techniques which allow us to use this versatile platform to study a wide variety of phenomena, ranging from the physics of correlated electrons to interacting excitons. By embedding a TMD monolayer into an optical cavity, we can exploit the strong light matter interactions to observe exciton polaritons: new quasi-particles which are part light (photon), part matter (exciton). This allows us to create large populations of polaritons using a strong pump laser pulse. Using a subsequent weak probe laser pulse we can probe polariton interactions which are governed by their exciton character [3]. Finally, I will lay out how we can use electric field modulations to create quantum confinement for excitons in a TMD monolayer.

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QUANTUM NANOPHOTONICS WITH 2D MATERIALS

Antoine Reserbat-Plantey[1, 2], Carlotta Ciancico[2], Maximilian Heithoff[2], Alvaro Moreno[2], Iacopo Torre[2] & Frank Koppens[2].

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The field of two-dimensional (2D) materials-based nanophotonics has been growing at a rapid pace, triggered by the ability to design nanophotonic systems with in situ control, unprecedented number of degrees of freedom, and to build material heterostructures from the bottom up with atomic precision [1]. A wide palette of polaritonic classes have been identified, comprising ultraconfined optical fields, even approaching characteristic length-scales of a single atom. These advances have been a real boost for the emerging field of quantum nanophotonics, enabling quantum technologies harnessing single-photon generation, manipulation, and detection using 2D materials. At this GDR meeting, I will show several hybrid systems consisting in lifetime-limited single emitters [2, 3] (linewidth ~ 40 MHz) and 2D materials at sub-wavelength separation without degradation of the emission properties [4]. We have demonstrated that their nanoscale dimensions enable ultra-broadband tuning (tuning range > 400 GHz) and fast modulation (frequency ~ 100 MHz) of the emission energy [5], which renders it an integrated, ultra-compact tuneable SPS. I will also present recent results on unusual Stark tuning of ultra-narrow quantum emitter located at the edge of a graphene transistor and electrostatic engineering of excitons in 2D semiconductors.

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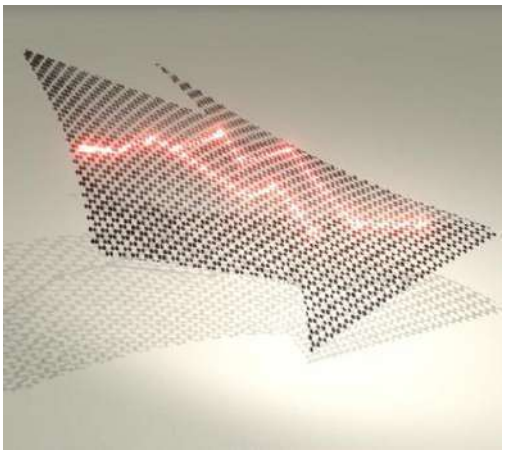

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STRAIN CONTROL OF CHARGE-, VALLEY-, AND SPIN DEGREES OF FREEDOM IN TMDS

K.I. Bolotin[1]

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We discuss new nanomechanical approaches to manipulate excitons in TMDs. We show how mechanical strain fields are used to move excitons around, convert between their different types, create new hybridized excitonic states, and manipulate spin/valley degrees of freedom.

First, we develop a experimental approach to generate tunable spatially non-uniform strain fields and explore their effects. We show that the presence of such a strain results in the transport of excitons to the position of the highest strain. In addition, we find that in presence of non-uniform strain, neutral excitons are effectively converted into their charged counterparts. Second, we develop an approach to generate high strain up to 3% in high-quality WSe2 at cryogenic temperatures. We demonstrate that at specific strain values, dark excitons are brought into resonance with defect-related states. In that situation, a new hybrid state with giant oscillator strength is formed. We show the control of that state and explain how its presence explains many traits of single quantum emitters in WSe2. Finally, we examine the effect of strain on spin- and valley- degrees of freedom. We use mechanical strain to controllably transfer spin information between free- and defect-bound excitons. This, in turn, allows long-term storage of spin information.

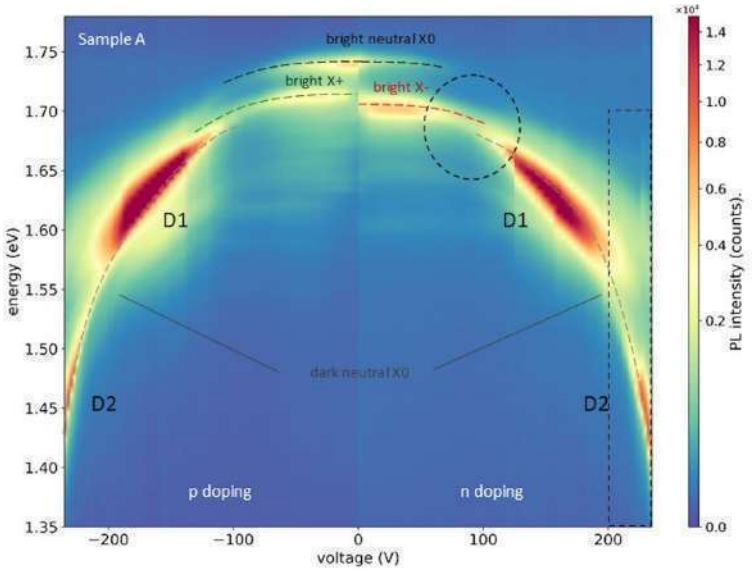

Figure 1: The evolution of excitonic states in WSe2 under strain. A new hybridized state (labelled D1) becomes visible at high strain.

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HIGH MAGNETIC FIELD SPIN-VALLEY SPLIT SHUBNIKOV–DE HAAS OSCILLATIONS IN A WSe_2 MONOLAYER

Banan Kerdi[1], Mathieu Pierre[1], Robin Cours[2], Bénédicte Warot-Fonrose[2], Michel Goiran[1] and Walter Escoffier[1]

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We study Shubnikov-de Haas oscillations in a p-type WSe_2 monolayer under very high magnetic field. The oscillation pattern is complex due to a large spin and valley splitting, in the non-fully-resolved Landau level regime. Our experimental data can be reproduced with a model in which the main parameter is the ratio between the Zeeman energy and the cyclotron energy. The model considers the Landau levels from both valleys with the same Gaussian broadening, which allows predicting the relative amplitude of the resistance oscillation originating from each valley. The Zeeman energy is found to be several times larger than the cyclotron energy. It translates into a large and increasing effective Landé factor as the hole density decreases, in the continuity of the values reported in the literature at lower carrier density.

References

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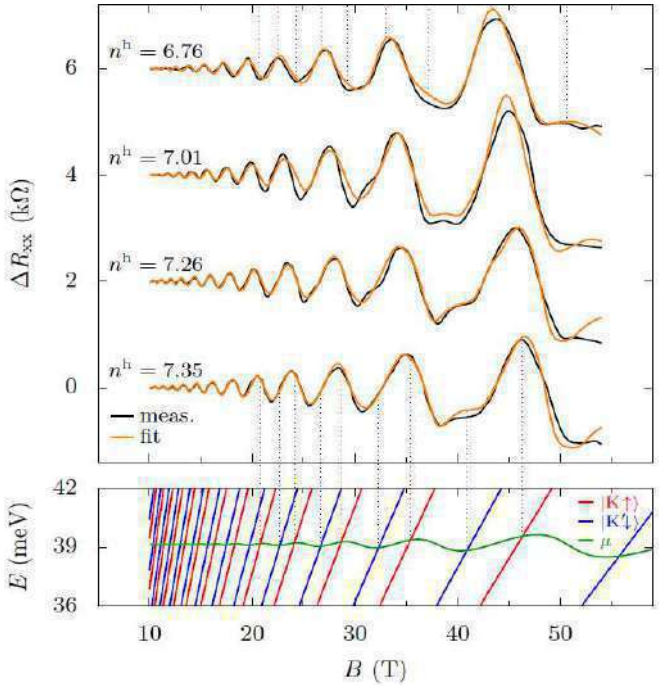

Figure 1: Experimental magneto-resistance (black lines) are compared to the model output (orange lines) for selected hole densities nh (given in unit of 10^{12} cm^{-2}). Bottom frame: Landau level spectrum and evolution of the chemical potential μ(B) for $n_h = 7.35\times10^{12}$ cm^{-2}.

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GDR HOWDI 2022 MEETING:
STRAIN SWITCHING IN VAN DER WAALS HETEROSTRUCTURES BY INCORPORATING SPIN-CROSSOVER MATERIALS

Carla Boix-Constant[1], Víctor García-López[1], Efrén Navarro-Moratalla[1], Miguel Clemente-León[1], José Luis Zafra[2], Juan Casado[2], Francisco Guinea[3], Samuel Mañas-Valero[1], Eugenio Coronado[1].

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Van der Waals heterostructures (vdWHs) provide the possibility of engineering new materials with emergent functionalities that are not accessible in another way. These heterostructures are formed by assembling layers of different materials used as building blocks. Beyond inorganic 2D crystals, layered molecular materials remain still rather unexplored, with only few examples regarding their isolation as atomically thin layers. In this work, the family of van der Waals heterostructures is enlarged by introducing a molecular building block able to produce strain: the spin-crossover (SCO). In these metal–organic materials, a spin transition can be induced by applying external stimuli like light, temperature, pressure, or an electric field. In particular, smart vdWHs are prepared in which the electronic and optical properties of the 2D material (graphene and WSe_2) are clearly switched by the strain caused by the spin transition. These molecular/inorganic vdWHs represent the deterministic incorporation of bistable molecular layers with other 2D crystals of interest in the emergent fields of straintronics and band engineering in low-dimensional materials.

References

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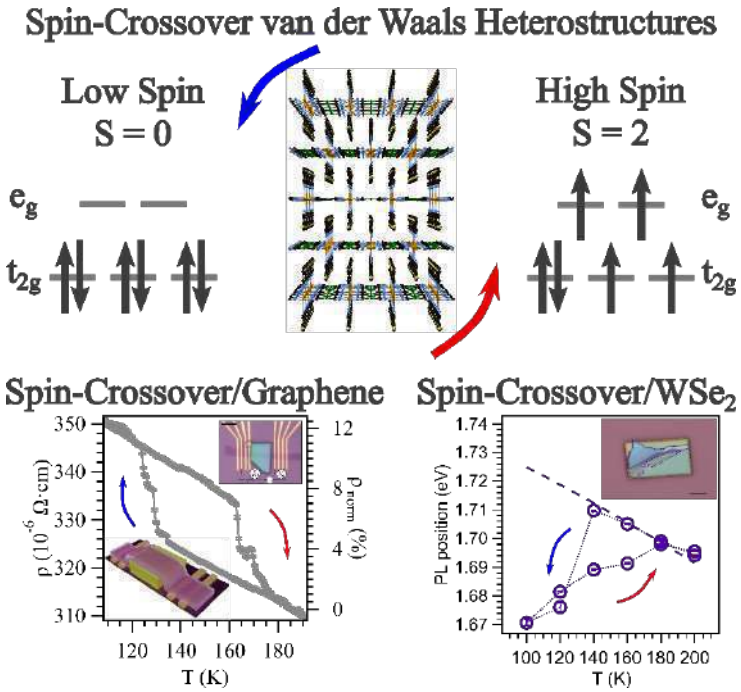

Figure 1. Upper figure: Scheme of the spin-crossover phenomenon for a d^6 (Fe^{2+}) metal complex. Bottom left: Thermal dependence of the resistivity for a vdWH. Bottom right: Thermal dependence of the PL position for the vdWH and a reference WSe_2 monolayer.

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ELECTRONIC TRANSPORT IN CORRUGATED GRAPHENE

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Graphene is known for its unique band structure, making it a great candidate for many electronic applications. However, it presents also astonishing mechanical properties [1], which can modify the usual behavior of the 2D material. Here, we report on the investigation of charge transport in corrugated hBN-encapsulated graphene devices (Fig. 1. a) and b)). We investigate our device by Raman measurements (Fig 1 c). Raman spectra show a periodic response due to the presence of the corrugation. Moreover, the position of peak 2D and G are clearly correlated, which is typical of the presence of strain in graphene [2]. From low-bias transport measurements at 4 K, we observe a clear signature of strain effects on transport properties by the emergence of a broad peak at high Vg., in contrast with unstrained graphene (Fig. 1 d)) [4]. The graphene is under a periodic stress, which can be seen as a Hamiltonian perturbation equivalent to applying periodic effective potentials to the graphene: a scalar potential and a pseudo vectorial potential [3]. We develop a model for ballistic transport through a strain barrier in graphene, showing that strain can induce valley separation (Fig 1 e)). This model reproduces both qualitatively and quantitatively the measured gate dependence of the resistance.

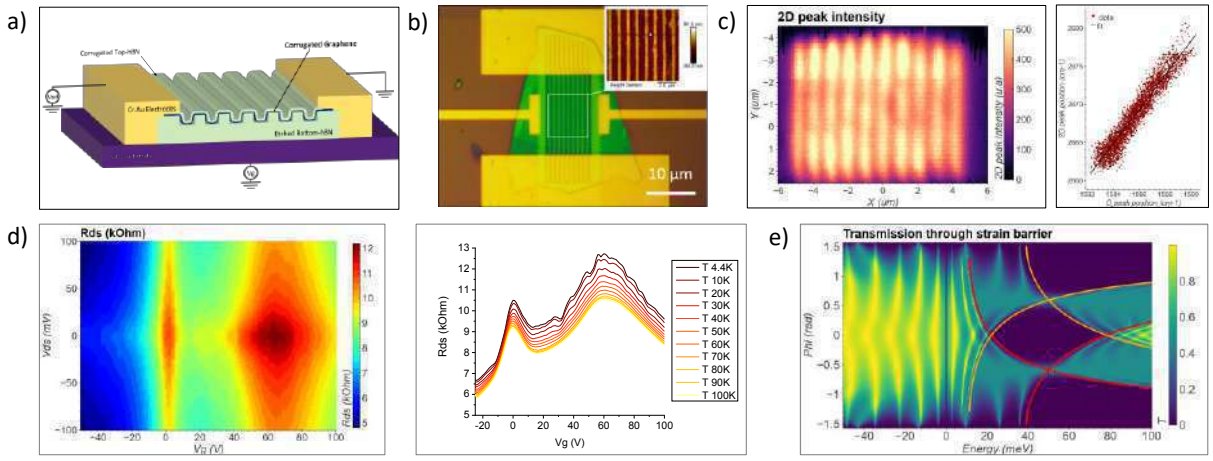

Fig. 1. a) - Principle *Schematic view of the corrugated hBN/graphene/hBN device* ***b) - Fabrication*** *Optical image of an encapsulated corrugated graphene. Inset: an AFM image of the corrugation* ***c) Raman spectroscopy*** *Map of the intensity of the 2D peak and correlation between the 2D and G peaks positions over the corrugated area* ***d) – Transport characterization*** *Left: Map of differential resistance R_{ds} as a function of the gate voltage V_g and of the bias voltage V_{ds} at T = 4.4 K Right: R_{ds} as a function of V_g at zero-biais for different temperatures (T = 4.4 K, 10 K, 20 K, 30 K, 40 K, 50K, 60 K, 70 K, 80 K, 90 K, 100 K).* ***e) – Theory*** *Transmission probability through a 150nm long strain barrier with uniaxial strain ε= 2% in the zigzag direction as a function of the electron energy E and the incidence angle on the barrier φ,. Red lines correspond to the limits of authorized incident angles for valley K and the orange ones for valley K'*

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GDR HOWDI 2022 MEETING: BN GROWTH ON NICKEL UNDER ULTRA-HIGH VACUUM CONDITIONS FROM BORAZINE

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Graphene is a 2D material, famous for its exceptional electronic properties. However, to exploit these properties in real devices, the electronic coupling with the substrate and with any surrounding material must be strongly reduced. Hexagonal boron nitride (hBN), another 2D material, is very promising for this purpose [1]. It could be used both to insulate graphene from the substrate and as a gate dielectric material. Although devices obtained by mechanical exfoliation and transfer did confirm the strong potentialities of graphene/hBN heterostructures [2], a scalable and reliable growth technique remains to be demonstrated: the development of new approaches to the fabrication of graphene/BN 2D heterostructures is of high importance. If scalable graphene growth is now well documented, this is not yet the case for BN [3]. The ultimate goal is to be able to grow BN film with accurate thickness control from one to few layers on graphene as well as on technologically compatible substrates.

Towards this goal, we have started to study the growth of BN on Ni substrates from the gaseous borazine precursor ($B_3N_3H_6$), used alone [4] or combined with a complementary source of N provided by a plasma cell. Experiments were done in a molecular beam epitaxy chamber. A continuous BN film is obtained using only the borazine precursor, with a self-limited thickness of one monolayer [5]. The strong orbital hybridization between the Ni 3d and BN π states at the interface [6] disappears after transfer on Si. When using combined borazine-nitrogen sources, high quality material is locally obtained but with a rather heterogeneous thickness and a structure dependent on the Ni crystallographic orientation.

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Advances in selfstanding hBN crystal synthesis via the PDC route

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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 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 crystal 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 and 1c) 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 routine 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 linewidths 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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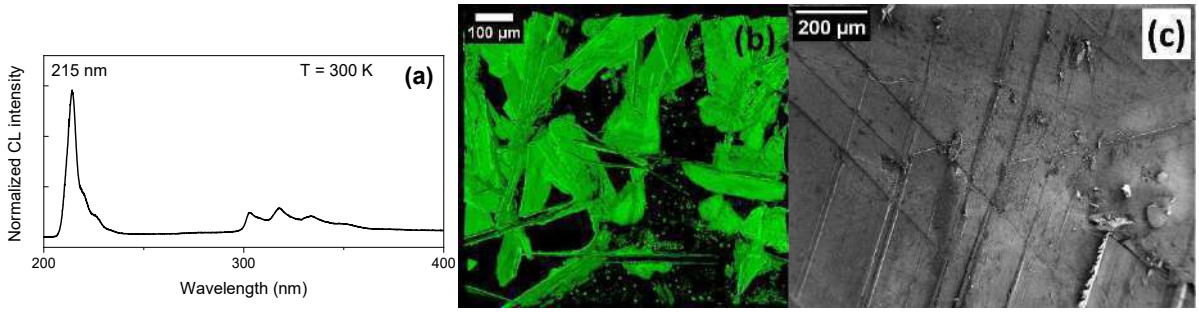

Figure 1: (a) Cathodoluminescence measurement of a PDC hBN crystal [2]; (b) 3D extracted view of entangled crystals inside the as-obtained ingot from X-ray tomography; (c) low magnification SEM view of the crystal surface

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CONCEPTUAL DESIGN OF INDUCTIVELY HEATED CVD REACTOR FOR HEXAGONAL BORON NITIDE SYNTHESIS

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Due to their atomically smooth surface and free dangling bonds, mono and few layer hexagonal boron nitride (h-BN) have a significant potential to be used as two-dimensional dielectric materials in functional 2D heterostructures devices [1]. Similar to graphene, controlled synthesis of large-area high-quality h-BN is important from both fundamental and applications point of views. Indeed, such applications require large scale continuous h-BN films not yet available from standard cleavage techniques. Here, we investigate the conceptual design of a new reactor built for CVD h-BN single crystals growth on copper substrates inductively heated [2]. We mainly designed a new feed system to incorporate suitable solid and liquid precursors allowing more versatility and flexibility to the process. Specifically, our design uses solid ammonia borane (AB) with independent heating control upstream of the h-BN growth, and the growth can be assisted by liquid water [3]. The choice of ammonia borane H_3BNH_3 as source material is justified by its stoichiometric quantities of boron and nitrogen, whereas water allows controlling nucleation density thereby improving h-BN grain size up to 330 µm [3]. Nevertheless, as highlighted by several reports, heating method of AB constitute the major engineering challenge towards full process control. Polymerization and foaming of AB present an additional challenge. Due to the complexity of AB decomposition, we performed a systematic thermochemical study by using *Chemkin-Pro* software to explore homogeneous gas mixture in H B N O system issued from AB precursor decomposition in argon at standard temperature of 60 °C up to h-BN growth temperature of 1140°C - beyond copper melting point. Note that at temperatures above 100 °C the ammonia borane was found to melt, coating the chamber in a white layer. In our approach, detailed model including 62 boro-nitrogen-oxygen species is performed in the specific growth condition to understand how species behaves upon vaporization from the AB precursor down to the hot regions in the vicinity of the copper substrate. Our calculation gives insight into the relative concentrations of h-BN precursor growth such as borazine ($H_3N_3B_3H_3$) as well as nucleation density regulator (HBO) Figure 1 (a-b) respectively. Elucidation of these details facilitated synthesis of high quality large area monolayer hexagonal boron nitride with safety and operational precautions considerations.

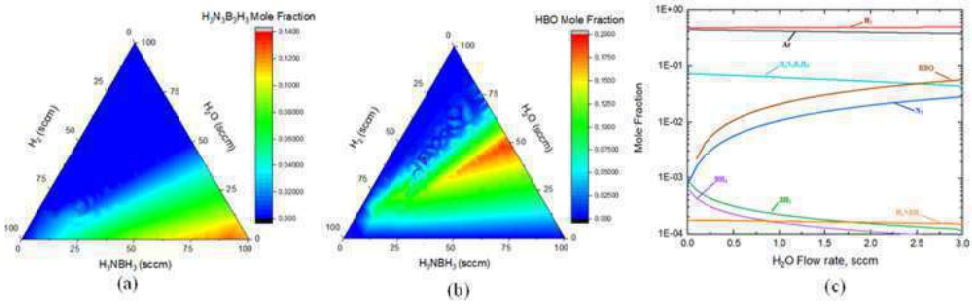

Figure 1: Ternary contour plots of (a) borazine ($H_3N_3B_3H_3$) and; (b) (HBO). Calculated at different gases flow rates at 1140°C, 1 bar and constant argon flow rate of 20 sccm. (c) Effect of water flow rate on major species distribution calculated with input flowrates H_2=1.5 sccm and AB=10 sccm.

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CROISSANCE D'HETEROSTRUCTURES VAN DER WAALS PAR ABLATION LASER PULSE

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Les matériaux bidimensionnels (2D) sont aujourd'hui au cœur de plusieurs développements en électronique, optoélectronique et spintronique. Assemblés en hétérostructures, la combinaison de leurs propriétés conduisent à de nouvelles architectures d'épaisseur ultime comme des puits quantiques ou de super-réseaux verticaux. Jusqu'à présent, les matériaux 2D ont été principalement élaborés par voie chimique en phase vapeur (Chemical Vapor Deposition), qui a rendu possible leur démocratisation et l'obtention de films 2D sur de grandes échelles (m²). Cependant, la forte dépendance de cette méthode au substrat de croissance limite les options d'intégration et rend très complexe la croissance d'hétérostructures 2D. Ainsi, de nombreux groupes cherchent aujourd'hui à développer de nouvelles solutions (MBE…). Nous présentons ici une approche flexible et innovante utilisant l'ablation laser pulsée (Pulsed Laser Deposition - PLD) pour faire croître des hétérostructures de TMDs (dichalcogenures de métaux de transition) sur différents substrats [1] et les intégrer *in-situ* dans des dispositifs hybrides compatibles CMOS [2]. Nous avons ainsi d'abord démontré la possibilité de faire croitre des films 2D de disulfure de tungstène (WS_2) et de diséléniure de tungstène (WSe_2). Nous avons ensuite réussi la croissance d'une hétérostructure (WSe_2 /WS_2) à grande échelle (cm²) combinant ces deux matériaux 2D (Figure 1.a et 1.b). La qualité cristalline de ces couches a été caractérisée par XPS (spectroscopie photoélectronique à rayons X), spectroscopie Raman, TEM (microscopie électronique à transmission) et EDX (spectroscopie X à dispersion d'énergie). Enfin, forts de ses résultats nous avons démontré l'intégration de ces matériaux dans des dispositifs actifs dont les caractérisations électriques (Figure 1.c) montrent qu'il est possible grâce à l'ingénierie des bandes interdites de ces semi-conducteurs 2D d'obtenir la signature d'une résonance de puit quantique. Ces résultats montrent que la PLD offre une alternative très polyvalente et originale pour la croissance de matériaux 2D, leur intégration *in-situ* dans des hétérostructures par simple changement de cible et ouvre la voie à l'exploration de nouveaux dispositifs complexes de van der Waals pour l'électronique et la spintronique.

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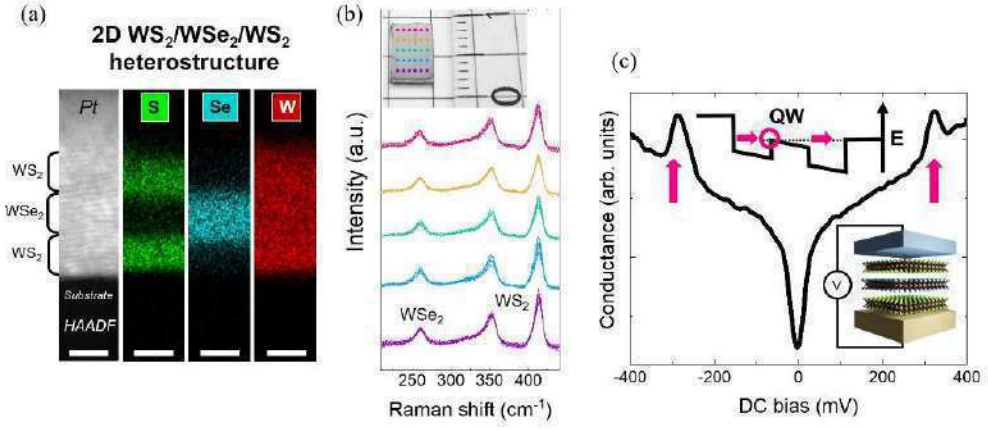

Figure 1 : (a) coupe TEM de l'hétérostructure $WS_2/WSe_2/WS_2$ et images EDX associées pour S, Se et W. (b) spectres Raman associés par couleur et superposés l'un sur l'autre pour points de chaque sur l'échantillon centimétrique (inset). (c) Conductance en fonction de la tension à travers cette hétérostructure. Schémas en inset.

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NOVEL NON-BENZENOID GRAPHENE ISOMERS BY ON-SURFACE SYNTHESIS

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The quest for planar sp^2-hybridized carbon allotropes other than graphene, such as phagraphene, graphenylene, and biphenylene network, has stimulated substantial research efforts because of the materials' predicted unique mechanical, electronic, and transport properties. However, their syntheses remain challenging due to the lack of reliable protocols for generating non-hexagonal rings during the in-plane tiling of carbon atoms. We have developed an on-surface synthesis strategy by which we first generate straight polymer chains, which then link to form the non-benzenoid graphene isomers. Using this approach, we achieved the bottom-up growth of ultraflat biphenylene network with periodically arranged four-, six-, and eight-membered rings of sp^2-hybridized carbon atoms, through on-surface inter-polymer dehydrofluorination (HF-zipping) reaction (Figure 1a). Apart from graphene, biphenylene network is the only experimentally known planar sp^2 carbon so far. Its characterization by scanning probe methods (STM, AFM, STS) confirms the non-benzenoid nature and reveals that it is metallic rather than a dielectric already at very small dimensions. While HF-zipping generates the four- and eight-membered rings during the on-surface reaction, the non-benzenoid structural elements may already be contained in the precursor: using an azulene-based precursor, we achieved sp^2 carbon nanostructures with odd-numbered rings, such as phagraphene nanoribbons containing five-, six- and seven-membered rings (Figure 1b). Additional non-benzenoid four- and seven-membered rings can be formed during dehydrogenative C-C coupling of the intermediate 2,6-polyazulene chains, resulting in tetra-penta-hepta(TPH)-graphene (Figure 1c) with metallic properties.

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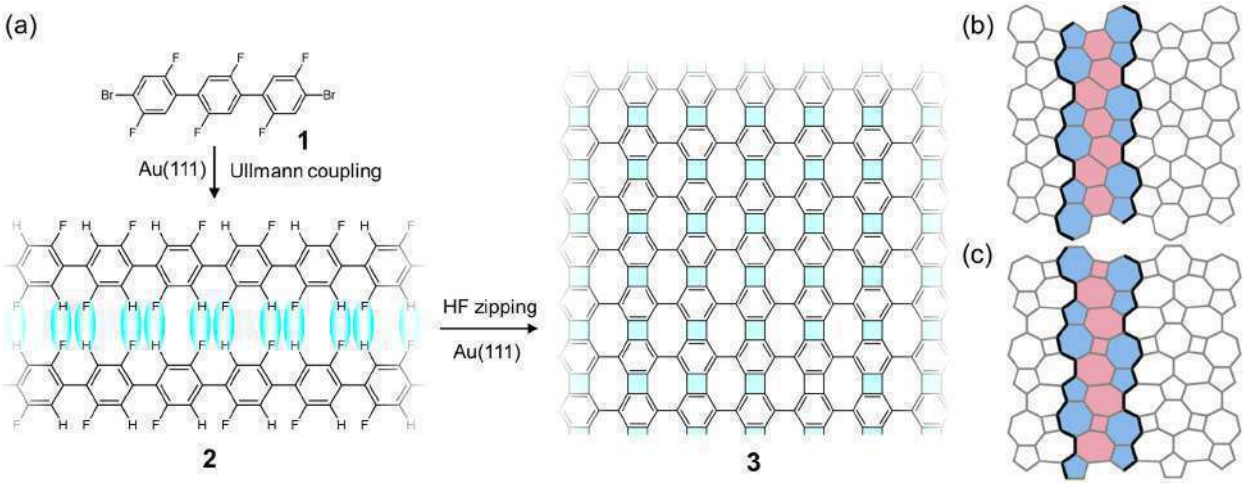

*Figure 1: (a) On-surface synthesis of biphenylene network **3** from 4,4''-dibromo-2,2',2'',5,5',5''-hexafluoro-1,1':4',1''-terphenyl **1** by HF-zipping of the intermediate poly(p-phenylene) polymer **2**. (b) Phagraphene and (c) tetra-penta-hepta(TPH)-graphene..*

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GDR HOWDI 2022 MEETING: SYNTHESIS AND OPTICAL PROPERTIES OF ROD-SHAPED GRAPHENE NANOPARTICLES

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Since its discovery, graphene has been positioned as a promising material because of its good mechanical, thermal and electrical properties, among others. Nonetheless, applications in optics and optoelectronics remain a challenge because of the absence of a bandgap. A solution to this problem is to reduce the size of graphene to a nanometric scale; thus, we shine our interest in Graphene Quantum Dots (GQDs). There are two general approaches for the synthesis of GQDs: top-down and bottom-up. On the one hand, top-down synthesizing (lithography, hydrothermal and electrochemical approaches) can be cheap and efficient at the expense of precise control of the size, shape, and edges of the GQDs.[1] On the other hand, bottom-up synthesis yields precise and controlled structures. Bottom-up graphene materials have developed exponentially for the last decade with the synthesis of highly controlled graphene nanoribbon structures and moderately soluble graphene quantum dots.[2,3] Our group demonstrated that bottom-up GQDs could act as single-photon emitters exhibiting high brightness and stability.[4]

To better understand the structure-optical properties relationship, we designed a series of elongated rod-shaped graphene nanoparticles that differ only by length while keeping the same morphology, symmetry, and edge states (see figure). These nanoparticles exhibit a high solubility, which facilitates their purification and individualization in solution giving well-defined absorption spectra. Here, we report on the synthesis of these GQDs and present results on their advanced optical characterization complemented with their theoretical description.[5]

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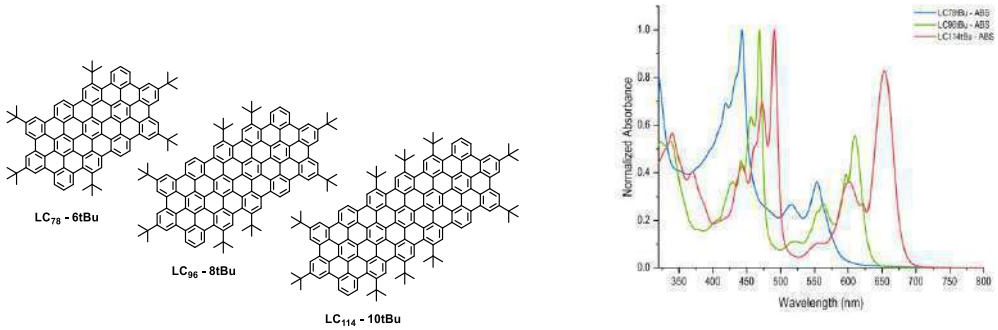

Figure 1: Structures and absorption spectra of rod-shaped GQDs: LC_{78} - 6t-Bu (blue), LC_{96} - 8t-Bu (green) and LC_{114} - 10t-Bu (red).

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HYDROGENATION OF GRAPHENES FROM H RADICALS

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The hydrogenation of single layer graphene (1LG) is controversial as its confirmation is difficult to obtain, and many reports claim for the related sp^2-C to sp^3-C transformation without clear evidence or based on inconsistent observations [1].

Here, a simple but very efficient hydrogenation route was used. The decomposition of H_2 at high temperature on tungsten heating wires was carried out to deposit H radicals on either bilayer graphene (2LG) deposited on a transmission electron microscopy (TEM) Cu grid or various graphenes (from 1LG to few-layer graphene (FLG), exfoliated from HOPG) deposited on an Si-based interferential substrate as reported on figure 1.

TEM characterization of such materials is limited because hydrogenated layers are not stable under the energy range of the electron beams currently used (typically, > 50 keV). Consistently, very low energy electron diffraction (5 keV) was able to discriminate between hydrogenated and non-hydrogenated graphene, and between various stacking sequences as well [2]. Based on this method, a new approach able to take into account misorientations is proposed, which makes the analysis of the diffraction patterns accessible even if the material is affected by local distortions. We will present these results in detail, before (see figure 2) and after hydrogenation.

On the other hand, multi-wavelength Raman spectroscopy succeeded in demonstrating the actual conversion of 2LG into diamane [3], thanks to the sensitivity of visible light excitation to C(sp^2) domains and that of UV light excitation to C(sp^3) domains. It is complementary to Infrared microscopy which is able to reveal C(sp^3)-H but remains qualitative only as the conversion rate is not accessible. The interferential substrate was useful to optically reveal the hydrogenation-promoted C(sp^2)-to-C(sp^3) conversion by a mere color change while enabling Raman spectroscopy. Whereas obtaining the signal of both D and G bands after hydrogenation is a clear signature of partial conversion only, we show that 1LG exposed to hydrogen radicals becomes transparent in the visible light range without exhibiting any Raman signal. We also discuss the case of the partial hydrogenation of 2LG (either AB stacked or twisted considering thermodynamics considerations proposed by Erohin et al [4].

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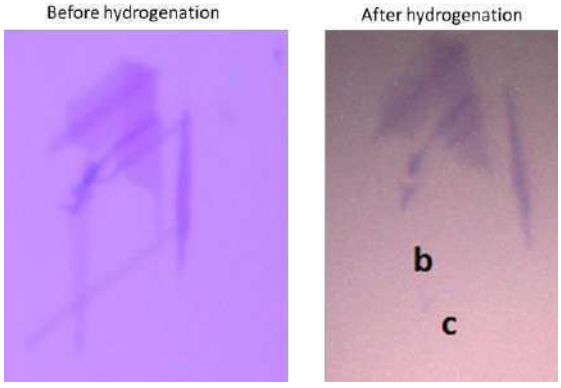

Figure 1: Contrast change after hydrogenation. (b) 1LG, (c) twisted 2LG.

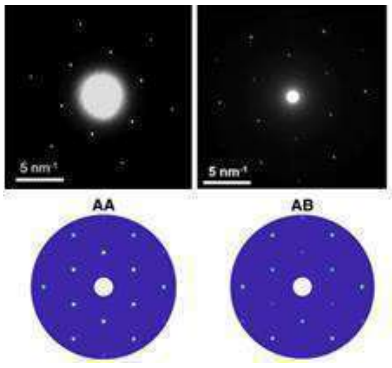

Figure 2: low voltage (5 keV) diffraction patterns for 2LG with AA and AB stacking. Top: experimental; bottom: calculated.

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STRUCTURE, CHEMISTRY AND CHARGE DENSITY IN MBE GROWN TMDS INVESTIGATED BY 4D-STEM

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Epitaxial growth is a route to achieve highly crystalline continuous 2D layers. Molecular beam epitaxy (MBE) could lead to the fabrication of large scale and well-oriented single crystals with a great flexibility in the choice of elements and a potential in building van der Waals stacks, alloys or 2D layers doped either electrically or with magnetic elements. In order to achieve the synthesis of the desired complex materials and to explore their functionalities, the ability to survey the structural configuration and their properties at the atomic scale is essential. High resolution scanning transmission electron microscopy (STEM) has become the most powerful technique for providing detailed atomic structure by Z-contrast direct imaging and the associated chemical information by electron energy loss spectroscopy (EELS). While charge density is among the most fundamental solid-state properties determining chemical and electrical characteristics, measuring local charge density together with detailed atomic structure poses a challenge in advanced microscopy for atomistic understanding of 2D materials. A new STEM acquisition technique so-called four-dimensional STEM (4D-STEM) consists in recording a diffraction pattern for each position that the electron probe scans on the sample in order to map multiple information found in reciprocal space [1]. Analyzing the deviation (Center of Mass: CoM) of the transmitted beam position gives access to the electric field with atomic resolution, and to the electrostatic potential and the charge density through Poisson's equation [2-3].

In this work, we first demonstrate a multi-scale analysis of MBE grown WSe_2 using the orientation and 1H-1T' phase maps reconstructed by the 4D-STEM diffraction datasets obtained over micron areas. A histogram of the orientation angle was generated for direct comparison with X-ray diffraction (XRD) data acquired at the mm scale. This step makes it possible to link large- and atomic-scale diagnostics and finally to explain the mis-orientation in layers investigated by the XRD relating to their atomic structures. Secondly, the electric field map around single dopant vanadium atoms incorporated in WSe_2 was reconstructed by the CoM measurements and then converted into local electrostatic potential and charge density maps. The quantitative interpretation of the experimentally obtained charge density was studied by comparison with the DFT calculation and the ability to identify a single impurity atom is discussed by comparing with z-contrast imaging and EELS spectrum imaging.

This 4D-STEM technique is still exploratory and far from being used in a standard way to study synthesized 2D materials. The methodology highlighted here will open the use of electron microscopy to provide atomic scale multiple information on structure, chemical and electric characteristics appearing in 2D layers and their heterostructures.

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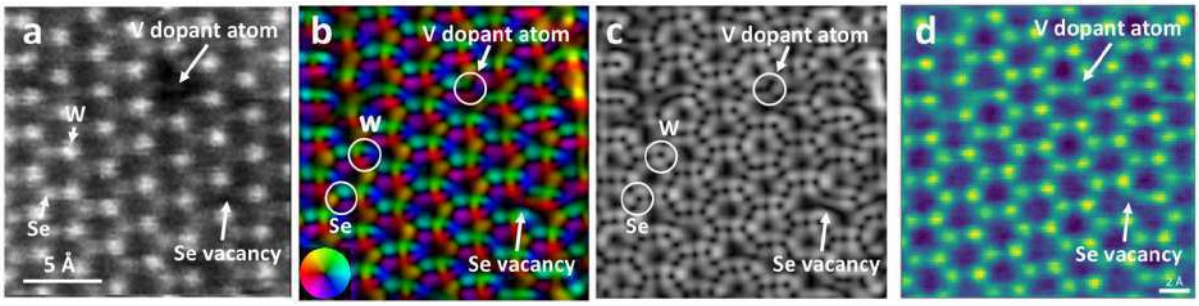

Figure: (a) Virtual HAADF image, (b) projected electric fields vector map, (c) projected electric field strength map (0-65V) and (d) projected electrostatic potential map; of vanadium doped WSe_2 monolayer grown by MBE. All maps were reconstructed from a 4D-STEM dataset.

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TWISTED BILAYERS OF HEXAGONAL BORON NITRIDE

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Since the last decade, **twisted bilayers of graphene** (stackings of two graphene planes, with a non crystallographic rotation angle, also called *moires*) have attracted attention because novel -and quite fascinating- behaviours have been reported on these structures, especially when the angle of rotation is small [1]. Flat bands arise in electronic structure linked to different zones of the supercell, with local AA or AB stackings, and the resulting properties, such as Mott transition or tunable superconductivity, are controlled by a subtle interplay between the radius of these AA and AB stacking zones, the amplitude of interlayer interaction and the filling level.

More recently, the physical properties of **twisted bilayers of hexagonal boron nitride** (hBN) have been questioned. Differently to graphene, hBN is a wide band gap semiconductor (> 6 eV) and consequently attracts a growing interest for its strong UV photo-luminescence properties [2,3]. The optical properties of bulk as well as hBN layers are governed by strong excitonic effects. Theoretical studies of twisted hBN bilayer have been reported [Zhao, Wallet]. It has been shown for example that the rotation angle may be responsible for a geometric separation between the valence and conduction band states.

However, the geometries of stackings with a small angle of rotation require very large periodic cells, and the usual numerical approaches, mainly based on self consistent calculations, are restricted to a limited number of atoms in the calculation cell. In this context, and since we want to be able to calculate the electronic structure of twisted hBN bilayers with a wide range of rotation angles, only tight-binding (TB) approaches are tractable.

In the present work, we have extended a TB model originally developed for graphene moires [4] to the study of hBN twisted bilayers. First, the validation of this approach and its transferability to numerous systems will be discussed. More precisely, comparison with band structures of hBN bilayers calculated ab initio, for the smallest simulation cells will be presented including all the different stacking geometries which exist in such heteregenous BN system. In a second part, different electronic properties as well as optical properties will be investigated for various configurations, i.e. different angles and stackings.

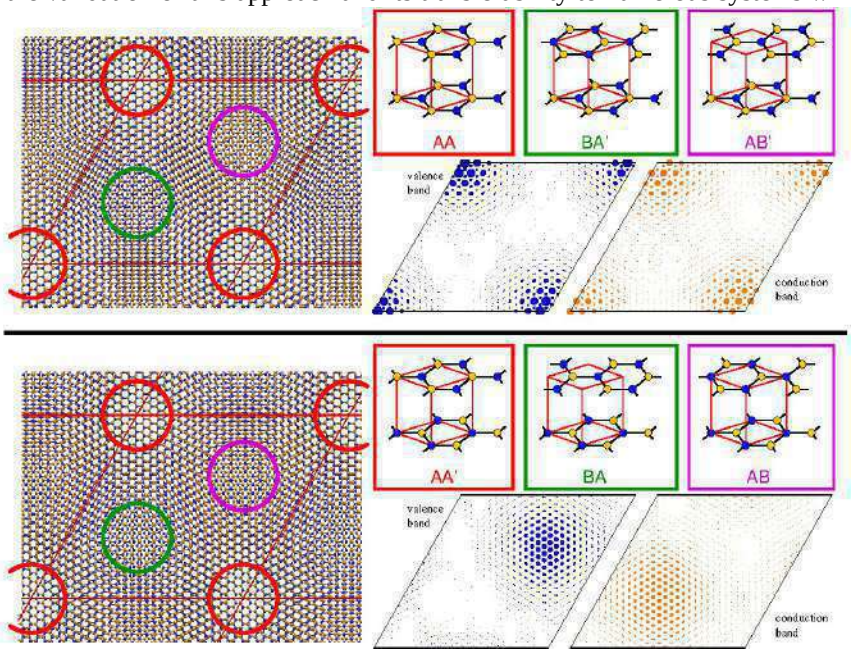

Figure : Electronic structure of two stacking geometries, with the same 2.7° angle (the only difference is a switch of B and N positions in the upper layer). Electronic states of both valence and conduction are localized in the high symmetry points areas. In the above case, valence and conduction belong to the same area. In the below case, eigenstates a geographically separated.

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INFLUENCE OF BIAS VOLTAGE ON THE OBSERVED MOIRÉ PATTERNS OF $MoTe_2$/GRAPHENE HETEROSTRUCTURE GROWN BY MOLECULAR BEAM EPITAXY

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In recent years, the importance of the rotation angle between layers of 2D material has come to the forefront of the research on 2D van der Waals heterostructures. Bi-layer graphene with small magic angles is a prime example with its superconducting behavior and the presence of solitons [1, 2]. In heterostructures with different lattice parameters such as $MoTe_2$/graphene, it is possible to observe high-indexed Moiré patterns that are more complex and less studied than the usual low-indexed ones. The STM images have then to be analyzed with great caution because topology and electronic effects are intertwined. These high-indexed patterns imply extra periodic potential modulations in the electronic system, which is at the heart of flat-band formation in van der Waals heterostructures.

In our study, we demonstrate that MBE grown $MoTe_2$ on graphene substrate favors various higher-indexed Moiré patterns for twist angles around 30° (see figure). These patterns have an unusually high degree of complexity, therefore their characterization had to be done rigorously in the full context of Moiré theory. Our analysis provides a useful example to researchers working in the field of how to identify and interpret higher-indexed patterns and also highlights the importance of the electronic effects in $MoTe_2$/graphene heterostructure.

The key findings emerging from our STM investigations combined with DFT calculations and the Moiré-analysis are:

- The Moiré patterns found in our STM measurements are remarkably sensitive to the bias voltage. When changing the bias voltage, the Moiré pattern transforms because of the entanglement with electronic effects, causing the apparent Moiré periodicity to be modified. Although such high-indexed Moiré patterns have been studied in details in theory, their appearance in STM images of real heterostructures is rather new.
- The complexity of the patterns is further increased if commensurate layers are analyzed. Besides the higher-indexed Moiré periodicity, the length of commensurate supercells also shows up with strong contrast in STM images, highlighting the influence of the small atomic deviations on the electronic properties.
- Exceptional variability of the spatial distributions of the charge density in the $MoTe_2$ layer is further investigated by DFT calculations, which also revealed the crucial role of the coupling with the underlying graphene substrate.

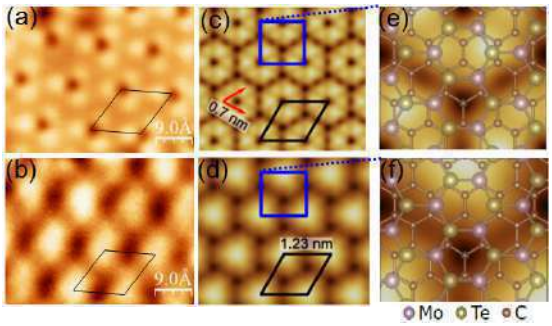

Figure: STM images of the Moiré 2√3R30° 1H-$MoTe_2$/graphene heterostructure recorded at 0.2V/200pA ***(a)*** *and 1.0V/100pA* ***(b)****;* ***(c, d)*** *simulated images calculated for the same +0.2V and +1V bias voltage;* ***(e, f)*** *the smaller spatial dimension zoomed on the blue square as marked in (c) and (d), respectively. C stands for the sp^2-bonded carbon in graphene on terminated 6H-SiC(0001). The Moiré supercell is marked by black rhombus on the corresponding image.*

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UNFOLDING
THE ELECTRONIC BANDS OF TWISTED 2D MATERIALS

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Two-dimensional (2D) heterostructures can be very effectively built by direct stacking of individual monolayers of different 2D materials. The extended range of functionalities of such heterostructures yields possible applications going from field effect tunneling transistors to optoelectronic devices. In order to control the ultimate performance of these systems it is fundamental to understand how the electronic properties of each layer are affected by the neighboring one. These effects can be reliably described in the framework of the Density Functional Theory (DFT) but the electronic structure derived from a moiré supercell model results in highly folded bands, which can be hardly linked to those of the reference unstacked lay that which provide an effective band structure, which has great interpretative value and can help for instance in the understanding of angle-resolved photoemission spectroscopy (ARPES) measurements.

As an example, here we show how band unfolding can correctly describe the appearance of additional gaps in the electronic structure of MoS_2 on top of black phosphorous which has been observed by ARPES. Band unfolding techniques have been further applied to the study of bilayer moiré structures of emergent optical materials such as BN and WSe_2. After discussing the dependence of the electronic structure on the twist angle, we combine this ground state information with simulations of the optical response obtained by a GW+BSE approach. Finally we discuss how the twist of the layers can affect the excitonic response of the bilayers.

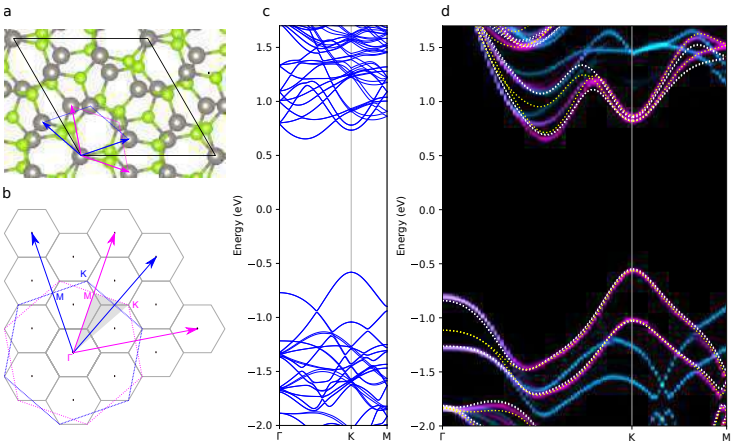

Figure 1: a) Structure of a moiré WSe2 supercell where the primitive unit cell of the top and bottom layer are indicated. (b) Reciprocal lattice vectors and Brillouin zones of the primitive cells of the individual layers, and the supercell Brillouin zones (grey hexagons). (c) Band structure calculated over the high symmetric direction of the moiré supercell. (d) Band structure of the moiré cell unfolded along the high symmetry direction of the reduced Brillouin zone shaded in (b). Blue and purple lines correspond to the unfolding using the reference primitive cell of the top and bottom layer respectively. The yellow and white lines are the band structure of WSe2 mono- and bi-layer respectively.

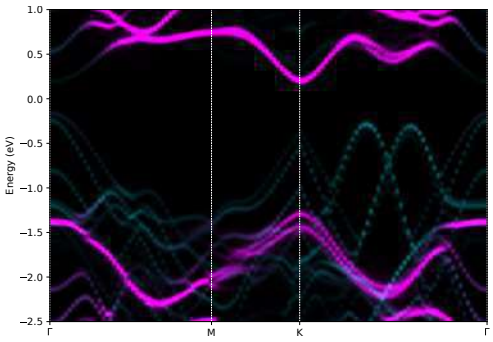

Figure 2: Electronic band structure of a stack of monolayer MoS_2 on top of black phosphorous unfolded using as reference the MoS_2 (purple lines) and the black phosphorous (cyan lines) primitive cells.

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RADIATIVE LIFETIME OF FREE EXCITONS IN HEXAGONAL BORON NITRIDE. [1]

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We have developed a new time-resolved cathodoluminescence (TRCL) system dedicated to the UV spectral range. It provides a first estimate of the radiative lifetime (τ_r) of free excitons in hBN, evaluated from a single experiment comparing hBN crystals issued from different synthesis routes (HPHT, APHT, PDC). On each sample, the internal quantum yield (η_i) was evaluated from the absolute luminescence intensity under continuous excitation [2], and the exciton lifetime (τ) was deduced from the decay time of free excitons in the time domain. Since $\eta_i = \tau / \tau_r$, we estimated τ_r at 27ns from the proportionality measured between τ and ηi, as shown in the Fig. (a). It is much shorter than in other indirect bandgap semiconductors [3][4], which is first explained first by the close proximity of the electron and the hole in the exciton complex, see Figure (b). The unusually high luminescence efficiency of hBN for an indirect bandgap is therefore semi-quantitatively understood. Beyond that, the demonstration of the intrinsic character of the radiative lifetime of the exciton has a practical application to compare quantitatively hBN samples. The linear relation between the free exciton lifetime and the internal quantum yield indeed provides a scaling of the sample quality, which can be obtained from a single experiment carried out at room temperature. This tool can be capitalized for linking hBN quality to the expected performances of 2D materials in devices using hBN layers.

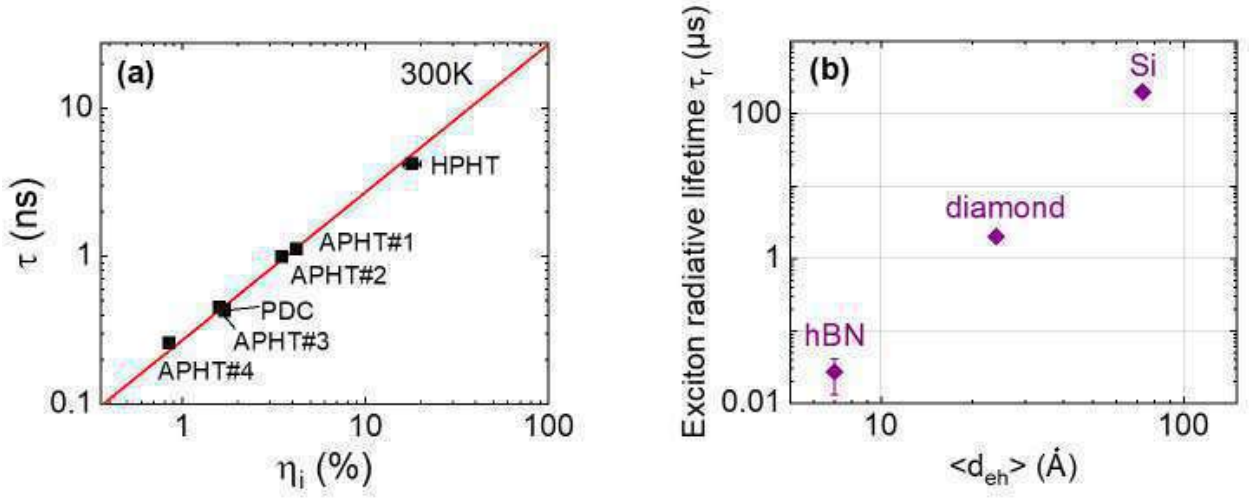

Figure (a) Free exciton lifetime (τ) as a function of the internal quantum yield (ηi) for the intrinsic luminescence in hBN. The radiative lifetime (τ_r) of hBN indirect excitons is estimated at 27 ns from the linear fit (red curve). (b) Radiative lifetimes of free excitons in silicon [3], diamond [4] and of hexagonal boron nitride as a function of the average distance between electron and hole forming the exciton. We observe an unusual short radiative lifetime of hBN exciton for an indirect exciton, which is explained in a first order by the close proximity between its constitutive electron and hole.

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OPTICAL SIGNATURES OF THE STRONG 3D ANISOTROPY IN BLACK PHOSPHORUS

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After reports of high mobility and a tunable bandgap covering a wide spectral range from the visible to the mid-infrared region, layered black phosphorus (BP) has emerged as a promising 2D material for high performance electronic and optoelectronic devices [1]. Owing to its orthorhombic crystallographic structure, black phosphorus expresses strong anisotropic properties [2,3]. While recent investigations on few-layers crystals have extensively explored the in-plane anisotropy, much less attention has been given to the out-of-plane direction.

In this work, we use polarization-resolved photoluminescence (PL) and Raman spectroscopies to investigate the band structure anisotropy of bulk BP along the in-plane (zigzag, armchair) and out-of-plane directions. An unexpected room-temperature luminescence is detected in the visible, and strongly polarized in the out-of-plane direction. This emission, detected at 1.75 eV far above the band gap (0.3 eV), is surprising as it violates Kasha's rule which favors light emission from the lowest energy states. To elucidate its origin, we have systematically examined the characteristics of this luminescence as a function of polarization, temperature and excitation energy. These results reveal an unreported out-of-plane resonance at 2.3 eV in both the PL and Raman responses. Polarization selection rules and density functional theory (DFT) calculations of the complex dielectric permittivity are used to understand the origin of the strongly polarized optical response and demonstrate the remarkable extent to which the anisotropy influences the optical properties and carrier dynamics in black phosphorus.

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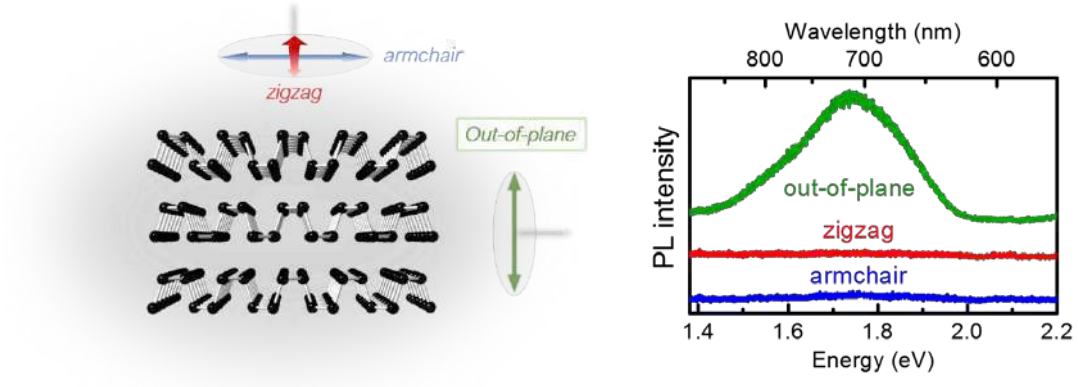

Figure 1: Left: Schematic illustration of the polarization-resolved spectroscopy experiments on bulk BP. Right: Room temperature PL spectra recorded along the out-of-plane (green), zigzag (red) and armchair (blue) directions.

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SEMICONDUCTING THIN LAYERS OF TRANSITION METAL DICHALCOGENIDES UNDER PRESSURE

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Semiconducting monolayers of transition metal dichalcogenides (mTMDCs) are intensely studied in the community of 2D materials owing to their manifold and unique properties for optoelectronics and photonics: artificially stacked van der Waals structure, moirée superlattice, high exciton binding energy, spatially separated electron-hole pair in heterostructure, spin-valley physics and so on. One particular hot topic in the field is the tuning of intralayer and interlayer exciton properties in multilayers heterostructure via tailoring the number of layers [1, 2] applied gate voltage [3], magnetic field [4], strain [5], and pressure [6, 7], all in order to achieve high-performance spin-valleytronics and excitonic devices.

In this context we elected to study mTMDCs heterostructures under pressure. We developed an experimental setup to study materials in extreme environment of low temperature, high magnetic field, and high pressure using a diamond anvil cell (DAC) reaching up to 10GPa [8]. The experimental setup offers novel and exciting possibilities to explore how optical properties (photoluminescence, Raman scattering, reflectivity) vary with interlayer distance and lattice parameters change when hydrostatic pressure is applied. In particular, the large polarisability in plane compared to out-of-plane and the drastic change in the dielectric environment completely modify the screening of the coulomb interaction between electrons and holes.

Several fundamental questions are raised by the possibility of applying pressure to a monolayer of 2D material. The first one being how is pressure transferred to a monolayer or to a van der Waals heterostructure ? Using low temperature optical spectroscopy on high quality TMDC encapsulated in hBN and inserted in a DAC, we investigate the exciton properties including its excited states series [10], and its evolution when applying high pressure. We will discuss the potential structural changes affecting the TMDC via Raman scattering analysis together with the changes of the dielectric environment [9] when reducing the van der Waals gaps.

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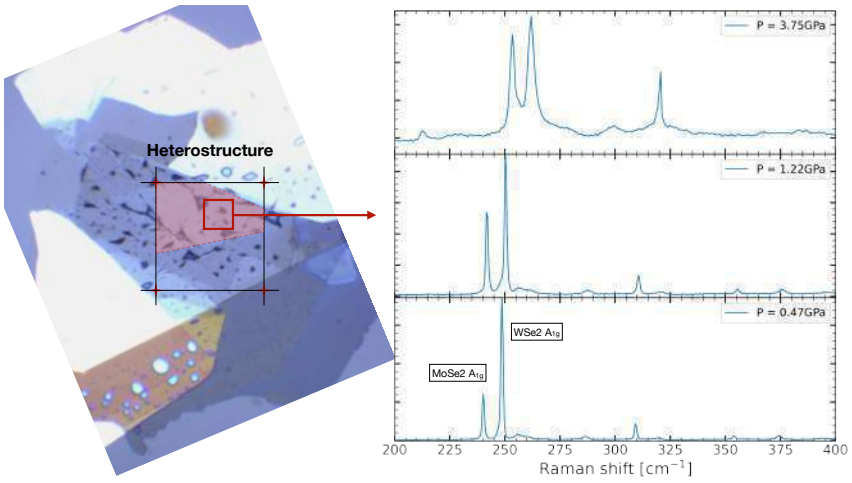

Figure 1: Raman spectra at different value of pressure inside the DAC. Each raman spectrum on the right panel is averaged over the area on the MoSe2/WSe2 heterostructure denoted by the red square on the picture.

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2D MoS_2 CAPACITORS AND TRANSISTORS STUDIED BY EXCITONIC REFLECTION MICROSCOPY

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Inverted reflection microscopy is a powerful tool to study nanomaterials undergoing *in situ* processes. Its configuration is highly compatible to work with solvents, and the use of metallic anti-reflection coatings can enhance sensitivity to changes in optical path length (OPL), in addition to serving as an electrode. We recently demonstrated some of its assets for the high-contrast observation of graphene oxide and its chemical modifications [1] as well as for the *in situ* study of ultrathin molecular film growth [1,2].

In the present work, we show how reflectance imaging can be used to study semiconductor devices of 2-dimensional (2D) MoS_2, a transition metal dichalcogenide (TMD) crystal, synthesized by chemical vapor deposition (CVD). As explained in [3], 2D TMDs exhibit gate-tunable optical properties (n,κ) near the exciton energies. Therefore, at appropriate wavelengths a reflectance change is correlated with the local charge density profile of a TMD device [4,5]. Based on this principle, we study MoS_2 device operation *in situ* for both capacitors and field-effect transistors (FET), in wide-field mode and with high throughput. In Figure 1a, a network of interconnected MoS_2 domains is capacitively charged, and reflectance change images are acquired as a function of time. In addition to local charge inhomogeneity imaging within each individual MoS_2 domain, this type of experiment informs on the domain-to-domain contact resistances through the RC charging delay they induce.

In Figure 1b, a FET example is shown, where an asymmetric drain-source charge profile is observed when switching the device polarity. In the proposed talk, we will show how such a technique opens the door to measuring high-throughput *in operando* device physics parameters of nanomaterial electronic systems, using readily accessible optical equipment.

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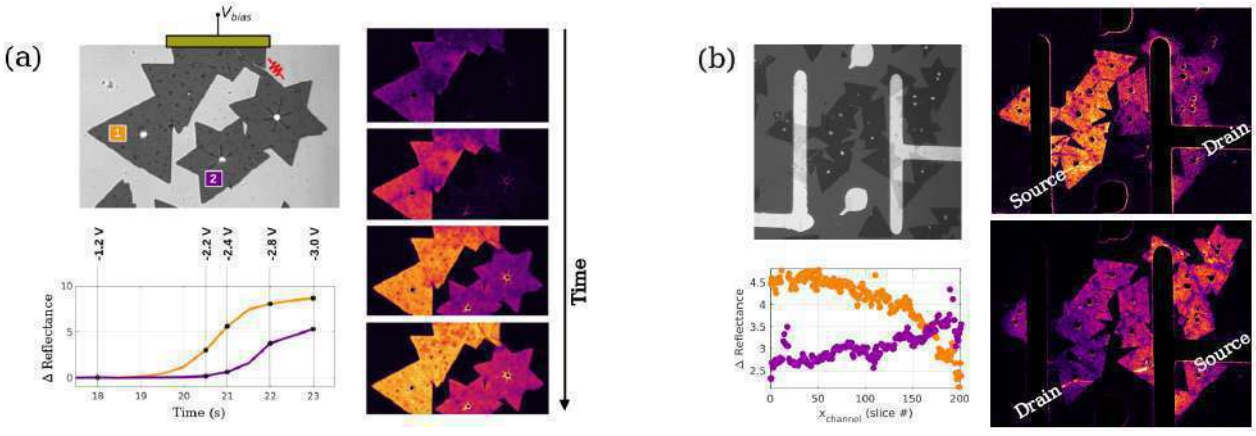

Figure 1: (a) Charging dynamics of MoS_2 capacitor network revealed by reflectance change. (b) Charge density profile of MoS_2 FET revealed by reflectance change, for different polarity.

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GDR HOWDI 2022 MEETING: A GLIMPSE INTO THE WORLD OF TOPOLOGICAL PHASES IN TWO DIMENSIONS

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Topology is a branch of mathematics which focuses on properties of objects insensitive to smooth deformations. Its first occurrence in the description of matter happened in the 70s: topological numbers allow to classify stable defects of various ordered phases, such as vortices, dislocations or skyrmions. The discovery of the Quantum Hall Effect in 1980, allowed to realize that a quantum electronic phase as a whole can be associated with a topological property. In this tutorial, I will introduce pedagogically the notion of a topological phase, starting from the pioneering works associated to the 2016 Nobel prize. Then I will turn to more recent use of topology to characterize matter, with a special focus on various two-dimensional phases, from quantum spin hall state to twisted bilayer graphene. In particular I will introduce the notion of insulators of a new kind, which are identified not by a standard broken symmetry but by a topological property of their ground state protected by a symmetry. I will then discuss the manifestation of these topological properties as edge states. Finally, I will discuss topological semi-metals, analogs in electronic phases of topological defects in ordered matter.

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GDR HOWDI 2022 MEETING:
METAL-INSULATOR TRANSITION IN ANNEALED MOS_2 DEVICES

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Single-layer MoS_2 has been widely studied due to its promising electronic and optoelectronic properties, which can be efficiently tuned by electrostatic doping in a transistor configuration [1]. To consider actual applications, a perfect understanding and control of the contacts and transport regime in the devices is required [2-3]. We present a systematic study of the transport characteristics of monolayer MoS_2 as a function of electron density and temperature. High quality MoS_2 flakes are grown by CVD on a Si/SiO_2 substrate, then plasma etched into the desired shape and top-contacted with Ti/Au through electron beam lithography (Fig. 1).

More than 10 devices were studied by electrical measurements after in-situ annealing at 600 K under vacuum. The 2- and 4-probe resistance was systematically recorded as a function of temperature (down to 20 K), gate voltage and source-drain voltage. In this presentation, we will focus on the intrinsic conductivity of the MoS_2 channel (4-probe measurements). For all the devices the conductivity increases with gate voltage and the apparent threshold voltage decreases with temperature. Insulating or metallic-type temperature dependencies are observed (without the need of top-gating or high-k dielectric capping) depending on carrier density (see Fig. 2), with a transition occurring around $2x10^{12}$ cm^{-2}. The devices exhibit high mobilities at low temperature (for CVD MoS_2 on SiO_2) on the order of 200 cm^2/Vs, with a nontrivial dependence between the gate voltage and the density of occupied states above the mobility edge (*i.e*, extended states).

A detailed analysis with different models fitting these results [3,4] will be presented to clearly elucidate the dominant transport mechanism for each doping and temperature range. For low gate voltages, thermally activated and variable-range hopping transport of in-gap states explain the drastic change in threshold voltage and the insulating transport [*e.g. Ref.* 2]. For higher gate voltages, the metallic behavior is well explained by phonon and static defects scattering, in agreement with a theoretical model done through a full energy- and momentum-dependent Boltzmann transport equation [5]. All these results are consistent with other device characterization such as Raman spectroscopy. We will show that this metal-insulator transition also matches more elaborate models involving quantum phase transitions. We will tentatively discuss how this approach can be reconciliated with the previous models, which are more consistent with the temperature and mobility ranges observed.

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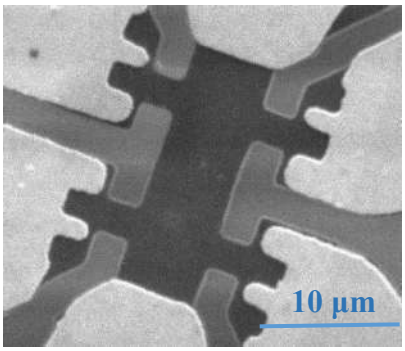

Figure 1: SEM Image of a typical device in Hall bar shape (MoS_2, SiO_2 and Au from dark to light gray).

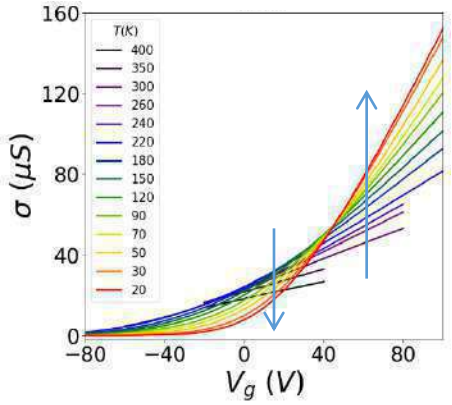

Figure 2: Typical conductivity versus gate voltage characteristic. One can notice that the conductivity increases with gate voltage (conductivity band doping), and either increases or decreases with temperature, corresponding to what is typically called a metallic or insulating behavior respectively.

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A graphene-based voltage-tunable Josephson parametric amplifier

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In recent years, 2D materials have shown their potential for quantum technologies. Applications range from single photon emitters, detectors, to quantum dots or superconducting circuits. The use of van der Waals materials brings new functionalities and enhanced performances. In the field of superconducting quantum circuits, graphene can allow gate tunability [1] and very efficient photons detectors [2]. The recent demonstration of a quantum bit based on a graphene Josephson junction has been a major milestone in this context [3].
In this work, we report the demonstration of the other key element of superconducting quantum circuit: a Josephson parametric amplifier. Tuning the critical current of the graphene Josephson junction with a simple gate voltage allows to tune the working frequency of the amplifier by about 1GHz around 5.5 GHz. We show that the performances of such amplifier (gain, saturation, noise) are on par with traditional implementations using superconducting tunnel junctions, with the additional electrical tunability in our device.
This development shows that van der Waals materials brings new opportunities in the field of superconducting quantum technologies and that they can be considered as realistic platforms for such applications.

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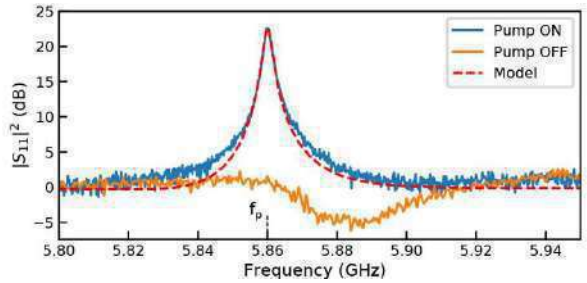

*Figure 1: **Parametric amplification**. Reflection of the device without (orange) and with (blue) an additional pump tone (at frequency f_p). In the absence of the pump, the dip indicates the resonance of the circuit. A gain exceeding 20 dB is achieved in the presence of the pump. The behavior is well reproduced with a model of parametric amplification using experimentally determined parameters (red dotted line).*

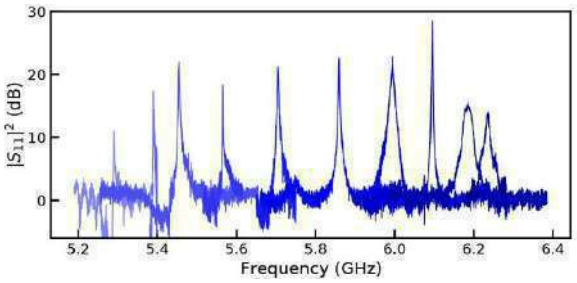

*Figure 2: **Tunability of the parametric amplifier**. Gain profile for different setpoints of the graphene Josephson junction. Tuning the gate voltage, we can change the working frequency from about 5.3 GHz (near the Dirac point) to 6.3 GHz at large carrier density.*

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QNAMI PROTEUSQ: A COMMERCIAL SOLUTION UNLOCKING MAGNETIC FIELD MEASURMENTS IN 2D MATERIALS

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The ability to resolve minute magnetic fields with nanoscale resolution makes scanning NV magnetometry an intriguing tool to analyze 2D materials. In this talk we discuss the capabilities of scanning NV magnetometry and how the technique can be applied to van-der-Waals magnets. We elaborate on the recent progress in the field and reveal potential future applications of scanning NV magnetometry. Finally, we discuss the specs of Qnami ProteusQ, the first commercially available scanning NV magnetometer, in the context of van-der-Waals heterostructures.

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GDR HOWDI 2022 MEETING: SCANNING NITROGEN-VACANCY MAGNETOMETRY OF VAN DER WAALS MAGNETS

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The recent discovery of two-dimensional (2D) magnetic materials [1] has sparked wide interest in the scientific community due to their potential for a novel, atomic-scale platform hosting exotic spin-textures [2]. Advancement in this field, however, relies on quantitative knowledge of the magnetic properties of van der Waals (vdW) magnets at the nanoscale.

In this talk I will present our work on nanoscale magnetic imaging of vdW materials using a quantum sensor based on single spins in diamond, specifically the Nitrogen-Vacancy (NV) center. In our measurements we employ a scanning technique with NV centers embedded in an all-diamond scanning probe to image nanoscale magnetization patterns with a special resolution of tens of nm. We have conducted quantitative studies of magnetism in the vdW magnet chromium triiodide (CrI3) [3], where we investigated the interlayer exchange coupling in this material and shed light on the correlation between structural order and magnetization of the material. Recently, we have extended our work to other 2D magnets, specifically to in-plane magnetic systems, where we study spin textures down to the monolayer limit. Our studies provide a solid basis for future fundamental experiments on low-dimensional magnetism and open the path for studying more exotic phenomena, such as magnetic excitations (magnons) in 2D magnets.

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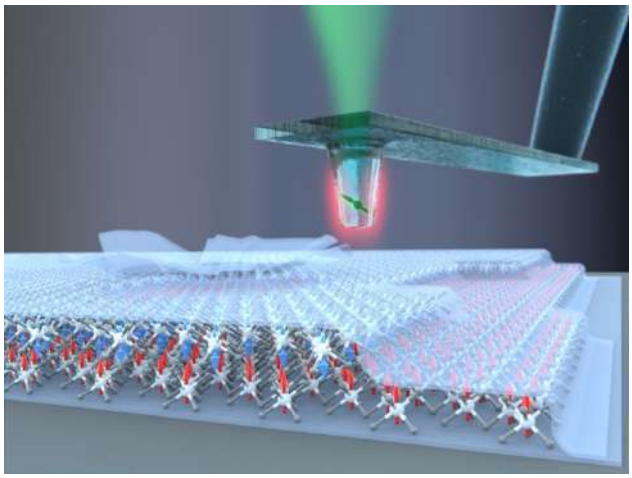

Figure 1: Nitrogen-Vacancy (NV) scanning probe technique for magnetic imaging. A single-spin NV center embedded in the tip of a diamond pillar scans over a 2D magnet while measuring the magnetic stray field.

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MAGNETIC ORDERING IN WEAKLY COUPLED VAN DER WAALS SYSTEMS, WITH APPLICATION TO VI_3

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Magnetic van der Waals (vdW) materials exhibit promising potential for high-tech magnetic, magneto-electric and magneto-optic applications in nanostructures [1]. Due to their intrinsic magnetocrystalline anisotropy, several vdW magnets could be thinned down to nanoscale thickness while overcoming the consequences of Mermin-Wagner theorem and still maintaining magnetic order. A prominent example of such materials are transition metal trihalides, in particular CrI_3, a first atomically thin ferromagnet, realized in 2017 [2].

In van der Waals materials exchange coupling between layers is rather weak and can be relatively easily modified. Regime of weak interlayer coupling represents a transition between the more explored cases of isotropic bulk-like exchange and the ideal 2D (monolayer) limit [3]. Here we examine general features of finite temperature magnetic order in this regime by atomistic spin dynamics methods. The method is applied to a particularly interesting system from this class, VI_3. It is a quasi 2D ferromagnetic semiconductor with T_C = 50 K, and a rather unusual magnetic anisotropy [4]. The anisotropy was reproduced by first-principles calculations only if lattice distortions present at its low temperature phases were taken into account [5]. The calculations also revealed an exceptionally large orbital momentum on V atoms, showing that the effect of spin-orbit interaction is more important than the crystal field in this case. Employing calculated exchange interactions we study how is the Curie temperature affected by interlayer coupling of this system and how much this solution differs from the mean-field model results. We also predict a possibility of magnetic order with parallel aligned spins inside layers that are magnetically decoupled from each other. This phase may occur at some temperatures above T_C in case that magnetic anisotropy and specific exchange interactions fall within a certain range of values.

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STRUCTURAL, MAGNETIC AND TRANSPORT PROPERTIES OF VAN DER WAALS CR_2TE_3 BASED HETEROSTRUCTURES

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Achieving the large-scale growth of 2D ferromagnetic materials with high Curie temperature and perpendicular magnetic anisotropy is highly desirable for the development of future ultra compact magnetic sensors or magnetic memories based on van der Waals (vdW) heterostructures. In this context, vdW materials in the class of $Cr_{1+x}Te_2$ compounds, which are stable in the range of $0 \leq x \leq 1$, appear as promising candidates [1]. Among them, Cr_2Te_3 exhibit strong perpendicular magnetic anisotropy and a Curie temperature in bulk of 180 K. With increasing chromium content, Curie temperature is augmented and magnetic anisotropy changes to an in-plane easy axis [2].

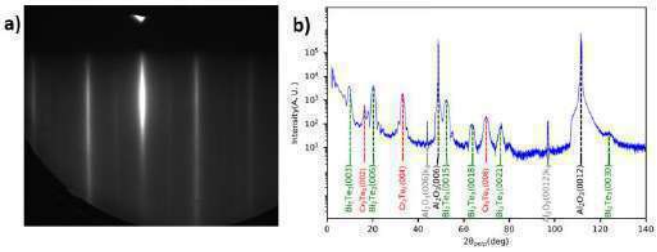

Figure 1: Structural properties of epitaxial Cr_2Te_3. a) RHEED image of Cr_2Te_3 grown on graphene/SiC. b) Specular x-ray diffraction of a vdW heterostructure of Cr_2Te_3 on Bi_2Te_3 on a sapphire (0001) surface.

Successful growth of vdW Cr_2Te_3 layers was achieved at the SPINTEC laboratory of CEA-Grenoble by molecular beam epitaxy (MBE). The growth was realized on various substrates such as epitaxial graphene on SiC(001), GaAs(111), WSe_2/GaAs(111) and Bi_2Te_3/Al_2O_3(0001). Systematic structural and magnetic analysis have been performed for each heterostructure. We obtained single crystalline growth on a centimeter scale surface, as can be seen by in situ reflection high-energy electron diffraction (RHEED) and ex situ x-ray diffraction (Figure 1), and well-defined magnetic properties (Figure 2). The surface morphology was studied by atomic force microscopy (AFM) and the stoichiometry of the layers was probed by Rutherford back scattering.

We observed - by SQUID magnetometry – perpendicular magnetic anisotropy and long range ferromagnetic order on vdW subtrates. We also found a decrease of the coercivity and an increase of the Curie temperature by post-growth annealing of the layers (Figure 2), that we attribute to a change of the stoichiometry (a raise of the chromium content symbolized by a positive ε in $Cr_{2+\varepsilon}Te_3$) as reported in thick films [2]. Following this method, we can expect to push the Curie temperature up to room temperature.

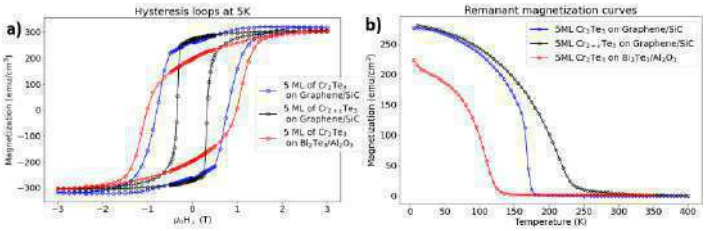

Figure 2: Magnetic properties of Cr_2Te_3 measured by SQUID magnetometry. a) Hysteresis loops at 5K with perpendicular applied magnetic field. b) Remanent magnetization obtained by heating the samples without any applied magnetic field starting from a saturated state.

Finally, magnetotransport measurements performed on Cr_2Te_3 epitaxially grown on graphene/SiC and on Bi_2Te_3/Al_2O_3 will be discussed with the purpose to study proximity effects and the topological Hall effect in these vdW heterostructures [3]. Despite the presence of out of plane chemical bonds in the Cr2Te3 crystal structure, we observe sharp interfaces with vdW materials and the Shubnikov de Haas oscillations in the graphene layer.

This study confirms Cr_2Te_3 and the class of $Cr_{1+x}Te_2$ materials as very promising candidates for future spintronic applications thanks to large scale single-crystalline growth, vdW interfaces with 2D materials and tunable Curie temperature possibly up to room temperature.

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A SCALING LAW FOR CHARGE TRANSPORT IN LAYERED 2D MATERIALS AND ITS APPLICATION TO REDUCED GRAPHENE OXIDE

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Advancements in the field of layered 2D materials not only open new venues for novel applications but they also bring new questions for basic science such as the possible scaling laws for transport in multilayer 2D materials. In terms of dimensionality, these materials lie between 2D and 3D. In addition, they are strongly anisotropic, that is interlayer interactions are much weaker than the intralayer ones. These van der Waals interactions define an extra transport length scale, interlayer diffusion length, which further complicates the transport phenomenon [1]. Motivated by these, we investigate charge transport in multilayer reduced graphene oxides (rGO). Multilayer rGO contain substantial amounts of disorder, which play a major role in transport. We follow a multiscale computational approach bridging first-principles calculations with large scale transport simulations, and investigate the relevant transport scaling laws. We observe a reversal in the hierarchy of transport regimes, between diffusion and localization. Namely, transmission in the localization regime can be higher than the values predicted by the diffusion formula. We also derive a scaling law for resistivity, depending on the number of layers. Our predictions compare very well with the experimental data [2]. Lastly, we show that the multilayer scaling law is valid not only for rGO but other multilayer 2D materials as well.

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GDR HOWDI 2022 MEETING:
2D SWITCHES FOR RF APPLICATION

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The observation of nonvolatile resistive switching in monolayers and multilayers materials [1] is promising for electronic applications. Because of the ultimate thickness of 2D layers, analogue RF switches based on 2D materials shows a favorable scaling of the cut-off frequency versus device size, compared to other emerging technologies [2]. Our RF switches are metal-insulator-metal structures consisting of a vertical junction made of metal electrodes separated by a 2D material. We fabricated devices using CVD grown hexagonal boron nitride (hBN) and molybdenum-disulfide (MoS2). The devices are embedded in a coplanar waveguide for RF measurements. The DC measurements show that the switch is in a high-resistance state until the application of a SET voltage (~2V for the MoS_2 device and ~1.3V for hBN), which brings the device into a low-resistance state. This state persists until a negative bias is applied (RESET) to force the switch into a high-resistance state. This switch being nonvolatile, the state of the switch remains after the voltage pulse, with a retention time that exceed 12 months. From the S-parameters measured in 0.25 to 320GHz band, we found low power loss due to the switch (insertion loss) in the ON state around -1dB @ 300GHz - and large attenuation across the switch in the OFF state (isolation), around -20dB @300GHz. The cut-off frequency $1/2\pi R_{ON}C_{OFF}$ exceeds 100THz. At high-bias, the static I-V characteristics of our devices exhibit a non-linear behavior. We quantify the non-linearity with a 2 tones measurement (F_1=2.365GHz and F_2 = 2.415GHz) from which we extract the Input Third-order Intercept Point (IIP3), which exceed 46dBm for hBN devices and 37dBm for MoS_2 devices. Finally, we demonstrate the potential of our devices for telecommunications applications by conducting a data communication experiment where a 100Gbit/s data rate signal encoded with a QAM16 vectorial modulation at 300GHz carrier was transmitted across our switch.

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A VAN DER WAALS HETEROJUNCTION BASED ON MONOLAYERS OF MoS_2 AND WSe_2 FOR SOLAR WATER SPLITTING

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The production of clean, sustainable and economical hydrogen is one of the major challenges to face the depletion of fossil fuels and their detrimental environmental impacts. Among others, solar water splitting (SWS) has been widely studied as a promising technology for generating carbon-free hydrogen. Here, we propose a monolithic SWS system based on a *Z-Scheme* van der Waals heterojunction (vdWH) using monolayers of transition metal dichalcogenides (TMD) as active core materials (Fig 1). This structure provides the bias required for electrolysis ($V_{oc} > 2$ V) while maximising the absorption of solar energy[1] with small bandgaps. MoS_2 and WSe_2 are *a priori* chosen for the anode and cathode respectively because of their electrochemical[2, 3, 4, 5] and optical[6, 7] properties. Two distinct regions make up the active core. The first is a $MoS_2/hBN/WSe_2$ heterojunction (Fig 2). Hexagonal boron nitride (hBN) is used to isolate the two TMDs[8]. The electrons (holes) photogenerated in WSe_2 (MoS_2) are consumed by the hydrogen (oxygen) evolution reaction. In the second region, hBN is removed to ensure the recombination of the extra carriers (i.e. holes in WSe_2 and electrons in MoS_2). Membranes of mesoporous transparent metal oxides support the heterojunction and enable water to reach the active part. To understand the behaviour of our system, we developed a multiphysics model that computes the solar-to-hydrogen (STH) efficiency of the system. In this model, we use *ab initio* calculation to determine the optical porperties of the active materials and we implement the detailed balance method and the Butler-Volmer kinetics to simulate the photoelectrochemical response. Under realistic operating conditions, the system achieves an STH efficiency greater than 15%. Since our system is wireless and requires simple manufacturing processes (exfoliation), this result is remarkable.

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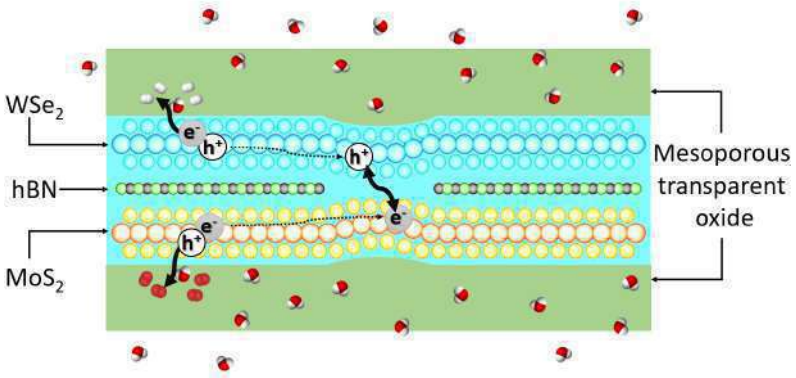

Figure 1: Schematic representation of the SWS system. The active core is based on a $MoS_2/hBN/WSe_2$ vdWH and a MoS_2/WSe_2 vdWH. The former enables the carrier generation and the electrochemical reactions and the latter ensures the extra carriers recombination. A transparent mesoporous oxide supports and protects the active core.

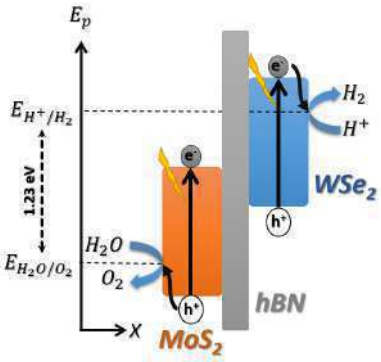

Figure 2: Sketch of the band diagram in the first region where MoS_2 and WSe_2 are isolated by hBN. E_{H^+/H_2} and E_{H_2O/O_2} are respectively the reaction potentials of the reduction of H^+ in H_2 and of the oxidation of H_2O in O_2.

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GDR HOWDI 2022 MEETING: PROXIMITY-INDUCED SPIN-ORBIT PHENOMENA IN GRAPHENE-BASED HETEROSTRUCTURES

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Van der Waals heterostructures consisting on the layered stacking of two-dimensional (2D) materials, enable atomic-scale tunability of electronic properties. They provide great advantages to develop compact hybrid heterostructures, that have led to the emergence of new phenomena not accessible in other platforms [1]. In the field of spintronics, graphene constitutes a promising 2D material because it enables the transport of spin signals over larger distances compared to other systems [2]. However, its low intrinsic spin-orbit coupling prevents spin signal manipulation, which has prevented the fast application of graphene for spintronic devices.

In this talk, I will describe two recent studies performed in graphene-based heterostructures, where we demonstrate that spin signals can be generated and manipulated by means of proximity effects induced by spin-orbit phenomena. In the first part, I will show how the imprinted spin texture in graphene interfaced with a transition metal dichalcogenide give rise to an anisotropic spin relaxation, where the spin lifetime for spins oriented out-of-plane is one order of magnitude larger than those oriented in-plane [3]. In the second part, I will show how such proximity-induced effects can be used to generate spin signals in graphene that can also be controlled by electrical gating with one of the highest efficiencies reported to date at room temperature [4]. These results provide the building blocks for development of ultra-compact devices made of two-dimensional materials.

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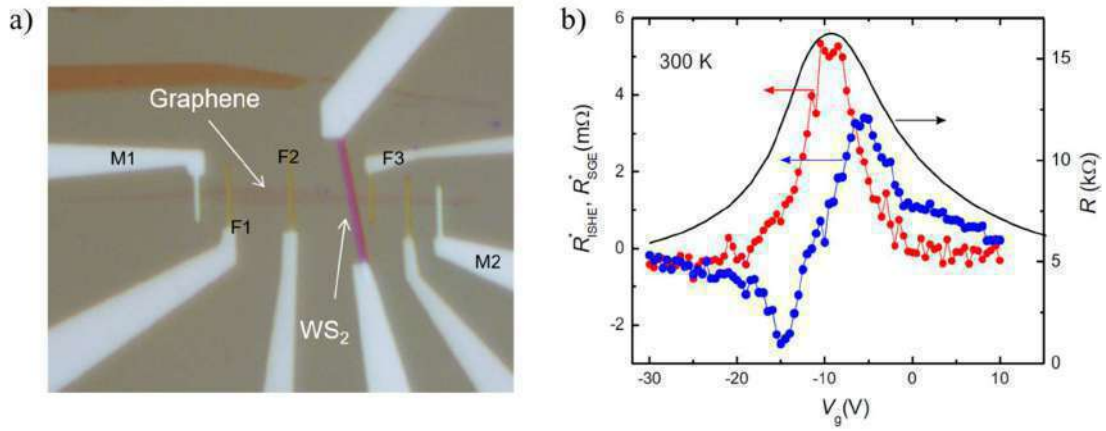

Figure 1: a) Optical micrograph of the graphene/WS_2 heterostructure used for studying anisotropic spin lifetime relaxation in graphene. F1, F2, F3 and M1,M2 are ferromagnetic and metallic contacts respectively. b) Electrical gating dependence of spin signals induced in graphene by proximity effects. Red and blue points display signal amplitudes due to the inverse spin Hall effect (ISHE) and the spin galvanic effect (SGE) respectively. Black line corresponds to the back-gate dependence of the graphene resistance.

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SPIN CURRENT IN VAN DER WAALS FERROMAGNET FE_3GETE_2

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The control of spin current is pivotal for spintronic applications, especially for spin-orbit torque devices. Spin Hall effect (SHE) is a prevalent method to generate spin current. However, it is difficult to manipulate its spin polarization in nonmagnet [1]. Recently, the discovery of spin current in ferromagnet offers opportunity to realize the manipulation [2, 3]. In the present work, the spin current in van der Waals ferromagnet Fe_3GeTe_2 (FGT) with varying magnetization is systematically investigated using *ab initio* calculations [4]. It has been observed that the spin current in FGT presents a nonlinear behavior with respect to magnetization. The in-plane and out-of-plane spin polarizations emerge simultaneously, and the bilayer FGT can even exhibit arbitrary polarization thanks to the reduced symmetry. More intriguingly, the correlation between anomalous Hall effect (AHE) and spin anomalous Hall effect (SAHE) has been interpreted from the aspect of Berry curvature and spin. An effective $k \cdot p$ model illustrates that the orbital hybridization is essential for Berry curvatures. This work illustrates that the interplay of magnetism and symmetry can effectively control the magnitude and polarization of the spin current, providing a practical method to realize exotic spin-orbit torques.

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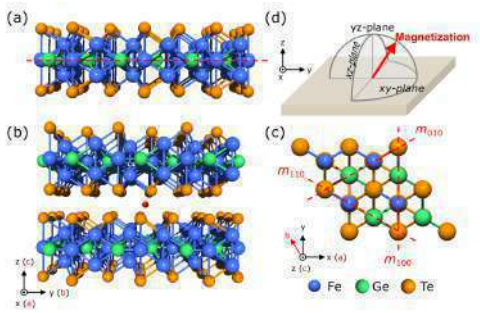

Figure 1: (a) Atomic model of monolayer FGT with a mirror symmetry (the red dashed line). (b) Atomic model of bilayer FGT with an inversion center (the red point). (c) Top view of bilayer FGT including mirror symmetries. (d) Illustration of the magnetization evolution in different planes.

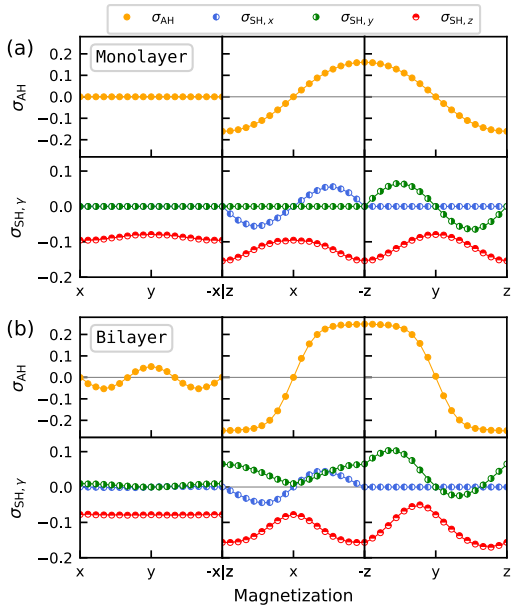

Figure 2: AHE and SHE of (a) monolayer and (b) bilayer FGT with magnetization rotating inside *xy*-, *xz*-, and *yz*-planes. σ_{AH} of *xy*-magnetization is magnified 10 times in (b).

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OPTICAL DETECTION OF LONG ELECTRON SPIN TRANSPORT LENGTHS IN A MONOLAYER SEMICONDUCTOR

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In semiconductor monolayer based on transition metal dichalcogenide, spin and valley degree of freedom of carrier are coupled. Here we report on the observation of spin (and thus valley) transport of electrons over tens of micrometers in a WSe_2 monolayer. The lateral spin diffusion is investigated with an original spatially-resolved pump-probe experiment (described in Fig 1) where a circularly polarized laser yields a very efficient local spin/valley pumping of resident electrons [1], reaching polarization up to 75%. The circular polarization of the photoluminescence of charged excitons induced by a weak linearly polarized probe beam, at a distance d from the pump, is a direct measurement of the two-dimensional electron gas spin polarization. It reaches values as large as 25% for a distance d=20 µm. Measurements as a function of d give a long spin diffusion length of L_s=18 ± 3 µm (shown in Fig 2), resulting from the spin valley locking effect in this transition metal dichalcogenide material. The measured temperature dependence highlights the key role played by the spin relaxation time [2] on both the spin pumping efficiency and the spin transport properties.

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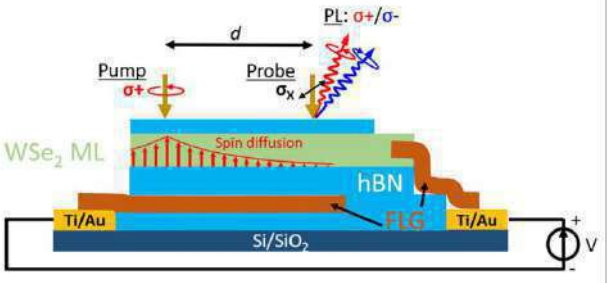

Figure 1: Sketch of the charge tunable WSe_2 ML. Two laser spots (pump and probe) are focused on the sample separated by a distance d. The pump is circularly polarized σ+ and dynamically polarizes the resident electrons in the K' valley with spin up. This spin/valley information propagates over long distances and is detected by a linearly polarized σ_X probe. The circular polarization of the probe-induced X^{S-} and X^{T-} PL provides a quantitative measurement of the polarization of the 2D electron sea at the location of the probe spot.

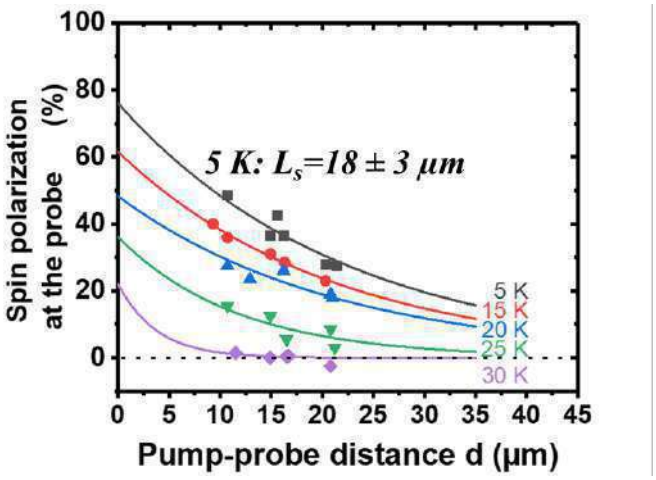

Figure 2: Temperature dependence of the spin polarization of the resident electrons at the probe location as a function of the pump-probe distance, which clearly shows the spin diffusion.

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THEORETICAL INVESTIGATIONS OF OPTICAL PROPERTIES OF 2D SEMICONDUCTORS IN VAN DER WAALS HETEROSTRUCTURES

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Stacking 2D materials to build van der Waals heterostructures provides an interesting approach toward creating artificial lattices with desired band structures and possible new functionalities. In transition metal dichalcogenide (TMD) monolayers the optical absorption is strong, but the transition energy cannot be tuned as the neutral exciton has essentially no out-of-plane static electric dipole. In contrast, for homo-bilayers systems hole delocalization over the bilayer is only allowed in *2H* stacking and results in strong interlayer exciton absorption and also in a larger A-B exciton separation as compared to *3R* bilayers [1]. *GW*+BSE calculation scheme confirm signatures of efficient interlayer coupling for *2H* stacking for the MoS_2 bilayer case [2], when theoretical investigations of interlayer exciton properties for others TMD bilayers show interesting features. Besides, interlayer exciton transitions are widely tunable in applied electric fields [3] allowing to investigate the interaction between intra and interlayer excitons [4].

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INTERLAYER EXCITONS OF $MOSE_2$-WSE_2 HETERO-BILAYERS

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Monolayers of transition metal dichalcogenides (TMDs) exhibit remarkable optical properties. These rely on Coulomb bound electron-hole pairs realising model two-dimensional excitons. Monolayer excitons are characterised by strong optical absorption/emission, combined to binding energies possibly reaching a few 100 meV. Through the photoluminescence (PL) they radiate, excitons are then strikingly observable up to room temperature. In the low temperature limit, the exciton PL reaches the Fourier limit where its spectral width, of around 2 meV, is given by the very fast electron-hole recombination rate. The latter is then characterised by a time constant in the pico-second domain, which excludes that excitonic fluids are studied at thermodynamic equilibrium where quantum statistical correlations possibly emerge at sufficiently low temperatures ($\lesssim$ 10 K).

By interfacing two distinct TMD monolayers, thus realising a so-called hetero-bilayer, minimum energy states for electrons and holes possibly lie in a different layer. This geometry then favours the buildup of interlayer excitons made by opposite charge carriers confined in a distinct monolayer (Fig.1). The overlap between the carriers wave-functions is then greatly reduced so that interlayer excitons have radiative lifetimes extending beyond 100 ns. Furthermore, in hetero-bilayers excitons are characterised by a well oriented electric dipole, given by the separation between electrons and holes. They experience then repulsive dipolar interactions and explore at the same time a periodic two-dimensional confinement. Indeed, a triangular moiré lattice forms spontaneously due to both the mismatch between the monolayers lattice constants and the angle between their crytstalline axis. Remarkably both the period and the depth of the moiré potential are easily tuned by suitable hetero-bilayer engineering. Thus, interlayer excitons in moiré potentials provide a promising platform to explore the physics of the Bose-Hubbard Hamiltonian in the solid-state [1, 2, 3].

Here we study optically a $MoSe_2$-WSe_2 hetero-bilayer encapsulated in hBN (Fig.1). At low temperature ($\sim$5 K) interlayer excitons are directly evidenced by their low-energy PL emission, around 300 meV below that of intralayer excitons of individual $MoSe_2$ and WSe_2 monolayers. Importantly, we probe the role of the optical excitation, by comparing the situation where electrons and holes are non-resonantly injected, by exciting above the bandgap energies of $MoSe_2$ and WSe_2, to a resonant excitation of the $MoSe_2$ excitonic absorption. We observe that the latter excitation optimises both the PL intensity and its spectroscopic features. Thus, at low excitation powers, i.e. for very dilute excitonic fluids, we evidence that the PL spectrum is made of narrow-band emission lines, separated by a few 10 meV (right panel of Fig.1). Performing polarisation resolved excitation/detection spectroscopy, we observe that PL lines display the same degree of circular polarisation as the one of the excitation laser injecting electronic carriers. This behaviour reveals that interlayer excitons are delocalised, nevertheless we also resolve unpolarised PL lines marking the radiative recombination of localised excitons. We then discuss the role that the moiré potential can play in our experiments.

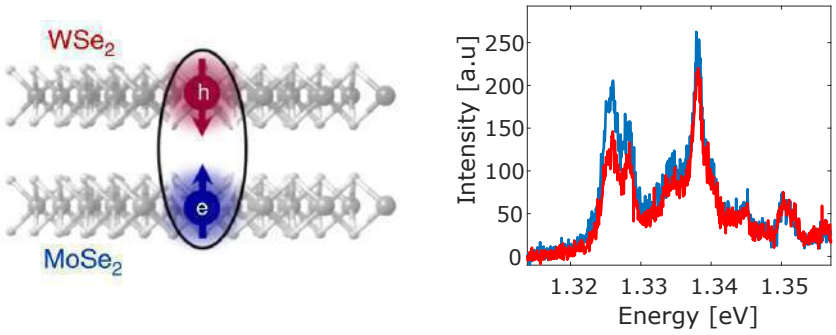

Figure 1: *(left)* We study a $MoSe_2$-WSe_2 hetero-bilayer hosting interlayer excitons resulting from the Coulomb attraction between electrons confined in a $MoSe_2$ monolayer and holes in the WSe_2 one. *(right)* Polarisation resolved PL spectrum of interlayer excitons at 5K. In these experiments electronic carriers are injected by a circularly polarised (σ^+) excitation at 1.62 eV, with an average power set to 50 nW. The PL is collected from the 1 μm wide region which is laser excited. The blue spectrum has the the same circular polarisation as the laser excitation, whereas the red one is detected along the orthogonal one.

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DIELECTRIC SCREENING IN VAN DER WAALS MATERIALS PROBED THROUGH RAMAN SPECTROSCOPY

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Van der Waals heterostructures provide a unique platform to investigate and engineer near-field coupling and proximity effects in two-dimensions. These complex phenomena require sensitive and high throughput experimental probes. In this context, Raman spectroscopy stands out as a powerful characterization tool, that has been widely used to probe strain fields, doping or dielectric screening, in particular in graphene layers [1]. These characteristics can be finely engineered using van der Waals (vdW) heterostructures [2]. Here, using a large variety of graphene-based vdW heterostructures, we show that the well-known Raman 2D mode of graphene is uniquely sensitive to dielectric screening and undergoes a sizeable upshift in excess of 15 cm^{-1} when comparing a bare suspended graphene monolayer with a graphene/transition metal dichalcogenide (TMD) heterostructure (Fig. 2). This upshift stems from the smearing of the Kohn anomaly that affects transverse optical phonons at the K point of the Brillouin zone [3]. Our results show that a single TMD monolayer smears the Kohn anomaly more efficiently than bulk Boron Nitride (Fig. 2).

Interestingly, the Raman G mode of graphene is not affected by this effect (Fig. 2). Preliminary theoretical investigations suggests that this absence of blueshift for the G mode frequency points toward an effect originating from π-bands only, which are symmetry protected from the effects of dielectric screening.

As an outlook we will introduce our ongoing efforts to mechanically tune interlayer coupling in vdW heterostructures and more broadly light-matter interactions in nanomechanical resonators [4, 5] made from suspended graphene/TMD heterostructures.

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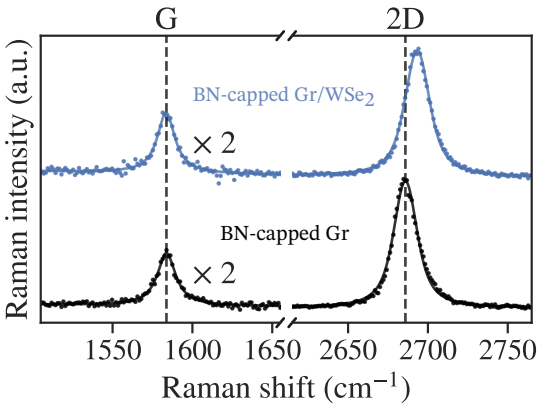

Figure 1: Typical Raman spectrum of graphene for a hexagonal Boron Nitride (BN) capped graphene/WSe_2 heterostructure showing a blueshift of the 2D mode relative to the case of a BN-capped graphene sample.

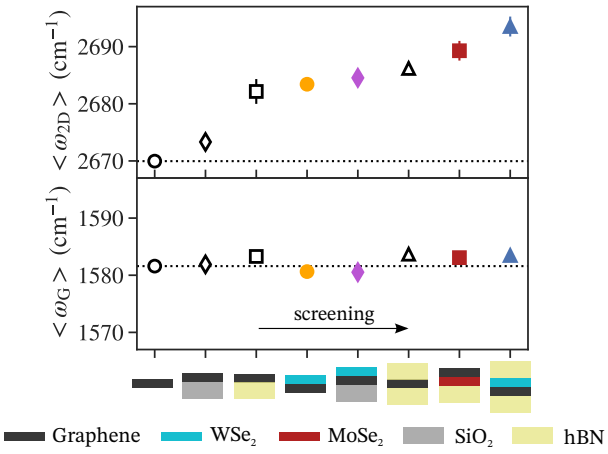

Figure 2: Top (bottom): spatially averaged 2D (G) mode frequency in graphene monolayers in various dielectric environments.

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AB INITIO STUDY OF GRAPHENE/BN VAN DER WAALS HETEROSTRUCTURE: EFFECT OF ELECTRIC FIELD, TWIST ANGLES AND P-N DOPING ON THE ELECTRONIC PROPERTIES

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One of the most important and attractive property of 2D materials is the possibility to design brand-new structures, without a bulk counterpart, with innovative features. These systems, known as Van der Waals heterostructures, are characterized by strong covalent bonds between atoms in the same plane and weak Van der Waals interaction among the layers. The key point in the design of new Van der Waals heterostructures lies in the possibility of finely tuning the optoelectronic properties of the system by changing structural parameters[1, 2] like stacking sequences, number of layers and different rotation angles. This aspect is one of the most widely used approaches in the study of novel graphene-based nanodevices. The aim of this work is to study, via DFT calculations, performed with the Quantum ESPRESSO suite, Van der Waals heterostructures based on graphene and hexagonal boron nitride (hBN), two systems with a very similar crystal structure (they have almost the same lattice parameter), but with totally different electronic properties. The goal is to explore different ways to modify the electronic properties of graphene, altering the dispersion of its band structures near the K point of the first Brillouin zone. Starting from the monolayers, several VdW-hs have been designed changing both the number of layers and their relative rotation angle in the structure. In particular, the attention has been focused on the bilayer phase (CBN-AB), the quadrilayer (CBNBNC), and the coincidence lattice achieved by rotating graphene on hBN by 21.8°. For all these systems stability analysis, structural relaxation, band structure calculation and optical properties study have been performed. The intention is to investigate the changes induced by both the structural design itself and by the external environment, investigating the response to an external electric field. The calculations show a small but significant modification [3] of the electronic properties of graphene and hBN when they are paired in a Van der Waals heterostructures, that results in particular in the opening of a tunable [4] band gap at the Dirac cone of graphene, even if the electronic fingerprint of the starting monolayers is still preserved. The results depict the interaction between the C atoms in graphene layers and the B (or N, according to the stacking sequence) atoms in the BN layer as the main factor affecting the electronic behaviour near the Dirac cones. A proper choice of the stacking sequence can induce in the heterostructure a small intrinsic dipole that can further affect the dispersion of the band structure contributing to the opening of small and finely tunable band gap in the Dirac cones of graphene. This makes graphene/hBN hs exploitable for nanoelectronic applications like in THz devices.

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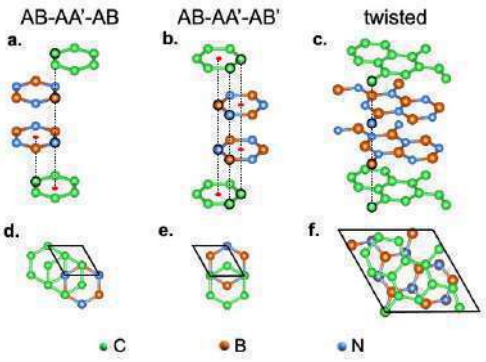

Figure 1: Geometry

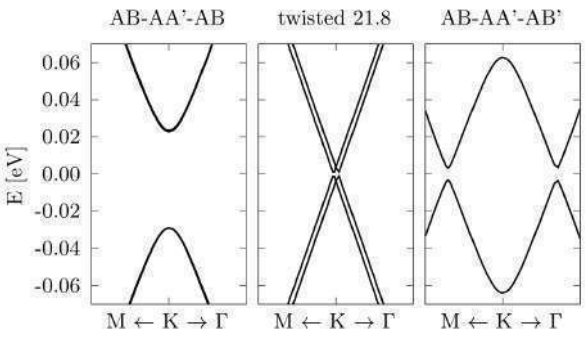

Figure 2: Bands

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1D HETEROSTRUCTURES BASED ON NANOTUBE TEMPLATES: CONFINEMENT OF 6T MOLECULES INSIDE BNNT FOR POLARIZED LIGHT EMISSION.

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Single walled carbon nanotubes (SWCNTs) have been used as a 1D template for assembling various molecules and inorganic compounds into well-defined shapes, thanks to their hollow, crystalline and cylindrical architectures.

In the context of fluorescent molecules assembly, it was unfortunately demonstrated that the overlap of the emission bands of the adsorbed dyes with the absorption bands of semiconducting nanotubes in the visible range (2-3 eV) leads to effective energy transfers that both readily quench the dyes fluorescence and sensitize the nanotube host. As an alternative, boron nitride nanotubes (BNNT) have been identified as a promising host template for fluorescent molecules because of their dielectric nature with wide-gap semiconductors of ~5.5 eV, opening the way for the design of fluorescent nano-hybrids.[1]

In this presentation we will focus on the impact of local order and stacking configuration of sexithiophene (6T) dyes confined inside BNNTs on the polarization properties of the fluorescence of the 6T: Combining ac-HRTEM and polarized fluorescence imaging on individual BNNT, we show that the fluorescence from the 6T assembly is stable and strongly polarized with extinction ratios as high as 700 at room temperature.[2] A statistical analysis of the 6T orientations inside BNNTs with inner diameter up to 1.5 nm shows that 80% of the encapsulated 6Ts exhibit a maximum deviation angle of less than 10° with respect to the BNNT axis.

Furthermore, our results reveal that the BNNT wall drives the alignment of the 6T by preferential adsorption in the competition molecule-molecule and molecule-BNNT interactions.

Finally, we show that the polarization properties at the nanoscale in 6T@BNNT can be expanded in thin films based on aligned 6T@BNNT inside polymeric matrix.

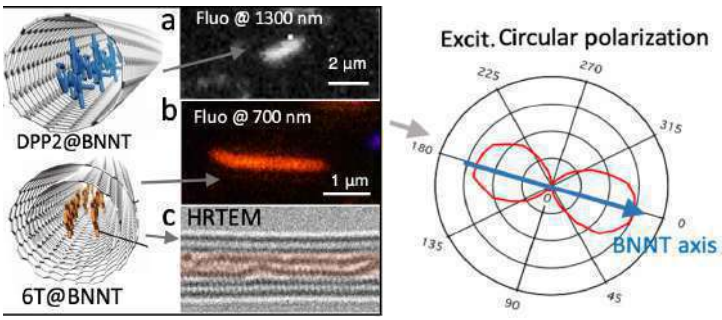

***Figure 1** : right **(a-b)** NIR bio-nanoprobes fluorescence pattern based on Dyes@BNNT. **(c)** Aberration corrected HRTEM image of a 6T@BNNT heterostructure. Left. Polarized fluorescence patterned from 10^3 molecules confined and aligned inside a BNNT*

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Diameter-dependent single- and double-file stacking of squarylium dyes inside single-wall carbon nanotubes

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The filling of single-wall carbon nanotubes (SWCNTs) with dyes has become a novel path to add and create new functionalities through the mutual interaction between the confined dyes and host SWCNTs. In particular cases, the encapsulated dyes form strongly interacting molecular arrays that result in severely altered optical properties of the dyes[1–3]. In this work we report for the first time the combination of extensive chirality-sorting[4] and dye filling, leading to the isolation of nearly single chiraliy squarylium-filled SWCNTs as shown in the photoluminescence-excitation (PLE) map presented in Figure 1.

For each dye@SWCNT chirality combination we observe a different absorption wavelength of the confined dyes, originating from the different dye stacking driven by the diameter of the surrounding SWCNT. This diameter-dependent dye absorption is experimentally determined through the measurement and detailed fitting of fluorescence-excitation maps of different chirality-sorted dye-filled SWCNT samples, where for each dye@SWCNT combination a different energy transfer peak is observed.

We therefore demonstrate that the diameter of the SWCNT is a lever to tune optical properties of the hybrids, paving the way for future applications in optoelectronics. Moreover, comparison with molecular models provides access to the possible different stacking configurations of the dyes inside the hollow space of SWCNTs with different diameters.

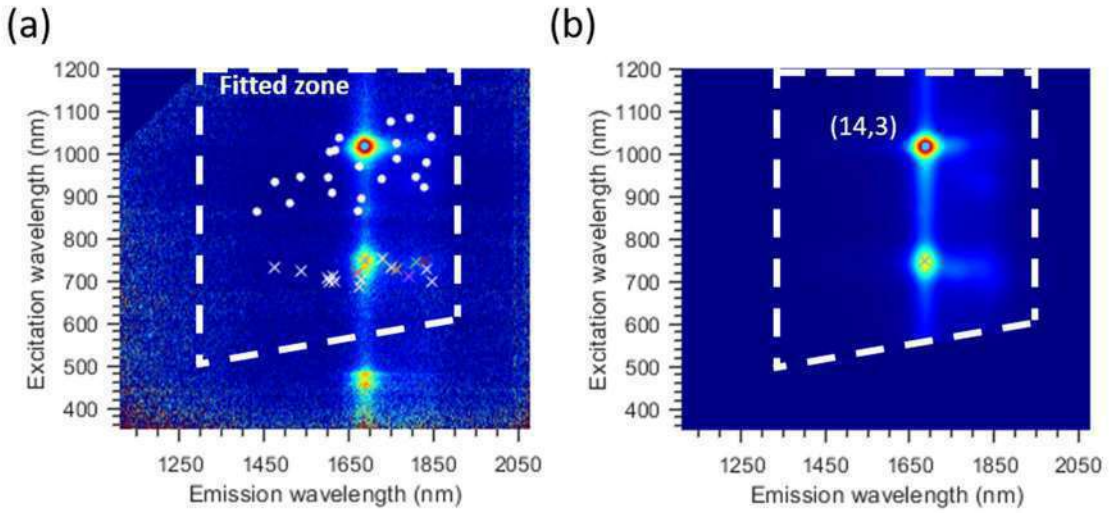

Figure 1 Example of a PLE map and the corresponding fit for one of the 15 samples: (a) Experimental PLE maps; The white dots represent all the chiralities that have been fitted and the crosses represent the energy transfer peaks. (b) Fitted PLE map, the most abundant chirality is labelled.

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SINGLE-WALLED CARBON NANOTUBES CHARGE MANAGEMENT BY CONTROLLED FUNCTIONALIZATION

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Managing the density of charges in carbon nanotubes opens new ways to tune their optical response, their transport properties, and their physico-chemical features. Charge transfer from molecules adsorbed onto the sidewall or filled within the hollow cavity of the nanotubes has already been demonstrated, yet a fine-tunable control of the surface coverage/filling fraction (and thus the amount of transferred charge) remains challenging to achieve. Alternatively, we developed an optically nonperturbing covalent functionalization technique based on the inclusion of a triazine derivative into the carbon network [1]. The nitrogen atom sustaining the attached group becomes an integrated part of the pi-conjugated network and contributes with its lone electron pair to uplifting the position of the Fermi level of the tube. Since the density of attached groups can be varied by adapting the synthetic conditions, this technique offers the advantage of controlling the amount of charge injected into the tubes. Additional groups attached onto the other end of the triazine moiety, moreover, are able to inject charge into the tubes as well. This, for example, allowed us to modulate the photoluminescence of the tubes, switching their emission on and off through the attachment of the switchable spiropyran/merocyanine system [2]. Here we focus on a class of charge-transfer agents that either donate or withdraw electrons depending on the arrangements of their building units [3] and how their decoration affects the properties of the tubes.

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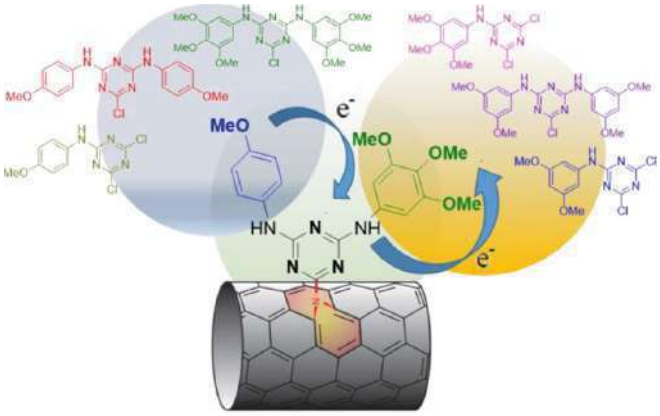

Figure 1: Different number of methoxy groups can be attached onto aniline at different positions, resulting in compounds that can either donate or withdraw electrons from the tubes they are attached onto [3].

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ULTRAFAST GENERATION OF ACOUSTIC WAVES IN WATER MEDIATED BY A CARBON NANOTUBE

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Photoacoustics, the study of acoustic waves triggered by an ultrafast laser pulse, gained new interest with the use of nanoparticles as transducers, with novel applications in biological systems where they can be introduced as imaging, thermal or mechanical agents with high localization and selectivity [1, 2]. Most approaches rely on water-dispersed metallic nanoparticles excited by nanosecond pulses and involve a photothermal effect. The laser pulse triggers an impulsive temperature rise in the nanoparticle, followed by the fast temperature increase of the surrounding water, leading to its thermal expansion and the launching of a pressure wave in water. However, the physics can significantly differ when dealing with carbon nanotubes (CNT).

Here, we theoretically investigate the transient photothermal and photoacoustic response of a CNT, multi- or single-walled, immersed in water. Given the time and length scales involved, the system requires a multi-physics, multi-scale approach [3]. Our simulations follow step-by-step the photo-thermal-acoustic stages involved, thus combining the optical, heat transfer and thermo-acoustic phenomena. The macro-physics equations are solved via Finite Element Methods with insertion of relevant microscopic parameter values, such as the CNT-water interface thermal boundary resistance [4] retrieved from dedicated molecular dynamics (MD) simulations [5].

The CNT geometry and laser pulse duration characteristics are discussed for the effective generation of propagative pressure waves in water. Most interestingly, we observe the emergence of a competitive new mechanism, which involves the generation of periodic vibration or impulsive dilation in the CNT upon pulsed excitation, and the direct mechanical launching of a pressure wave in water.

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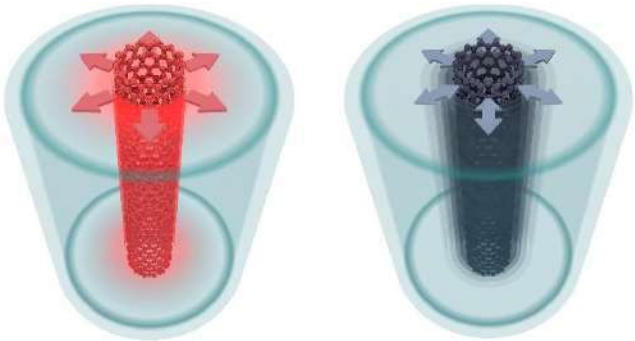

Figure 1: Schematic representation of the mechanisms for pressure wave generation in water upon nanotube pulsed light excitation. (Left) Wave triggered by photothermal dilation of surrounding water, referred to as thermophone. (Right) Wave triggered by mechanical expansion of the nanotube, referred to as mecanophone.

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Optical properties of h-BN: from bulk to monolayer

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Hexagonal boron nitride (h-BN) is a 2D material, iso-structural to graphite, with a wide band gap (~6eV). In 2004, h-BN demonstrated its ability to efficiently emit light in the deep ultra-violet (DUV) after the synthesis of high quality h-BN crystals in Japan [1]. The demonstration of lasing at 215 nm make of h-BN one of the most promising materials for DUV optoelectronics. However, its fundamental opto-electronic properties have not been fully understood.

In 2016, two photon-spectroscopy demonstrated that its fundamental exciton is of indirect nature and the resulting recombination process is assisted by phonons along M→K [2]. Nevertheless, there is a direct exciton at the K point with an energy slightly above the fundamental one. The interplay between the indirect and direct excitons in bulk h-BN was not fully understood because reflectivity and absorption experiments have been very limited in hBN. During this talk, I will present reflectivity measurements performed on bulk h-BN crystals at cryogenic temperatures and for an energy range between 5.5 eV and 7 eV. These results show the contribution of the indirect and direct excitons to the absorption process of bulk h-BN and reveal the effect of electronic flat bands to its optical response [3].

In h-BN, like in other 2D materials, when reducing the dimensionality from a 3D system (bulk) to a 2D system (monolayer), the nature of the gap changes. The calculations show a change from an indirect gap (bulk) to a direct gap (monolayer). This indirect-direct gap transition has never been observed in h-BN, and consequently the opto-electronic properties of the monolayer have never been studied experimentally. During this presentation, I will show the first experimental evidence of a direct gap transition in monolayer h-BN by presenting photoluminescence and reflectivity measurements performed on BN monolayer (mBN) grown by Molecular Beam Epitaxy (MBE) at high temperature on graphite substrates. Our results demonstrate for the first time the presence of an optical transition at 6.1 eV associated to the direct gap in mBN [4].

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Optical characterization of exfoliated monolayer boron nitride by means of hyperspectral microscopy in the deep-UV

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Hexagonal boron nitride (hBN) is an important material in many today technology [1] since the first fabrication of large single crystals by Watanabe et al. [2]. More specifically, hBN is a lamellar material made of sp2 bonded planes stacked through van der Waals interactions, which can be easily separated down to monolayer. This 2D material is a key compound in van der Waals heterostructures used both as a perfect dielectric barrier or as encapsulating layer to improve the properties of surrounding 2D materials [3]. Nonetheless, despite its large range of applications, little is known about the physic inherent to hexagonal boron nitride thin films and the monolayer [4].

By means of hyperspectral photoluminescence spectroscopy in the deep UV, we studied the optical properties of exfoliated hBN thin films down to a monolayer near the band gap energy (6eV) [5]. The hyperspectral images obtained allows us to identify distinct spectral signatures which, by comparing their spatial distribution to AFM data, are unambiguously associated to monolayer, few-layers and stacking faults emissions. We then observe modulations of the hBN photoluminescence spectrum with thickness and a strong bandgap crossover at the monolayer limit with a direct emission around 6.1eV. This work should bring a better understanding of the intrinsic properties of thin films boron nitride down to the monolayer.

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GDR HOWDI 2022 MEETING:

Exciton-phonon coupling and optical properties in hexagonal-BN

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Hexagonal boron nitride is an indirect band gap material with a strong luminescence intensity in the ultraviolet. This luminescence originates from bound excitons recombination assisted by different phonon modes[1.2]. The coupling between excitons and phonons is so strong that the resulting light emission is as efficient as the one of direct band gap materials[3]. In this talk I discuss different theoretical approaches to calculate exciton-phonon coupling and phonon-assisted luminescence[1.2]. Then I'll show how external strain[4], pressure[5] and the presence of a substrate[6] modify the coupling between excitons and phonons and the corresponding absorption/luminescence spectra.

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ATOMIC SCALE MAPPING OF THE ELECTRIC FIELD IN 1D AND 2D BN NANO-STRUCTURES BY 4D-STEM

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Variation at atomic scale of the electric field in 1D and 2D materials plays a key role in defining physical and chemical properties namely reactivity, interfaces effects and molecule rearrangement. However, the imaging of electric field fluctuations with single atom sensitivity still represents a challenge.

In this regard, four-dimensional scanning transmission electron microscopy imaging (4D-STEM) has recently appeared as a promising technique. In 4D-STEM experiments at every probe position a 2D convergent beam electron diffraction pattern is acquired, generating a 4D dataset. The displacements of the center of mass (COM) of the diffraction pattern is linked to the interaction between the electron beam and the electrostatic field as it propagates through the material. In case of weak phase objects, this technique is in principle quantitative providing space variation down to the atomic scale. This method has been successfully employed in the study of perfect and defective 2D materials but up to now only qualitative results have been presented without a precise estimation of the electric fields.

In this work, we present 4D-STEM analysis performed on several boron nitride (BN) based 1D and 2D structures, going from single and multi-walled nanotubes to mono and few layers h-BN crystals. We measure the electric field at sub-atomic scale, and we study its dependence as a function of the number of layers in few layers h-BN and curvatures effects in BN nanotubes. Furthermore, we investigate field modulations in presence of defects such as vacancies, adatoms and flake edges. These experimental results show an excellent agreement with theoretical estimation obtained from first principle simulations.

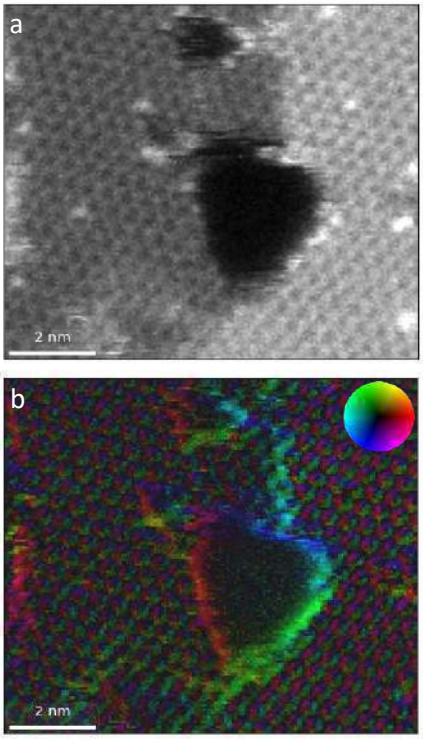

Figure 1: (a) ADF and (b) electric field orientation map images large defects and adatoms in a multi-layer h-BN.

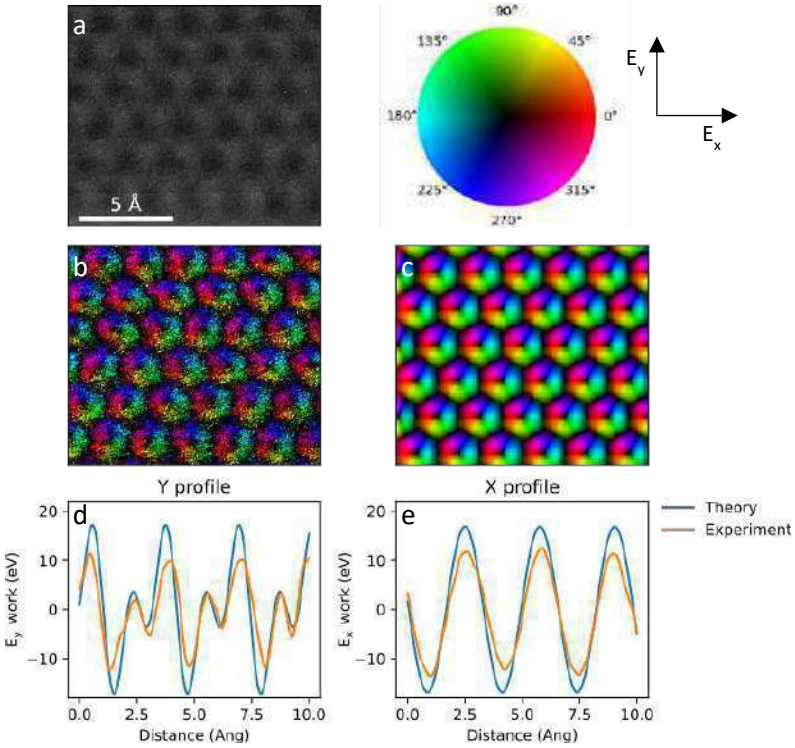

Figure 2: (a) ADF image and (b) electric field orientation map of h-BN monolayer compared with the electric field obtained by DFT integrated over the direction of propagation of the electrons (c). (d,e) Profiles of the electrical field intensity extracted along x and y direction.

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COHERENT JETTING FROM A GATE-DEFINED CHANNEL IN BILAYER GRAPHENE

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The quest to precisely control the valley degree of freedom to store, transport and readout binary information has been an important drive in valleytronics for more than a decade [1,2].
Using scanning gate microscopy, we image valley-polarized jets emanating from a gate-defined constriction in bilayer graphene at a mutual angle of 60°. The jets become visible via their interference pattern, and we observe no significant reduction of the conductance along the jets. We find that the angular distribution of the jets originates from a dispersion-related collimation of electron trajectories due to the trigonally warped bandstructure of bilayer graphene. The momentum distribution in the lowest-energy modes of the constriction enhances this collimation further and selectively activates the jets. This is in strong contrast to the small-angle scattering origin of electron branching observed in similar measurements on Ga(Al)As heterostructures [3, 4]. For arbitrary orientations of the channel with respect to the crystallographic orientation of the bilayer graphene, the jets may appear deformed. However, the angular distribution of the jets is a universal feature arising from the trigonally warped bilayer graphene dispersion and is stable against varying channel orientations, except for angles of 30°.
The general origin of the jets makes our observation relevant for carrier transport in all two-dimensional materials with a trigonally warped bandstructure, and opens new avenues for the design of novel quantum devices in various van-der Waals heterostructures, including bi- and multi-layer graphene [5], MoS_2 [6] and many more.

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PINCH-OFF RESISTANCE AND SCHWINGER EFFECT IN HBN-ENCAPSULATED GFETS

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Electronic transport in hBN-encapsulated graphene field effect transistors (GFETs) has already been characterized in details. [1] With increasing bias, the ohmic regime is first superseded by a velocity saturation regime due to electron scattering with optical phonons of hBN and graphene. Then, further increasing the bias leads to the appearance of an interband current due to Zener-Klein tunneling [2]. These phenomena are well-established in the doped regimes. (Figure 1, negative bias region)

However, near charge neutrality, we cannot ignore that the potential drop along the channel results in non-uniform chemical potential and doping profiles. These inhomogeneities play a critical role and give birth to peculiar transport properties at large bias. [3] As an illustration, in semiconductor MOSFETs, the application of a large bias nucleates an electronic depletion in the channel at the drain electrode. In graphene, a Dirac pinch-off (DPO) occurs as well, but the depletion region is limited due to the absence of gap. (See illustrations on fig. 1, and positive bias region)

We report on the low temperature experimental study of a high mobility hBN-encapsulated GFET with a close graphite backgate. The DPO occurs when the gate and drain voltages are equal, resulting in a zero charge carrier density at the drain side. At DPO, we observe a current plateau with bias which corresponds to a differential resistivity peak. Surprisingly, we observe that the resistance peak increases by two orders of magnitude (resistivity 400Ω→20MΩ) when increasing the gate voltage. This points to the formation of an insulating phase in the DPO region (~ 100nm) with electric fields around 10^7 V/m. At larger bias, an exponentially fast decrease occurs when reaching the bipolar regime.

We interprete the resistance peak as the result of an electronic field focusing effect. Beyond DPO, conductance is restored thanks to electron-hole pair creation at the drain side. This last regime is quantitatively described by the Schwinger theory of particle-antiparticle pair creation and makes the DPO regime an analogue to the breakdown of a relativistic vacuum in QED. Additional measurements of shot noise at DPO support this interpretation

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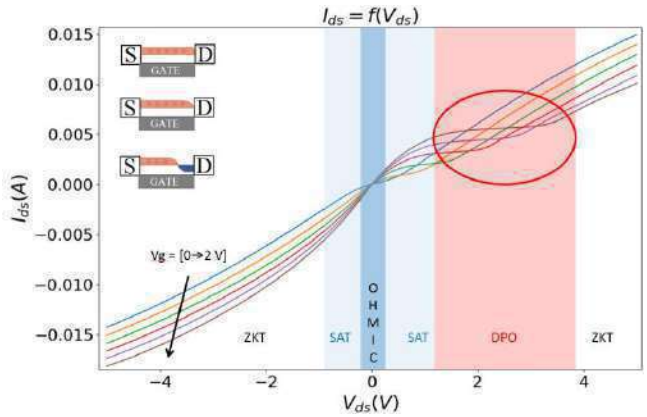

Figure 1: Experimental I-V curves of the GFET at various gate voltages showing the different transport regimes: ohmic behaviour, velocity saturation (SAT), Zener-Klein tunnelling (ZKT), and Dirac Pinch-off (DPO) in the positive bias region. Inset shows the doping profiles along the channel before DPO, at DPO and after DPO with positive doping (resp. negative) in red (resp. blue)

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ELECTRONIC WHISPERING-GALLERY RESONANT TRANSPORT IN GRAPHENE P-N JUNCTION

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Owing to the relativistic nature of charge carriers, electronic transport in graphene p-n junctions exhibits several features analogous to light rays in optical media, thus making them an ideal platform for developing electron optics devices [1]. Remarkably, the electron confinement in graphene circular p-n islands favors high angular momentum states, leading to rich geometrical patterns decorating the local density of states. In particular, the whispering gallery modes (WGMs) have been experimentally observed [2], offering promising perspectives to create a new class of sensors, owing to the inherent sensitivity of these geometrical resonances. However, exploiting these highly sensitive resonances requires the transduction of WGMs to the outside world through source and drain electrodes, a yet unreported configuration. A movable and tunable circular p-n island has been demonstrated in an encapsulated graphene using the polarized tip of a scanning gate microscope [3]. In addition, the quasi-confinement of Dirac fermions forming WGMs can be optimized by changing the potential barriers smoothness, *i.e.*, changing the tip-to-device distance [4]. Using numerical simulations, we demonstrate in this work [5] that by squeezing the created p-n island in an etched constriction, the device (Fig.1a) allows probing selectively the resulting WGM signatures (Fig.1b) in in-plane electronic transport, which translate as oscillations in the device resistance (Fig.1c). In addition, we explore selectivity of the active mode by displacing the p-n island with respect to the constriction. These results are experimentally confirmed by our transport measurements (*e.g.*, see Fig.1d), thereby constituting a proof of concept for graphene whisperitronics devices.

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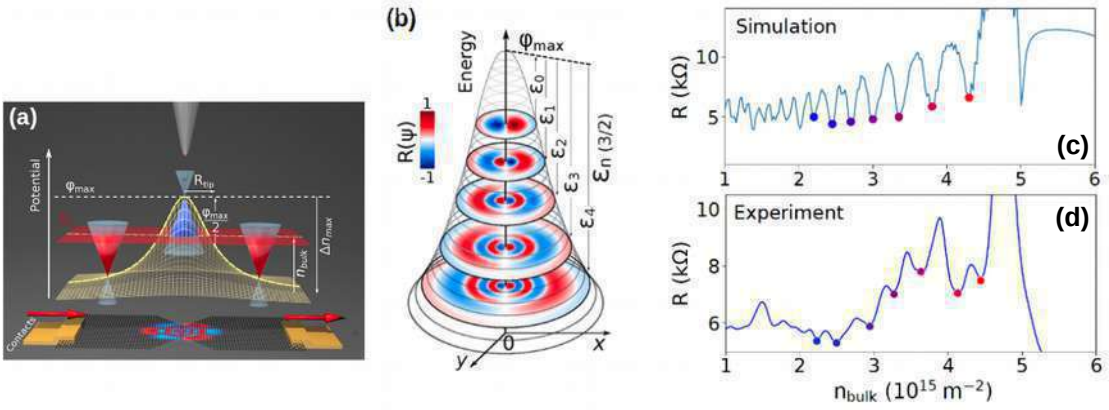

Figure 1: **(a)** *Model of the considered whisperitronics device: a polarized AFM tip is scanned above a constriction etched in a graphene device.* **(b)** *Wave function corresponding to the WGMs with angular momentum m = 3/2, for its different resonant energies.* **(c,d)** *Resistance of the device as a function of bulk carrier density, i.e., when tuning the back-gate voltage. The tip is placed above the center of the constriction.*

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AB-INITIO SIMULATION OF PHONON-ASSISTED ELECTRON TRANSPORT IN VAN DER WAALS HETEROSTRUCTURES

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Van der Waals (vdW) heterostrures are a promising option to design innovative electron devices due to their low defect densities, large tunneling currents and optimal electrostatic control [1]. In this work, we propose a first-principles study of electronic quantum transport in a vdW heterostructure tunnel-FET sketched in Fig. 1. In order to rigorously describe the material properties and quantum phenomena governing this device, we adopted a full *ab initio* methodology, and employed a density functional theory (DFT) Hamiltonian to self-consistently solve the quantum transport equations within the non-equilibrium Green's function (NEGF) formalism by coupling them with the 3D Poisson equation [2].
We focused on the system composed by 1T-$HfSe_2$ and 1T-SnS_2, two TMDs with a type II band alignment[3] and close to type III as illustrated by Fig. 2. To include dissipative scattering due to the electron-phonon interaction in our transport calculations, we first performed density functional perturbation theory (DFPT) and found that the dominating mode is the longitudinal optical (LO) phonon mode. We approximated the Fröhlich interaction of LO polar phonons through an effective deformation potential equivalent to the scattering rate computed with the 2D model of Ref. [4]. Phonon scattering was then included in the NEGF code with local self-energies and adopting the self-consistent Born approximation (SCBA).
Figure 3 shows the computed transfer characteristics for different values of the LO phonon scattering rate. It can be noticed that a stronger el-ph interaction degrades the sub-threshold swing and moreover it can increase the on-state current. These behaviors can be explained by inspecting the spectral current shown in Fig. 4 and Fig. 5 for the off- and on-state, respectively. The former highlights the role played by phonon absorption in the overlap region in increasing the off-state current, the latter illustrates the phonon emission in the drain responsible for inter-valley scattering and consequently in a current higher than in the ballistic case.

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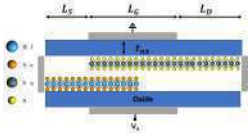

Figure 1: Sketch of the vdW Tunnel-FET with source/drain length of $L_{S/D}$=8 nm, and gate length of L_G=15 nm.

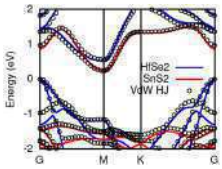

Figure 2: Band structure of 1T-SnS_2 and 1T-$HfSe_2$ and their VdW heterostructure

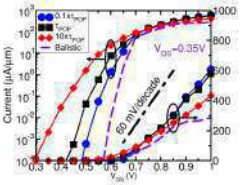

Figure 3: I-V curves for different scattering rate. V_{DS}=0.35 V.

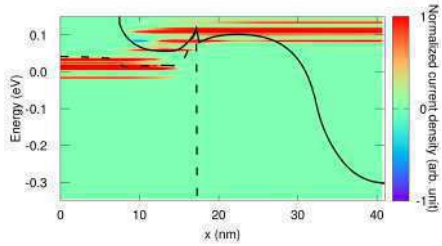

Figure 4: Spectral current density along the device in the off state.

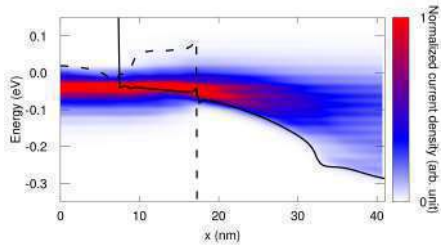

Figure 5: Spectral current density in ON state with a scattering rate at $10\times\tau_{POP}$

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Single photon emitters in hexagonal boron nitride for scalable quantum photonics

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In the context of photonic quantum information science, hexagonal boron nitride (hBN) has recently emerged as a very promising material. The bidimensional character of hBN renders it attractive for the realisation of compact heterostructures and integrated photonic devices. Moreover, this wide-gap material has been recently shown to host single photon emitters (SPEs) with appealing optical properties in the red and near infrared regions [1]. However, these deep defects 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.

Here we demonstrate a new approach towards deterministic positioning of SPEs with similar emission wavelengths, based on irradiation with an electron beam [4]. The SPEs are locally activated in exfoliated hBN flakes using a focused electron beam and subsequently characterised using microphotoluminescence (fig. 1). They exhibit narrow linewidth at low temperature (below the ~ 100 µeV resolution of the spectrometer) and a drastically reduced ensemble distribution of their emission wavelength ($\Delta\lambda < 1$ nm). Individual emitters display low $g^{(2)}(0)$ as well as high and stable count rates. Moreover, emission is observed up to room temperature.

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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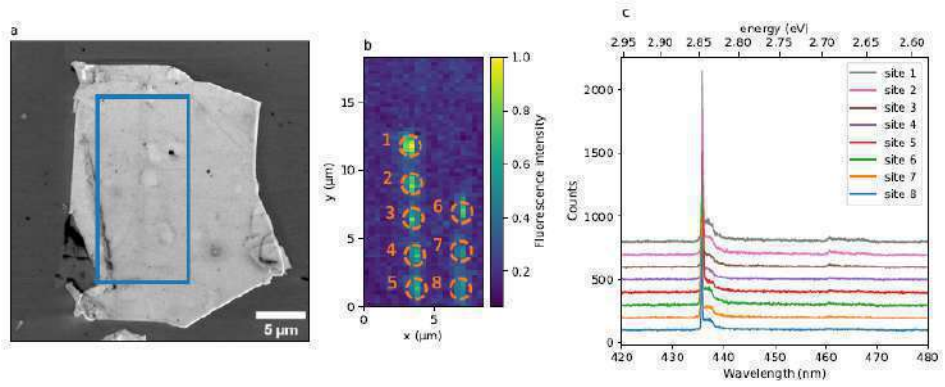

Fig. 1: hBN flake with eight irradiation sites and corresponding confocal map and spectra, displaying reduced statistical dispersion of the emission wavelength.

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OPTICAL SIGNALS OF QUBITS IN DEFECTED 2D TMDS

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Hard to avoid even in the best quality samples of 2D materials, vacancies and impurities are often present, even at non-negligible concentrations[1,2]. Their presence will alter intrinsic properties, so it becomes crucial to understand how we can take advantage of the presence of defects to generate functionality. In this work we employ many-body perturbation theory to obtain the optical absorption spectra of defected transition metal dichalcogenides using the yambo code[3]. New optical features arise in the presence of vacancies, especially in the largely unreported metal vacancies[4]. These show a large manifold of sub-optical-gap excitons, whose wave-functions are highly localized, making them good candidates for quantum dots. For the cases where isovalent substitutional defects are present, both the spin texture and the pristine excitonic energies are preserved, despite the strong interaction with the defects. There is, however, some redistribution of spectral weight between the A and B excitons which is visible in both cases and may allow for the quantification of the defect concentration. With this work we establish how excitonic signatures characterize defects in 2D materials and highlight vacancies as qubit candidates for quantum computing.

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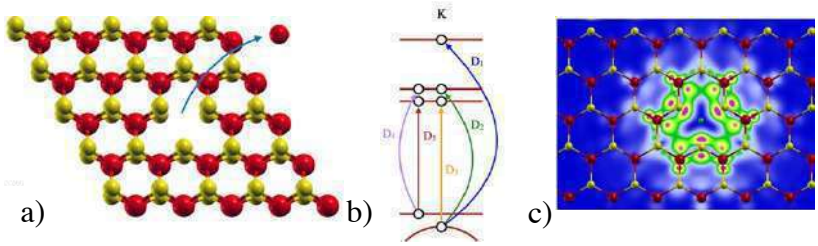

Figure 1: Removal of a tungsten ion (a) on a WS_2 monolayer leads to new, defect-bound in-gap states (b) in the electronic structure. These are responsible for new optical features in the absorption spectrum and lead to the formation of strongly localized qubits (c).

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OPTICAL INVESTIGATION OF C96 GRAPHENE QUANTUM DOTS

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2D graphene has established itself as an essential material in nanoelectronics thanks to its unique physical and electronic properties but suffers from an incompatibility for semiconductor applications due to its gapless electronic band structure. In this context, graphene quantum dots (GQDs), nano-pieces of graphene with a non-zero gap, is a fertile playground for controlled tunability of electronic properties. Bottom-up synthesis has enabled a precise control of the size, shape and edges of these objects, a crucial step towards the controlled engineering of their electronic properties [1]. Room-temperature experiments at the single-object level on a C_{96} triangular GQD (Fig. 1) have demonstrated bright and stable single-photon emission [2], giving promising prospects for its use as a quantum emitter at room-temperature.

Nevertheless, the fully unleash the potential of GQDs, important work remains ahead to understand their photophysics deeply. For example, theoretical calculations recently revealed that the fluorescence might arise from a symmetry-breaking of the GQD via vibrational deformations of the molecule, enabling appreciable emission from dark states [3]. In the perspective of unraveling the vibrational modes of the molecule, we performed low-temperature single-molecule experiments on the C_{96} GQD. By providing spectral resolution via spectral line-narrowing as shown in Fig. 2, this allows us to identify vibrational modes of the GQD. We thus discussed the nature of these modes and compared to theoretical predictions [4]. These results not only represent an important step towards deep understanding of the photophysics of GQDs, but also deliver new tools to unambiguously identify these objects for single-molecule experiments.

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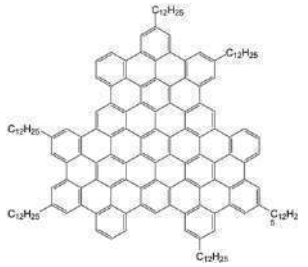

Figure 1: Chemical structure of C96 GQD.

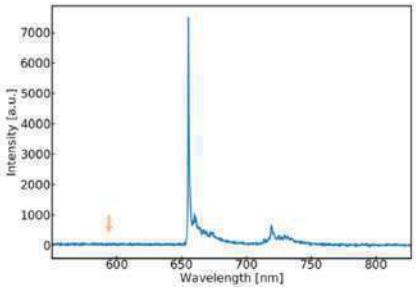

Figure 2: Low-temperature (7K) spectrum of C96 GQD (excited at 594nm).

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Posters session I – Tuesday, May 10

1.	Andrieux-Ledier A.	*CVD synthesis of sp2-hybridized multilayer boron nitride films*
2.	Baux D.	*Optical properties of metallic carbon nanotubes*
3.	Berciaud S.	*Exciton dynamics in atomically thin heterostructures made from graphene and transition metal dichalcogenides*
4.	Beret D.	*Effective negative diffusion of charged exciton in WSe2 monolayer*
5.	Canonico L.	*Nonlocal signals of orbital angular momentum transport in graphene*
6.	Caputo L.	*First-principles electronic and structural properties of bnc nanomaterials*
7.	Chapuis N. & Wallart X.	*GaP(111)B-Se surface for TMD epitaxial growth*
8.	Chiout A.	*Straintronics in 2D semiconductors*
9.	Costanza M.	*Electrical properties of graphene transferred on lithium niobate substrate*
10.	Cummings A.	*Design and optimization of graphene photothermoelectric detectors*
11.	Dieng M.	*Wet-chemical non-covalent functionalization of CVD-graphene: molecular doping and its effect on electrolyte-gated graphene field-effect transistor characteristics*
12.	Elias C.	*Optical spectroscopy of nonplanar graphene nanoribbons with fjord edges*
13.	Fiebor A.	*Photoswitching molecular conjugation on single-walled carbon nanotubes*
14.	Fournier C.	*Electrical control of deterministically-positionned quantum emitters in hBN*
15.	Galafassi R.	*Novel spectroscopic detection of reversible collapse of single walled carbon nanotubes at high pressure*
16.	Gautam S.	*Exciton dynamics study of hBN by time-resolved cathodoluminescence*
17.	Gloppe A.	*Magnon-exciton proximity coupling at a van der Waals heterointerface*
18.	Grillo S.	*Ab-initio investigation on the evolution of the electronic and optical properties of meta-stable allotropic forms of 2D tellurium of increasing number of layers*
19.	Hemmat M.	*Ultrafast terahertz photocurrents in semi-metal and semiconductor few layer PtSe2*
20.	Henrard L.	*Optical response of corrugated 2D materials and heterostructures*
21.	Lizee M.	*Phonon drag-electric current generation at the liquid-graphene interface*
22.	Marceau J.-B.	*Highly polarised fluorescent pattern of encapsulated dyes in BNNT: from nanoscale to thin film*
23.	Marty L.	*Laser heating of suspended graphene*
46.	Zhao M.	*Nanoscale wetting films on 2D materials*

Poster session II – Wednesday, May 11

24.	Mastropasqua C.	*Uniform cvd of graphene on 2'' SiC wafer*
25.	Matsoso J.	*Role of heteroatom domains on VOCs recogniton on B/N co-doped graphene*
26.	Medina Dueñas J.	*Copropagating edge states produced by the interaction between electrons and chiral phonons in two-dimensional materials*
27.	Milton K.	*Towards modelling realistic WS2/H2O/SiO2 interfaces*
29.	Pashayev S.	*Experimental methods for nanofluidics: focus on sealing technology for delicate nanomaterials*
30.	Pawbake A.	*High pressure tuning of the magnon-polaron resonance in the layered antiferromagnet FePS3*
31.	Pierret A.	*Dielectric permittivity, conductivity and breakdown field of hexagonal boron nitride`*
32.	Rajaji V	*Phonon signatures of graphene based systems under high-pressure conditions: suspended versus supported geometries*
33.	Rousseau A.	*First observation of bernal boron nitride single crystals*
34.	Roux S.	*Self-trapped excitons in twisted hBN heterostructures*
35.	Saïd Hassani S.	*Growth of hBN single crystals at atmospheric pressure*
36.	Schraeder C.	*CVD-graphene based transistor microarrays for biodetection of nucleic acid sequences*
37.	Serrano Richaud E.	*Modelling electronic and optical properties of graphene and boron-nitride nanoribbons*
38.	Sohier T.	*Mobility of gated TMDs as a function of valley profile*
39.	Susana L.	*X-ray excitated optical luminescence of boron nitride materials*
40.	Tharrault M.	*Ultra wide-band NIR-VIS micro-absorption characterization of PtSe2 thin films*
41.	Tailpied L.	*CVD synthesis of sp2-hybridized multilayer boron nitride films*
42.	Vu V. B.	*Theoretical studies of novel graphene based nanostructures*
43.	Wolff J.	*Nano-optomechanics of a few-layer FePS3 suspended membrane*
44.	Wu N.	*Revealing low frequency magnetic moment fluctuations of TbPc2 single-molecule magnets grafted on graphene*
45.	Yahia A.	*Thermodynamic calculations of CVD graphene growth from solid and gazeous precursors*
47.	Soliman M.	*Van der Waals heterostructure ferooelectric synapse*
48.	Brochard C.	*Heat transport in h-BN*

CVD SYNTHESIS OF SP²-HYBRIDIZED MULTILAYER BORON NITRIDE FILMS

Amandine Andrieux-Ledier[1], L.Taipied[2], F.Fossard[2], J.S.Mérot[2], J.M.Decams[3], A.Loiseau[2]

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Since graphene isolation in 2004, the 2D materials is a blooming research field. Due to its unique properties, sp² hybridized boron nitride (BN) has been acknowledge as a key towards integration of other 2D materials in devices. Indeed, it is structurally very close to graphene – their lattice mismatch is only 1.7%- a semiconductor, atomically flat and thermally and chemically inert. It is therefore a choice material to be used in the van der Waals heterostructures with other 2D materials either as a top layer to protect another 2D material from its environment [1], or as a dielectric interlayer [2] and mostly, as a flat substrate [3]. However, these applications have been demonstrated using mechanically exfoliated BN from low defective and highly crystalline single crystals. Yet, this process limits the size of the devices that can be created to sub millimeter scale. In order to develop devices at a wafer scale, it is therefore critical to master the synthesis sp² hybridized BN layers at low cost, large scale and high quality.

In that respect, the goal of the researches we have undertaken is to develop the synthesis of sp²-hybridized multilayer BN films with structural specifications fitting these requirements. We have already successfully obtained heteroepitaxial growth of a few nanometer-thick sp² hybridized BN film of well-stacked and flat layers on Ni (111) surface of polycrystalline substrate [4]. Here, we will present our work on Rapid Thermal CVD from Annealsys. We will show how we successfully adapt our growth process to this new reactor on centimeter monocrystalline nickel substrates. We will detail the crucial step of nickel surface preparation before the synthesis. We will present the results of the structural and quality characterization of the BN films from the macroscale to the nanoscale (OM, SEM, TEM, AFM, Raman and luminescence spectroscopies) on the growth substrate and after transfer onto dedicated substrate.

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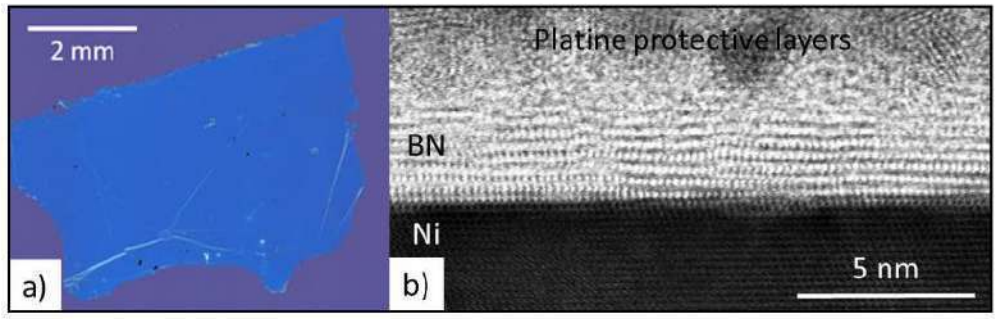

Figure 1: All the results present here are obtained on the Annealsys RTCVD (a) Optical microscopy image of a BN film grown on Ni(111)/YSZ/Si(111) pseudosubstrate and transferred on SiO2/Si, showing the large scale transfer. (b) HRTEM image of multilayers BN film grown on nickel (111) showing the thickness and the regular stacking of the BN layer (MATMECA, Titan G2 Centrale Supelec, 300 kV)

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OPTICAL PROPERTIES OF METALLIC CARBON NANOTUBES

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Carbon nanotubes are one-dimensional nano-objects that can have metallic or semiconducting behavior depending on their geometry. In order to study or predict the optical response of heterostructures made of metallic carbon nanotubes, it is essential to know precisely their dielectric constants over a wide spectral range at optical frequencies. Their optical properties are known for mixtures of metallic and semiconducting carbon nanotubes. However, in the literature, there are no experimental measurements of metallic carbon nanotubes dielectric constants at optical frequencies (mid and/or near-infrared) nor numerical calculations from Density Functional Theory which include intra-band transitions. Our measurements of the optical properties of sorted metallic and semiconducting carbon nanotubes [1] are based on reflectance/transmittance experiments, see figure 1, (from UV to far-infrared) of carbon nanotube films deposited on a CaF_2 substrate. An increase of reflectance between 0.08 eV and 0.5 eV is observed for metallic carbon nanotubes. It is attributed to intra-band transitions that characterize metallic material behavior and described by a Drude model. The experimental refractive index will be extracted from the reflectance measurements with the help of the Kramers-Kronig relations. [2-4]

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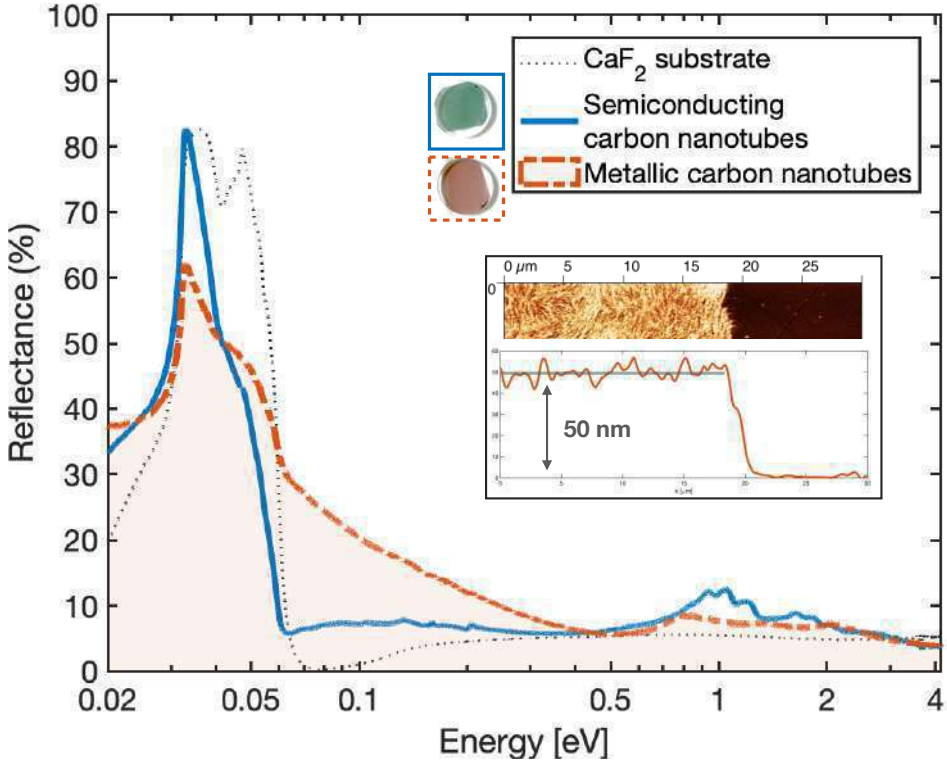

Figure 1: Reflectance (%) of 50 nm thick sorted carbon nanotube films (semiconducting and metallic) on a CaF_2 substrate.

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EXCITON DYNAMICS IN ATOMICALLY THIN HETEROSTRUCTURES MADE FROM GRAPHENE AND TRANSITION METAL DICHALCOGENIDES

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Two-dimensional materials compose a toolkit of atomically-thin crystals with remarkable electronic, optical, spin and valley properties. These assets can be enhanced by stacking 2D layers into so-called van der Waals heterostructures and thereby tailoring novel functionalities and devices. The performance of such devices is governed by near-field coupling through, e.g., interlayer charge and/or energy transfer. New concepts and experimental methodologies are needed to properly describe atomically sharp heterointerfaces. This poster will focus on model heterojunctions made from transition metal dichalcogenide (TMD) monolayers coupled to graphene monolayers. First, we will describe the most salient fingerprints of near-field coupling, namely fast (picosecond) energy transfer and slower, photoinduced extrinsic charge transfer to graphene [1,2]. Second, I will demonstrate that graphene does not only neutralize TMD monolayers leading to the complete absence of light emission from charged excitonic species but also enables selective energy transfer, leading to bright, single and narrow-line PL arising solely from TMD neutral excitons (X^0, see Fig. 1) [3]. Finally, we will discuss the implications of our results for opto-valleytronics and chiral optics, in light of our recent studies of large valley polarization and coherence in TMD-graphene heterostructures [4].

This work was done with E. Lorchat, L.E. Parra-Lopez, G. Froehlicher, S. Azzini, T. Chervy, T.W. Ebbesen and C. Genet at U. Strasbourg; C. Robert, D. Lagarde, and X. Marie at INSA Toulouse; C. Ferrante, G. Di Battista, G. Batignani, A. Virga, T. Scopigno at La Sapienza, Rome

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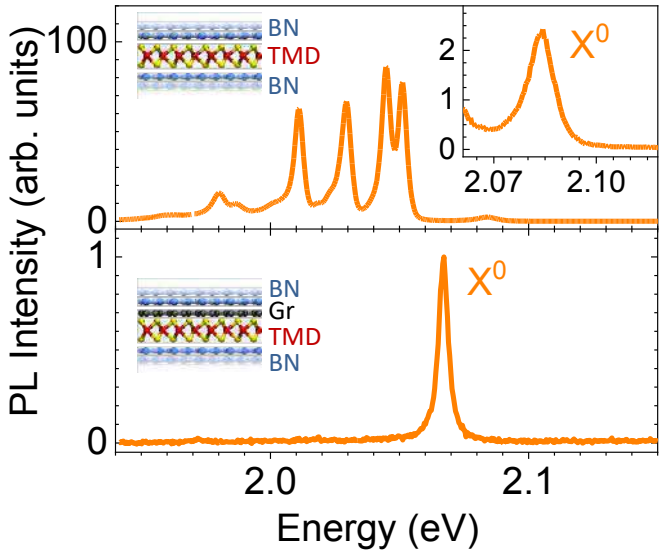

Figure 1: Bright, single narrow-line photoluminescence (PL) from a WS_2/Graphene heterostructure capped in hexagonal boron nitride (BN) (bottom). The PL of the BN-Capped WS_2 reference is shown in the upper pannel for comparison. Data from Ref. [3].

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EFFECTIVE NEGATIVE DIFFUSION OF CHARGED EXCITON IN WSE_2 MONOLAYER

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Here we investigate the transport properties of excitonic species in a charge adjustable WSe_2 monolayer device [1] ; more precisely we focus on the negatively charged exciton X^- (negative trion). Investigating the transport mechanism of X^- is appealing as the valley/spin properties of X^- are remarkable : the valley/spin polarization degree can reach values up to 90% [1]. The photoluminescence experiment we used is based on a diffraction-limited excitation spot that induces a lateral diffusion of the photogenerated species. We then used a Streak camera system with a temporal resolution of about 3 ps to record the time evolution of the PL profile [2]. The spatio-temporal information allows us to separate the transport and the recombination mechanisms. Moreover, it gives information on the trion formation mechanisms which are barely understood in this type of material.

First, we examined the width of the PL profile as a function of time, as shown in Figure 1(a-c). At the very early stage, the PL profile is already broader than the laser spot indicating a picosecond diffusion mechanism (even shorter than our temporal resolution at higher doping density). Within the next 20 picoseconds, there is a clear reduction in the width of the PL profile, indicating an effective negative diffusion process. Lastly, on a longer time scale, the negative diffusion process is weaker and becomes positive as the electron doping density increases.

Second, we observe that the trion PL signal arises after the neutral exciton X_0 PL one (Fig2). The delay time - on the order of picoseconds - is reduced when we increase the electron doping density; this would indicate a faster formation of the X^- trions coming from a bimolecular formation between the neutral excitons X_0 and resident electrons.

Finally, based on the previous observation and similar "negative" diffusion reported recently, we can model this unusual diffusion mechanism (see Fig. 1 (d)) by solving the rate equations of three populations: the neutral exciton population X_0, a trion population formed by either a bimolecular formation mechanism (binding of a bright exciton with one electron) or a geminate process (the photon directly photogenerate the trion).

We therefore observed an effective negative diffusion mechanism of the negatively charged exciton X^- that could be related to two different formation channels. Further studies will evidence the role of the doping density and the influence of the temperature.

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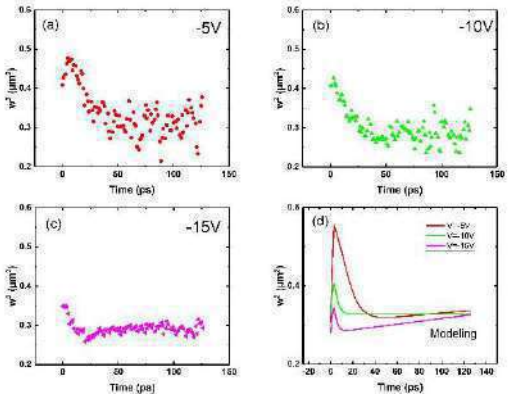

Figure 1: (a-c) Extracted squared width w of the PL profile as a function of time for different bias (i.e. electron doping density). (d) Example of modeled time evolutions of w.

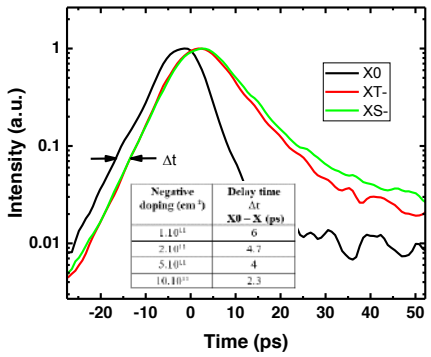

Figure 2 : TRPL dynamics of different excitonic species X_0, X_T- X_S- at -5V (i.e. ~$5.10^{11}cm^{-2}$). The table indicates the extracted delay time between the Exciton emission and the Trions emission for different voltages (i.e. electron doping density).

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NONLOCAL SIGNALS OF ORBITAL ANGULAR MOMENTUM TRANSPORT IN GRAPHENE

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In the last decades, the development and the successes accumulated by the field of spintronics demonstrated that harnessing the quantum degrees of freedom of the matter is the most prominent pathway for further technological development. Following the lines set by spintronics, orbitronics explore the possibility of manipulating the orbital angular momentum of the carriers to store and process information using the orbital Hall effect as its main lever. In resemblance to the spin Hall effect, the orbital Hall effect refers to the appearance of a transverse orbital angular momentum current after applying a longitudinal electrical field [1].

Contributions for the orbital Hall effect are separated as intra- and inter-atomic contributions since they refer to the localized atomic and motion orbital angular momentum, respectively [2,3]. Despite being studied for 3D systems, recent works on 2D materials demonstrated that materials with vanishing spin Hall conductivity such as mono- [4,5] and bilayers [6] of transition metal dichalcogenides and gaped graphene monolayers [7] exhibit finite orbital Hall conductivity, which is given by intra- and interatomic contributions, respectively. Using the Landauer-Büttiker formalism, we show that gapped graphene devices present sizable non-local resistance signals related to conduction through dispersive edge states. Investigating the effect of weak magnetic fields on these non-local signals, we find that they exhibit a chiral behaviour with the field direction. Our results suggest that the origin of the non-local resistance signals in gapped graphene devices are described more transparently in terms of orbital angular momentum currents.

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Figure 1: Schematic representation of the orbital-Hall effect.

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GDR HOWDI 2022 MEETING: FIRST-PRINCIPLES ELECTRONIC AND STRUCTURAL PROPERTIES OF BNC NANOMATERIALS

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Advanced Silicon-based device components are only moderately chemically tunable, which restricts the realistic prospect of current technology transitioning into flexible and miniaturized devices. Graphene is a promising candidate [1] to replace Silicon and heteroatom co-doping (i.e. with boron and/or nitrogen) has emerged as an appealing strategy to tune its electronic and structural properties and possibly inducing an electronic band gap in graphene. Since the existing BN-doped carbon-based materials are not periodically doped, their properties are not reproducible [2] hence a substantial challenge is to gain control in the incorporation of these BN rings in a reproducible manner. The present study aims to search for an entirely new class of BCN hybrid 2D materials in order to construct a high-accuracy reference database with key electronic and optical properties. This goal is achieved by using ab initio quantum mechanical calculations relying on density functional theory (DFT) and many-body perturbation theory (MBPT). A large set of BNC materials exhibiting different doping parameters (Figure 1) is considered in order to search for the best configuration in terms of both stability and band gap properties. For every doping parameter considered, these models display cohesive energies comparable with benchmark ideal periodic BCN systems with a decreasing linear trend for high concentrations of BN-rings. However, band gap values of borazine-doped graphene systems are found to be sensitive to the doping patterns and to be considerably larger for high concentration of BN rings with the same orientation. These predictions suggest that BN-ring doped graphene materials could be interesting candidates for the next-generation of opto-electronic devices and open new opportunities for their synthesis using chemical bottom-up approaches.

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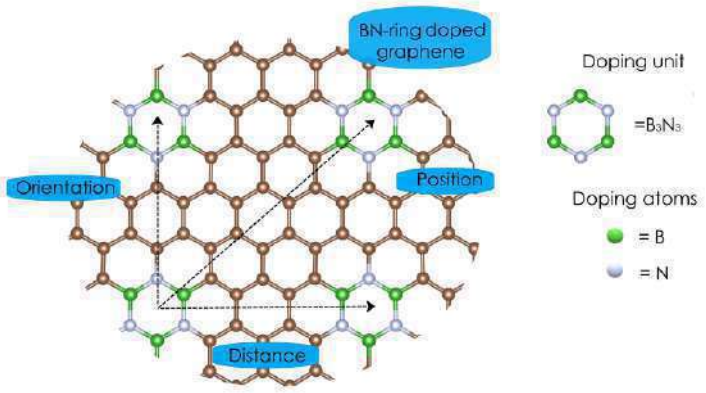

Figure 1: BN-ring doped graphene. Different doping parameters, such as orientation, position and distance, are considered herewith to search for an optimal doping configuration in terms of stability and band gap in order to possibly replace Silicon in future opto-electronic nanodevices.

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GDR HOWDI 2022 MEETING:
GAP(111)B-SE SURFACE FOR TMD EPITAXIAL GROWTH

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Over the past few years, 2D-Transition Metal Dichalcogenides (TMDs) have revealed great potential for optoelectronics and nanoelectronics devices, thanks to their exceptional properties, not encountered in other materials. They can be grown by van der Waals epitaxy allowing the use of materials with significant mismatch. Van der Waals epitaxy is usually performed on 2D substrates such as graphene, hBN or mica but 3D substrates can also be used after a proper surface passivation treatment, which for III-V semiconductor substrates has been applied successfully on GaAs(111)B surfaces. Since rather high growth temperatures are needed in order to get high quality-TMD layers **[1]**, GaP might represent an interesting alternative to GaAs considering its higher thermal stability. In this study, we present results relative to the preparation of n and p-type GaP(111)B surfaces and to their Selenium passivation.

The substrate is first deoxidized in a III-V MBE reactor under PH_3 and H_{at} fluxes to prepare a clean GaP(111)B surface before being transferred in a TMD epitaxial chamber where the surface is annealed under a Selenium flux with a Beam Equivalent Pressure in the 10^{-6}-10^{-5}T range. Samples are characterized *in-situ* by Reflexion High Energy Diffraction (RHEED), X-Ray and UV photoemission spectroscopies (XPS/UPS) and *ex-situ* by Atomic Force Microscopy (AFM).

After deoxidization, the GaP(111)B surface exhibits a (2x2) reconstruction before turning immediately to a (1x1) one under Selenium exposure, revealing the impact of Se on the atomic structure of the GaP surface. On the clean GaP(111)B surface, XPS reveals one main bulk component for the *Ga3d* and *P2p* core level lines (CL) and one surface component for the *P2p* one. After Selenium exposure, this surface component vanishes whereas a second component appears on the *Ga3d* spectrum evidencing the presence of Ga-Se bonds. The position of Selenium atoms in the atomic mesh compared to the initial GaP(111)B surface has been investigated using XPS photodiffraction. The evolution of the Ga3d and P2p XPS intensities with polar angle (Figure 1) are characteristics of a GaP(111)B surface whereas the lack of any intensity modulation for *Se3d* demonstrates that Se atoms stay in the outermost atomic plane. On p-type substrates, UPS measurements reveal a slight change in work function (from 5.05eV to 5.3eV) and an increase of the surface band bending of 0.15 eV after Selenium treatment. Contrarily, this latter has no influence on the surface morphology and roughness as evidenced in the AFM images of figures 2a and 2b where atomic steps, mean terrace length (280 nm) and mean RMS roughness (0.3 nm) remain unchanged.

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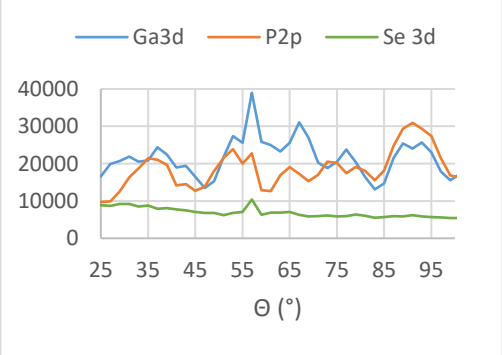

Figure 1: XPS photodiffracted intensities for polar angle variations along the <112> direction recorded on a GaP(111)B sample annealed at 700°C under Se flux

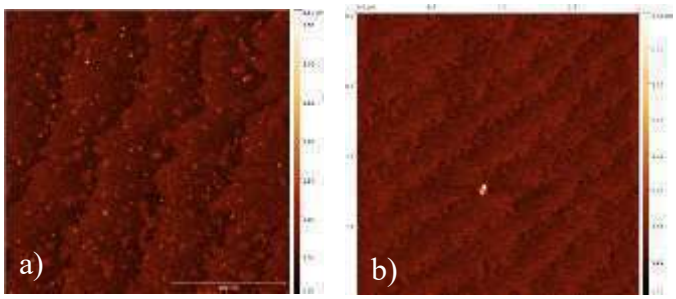

*Figure 1: AFM images (2µm*2µm) of GaP(111)B surfaces*
a) after deoxidizaton
b) after annealing at 700°C under Se flux

STRAINTRONICS IN 2D SEMICONDUCTORS

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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 MoS_2 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 sensitive device with a resolution of about 20mK.

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 $WS_{1.4}Se_{0.6}$ 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 excitons[2] and the conversion of excitons to trions[3].

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

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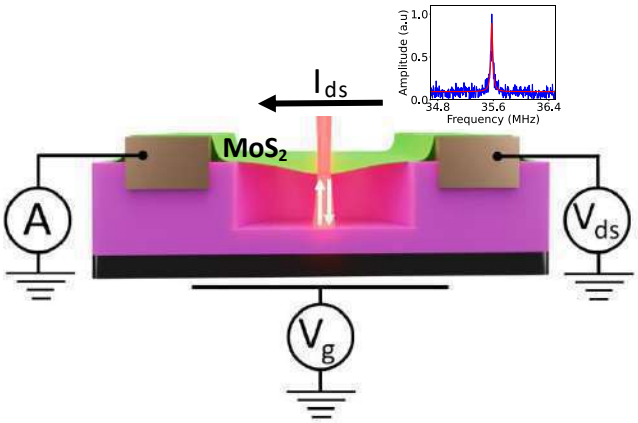

Figure 1: NOEM platform using electrical actuation and optical detection. Inset: resonant frequency of MoS_2 membrane

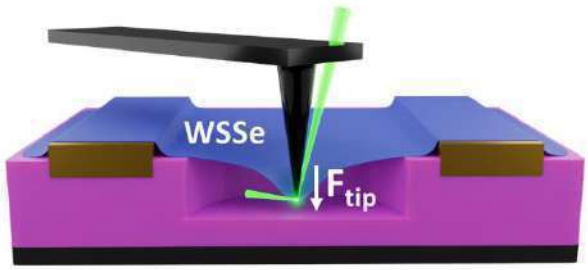

Figure 2: AFM tip indentation setup exploiting the TEPL

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ELECTRICAL PROPERTIES OF GRAPHENE TRANSFERRED ON LITHIUM NIOBATE SUBSTRATE

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Acoustic waves generated on piezoelectric substrates have been one of the most potent means for the miniaturization of telecom filters in cell phones. The principle is based on the transduction of an RF signal into an acoustic wave of relatively slow speed with respect to the electrical signal. It enables passive signal processing in the few GHz range. The impulse frequency response depends mainly on the geometry of interdigitated transducers (IDTs) [1]. The RF signal slowing provides other interesting architectures for signal processing. In particular, two IDTs facing each other reverse the time of the two counter-propagating waves. Mixing the two waves in a nonlinear medium can achieve analog signal convolution in the time domain. State-of-the-art devices have been made considering metallic or semiconducting films. Metal film losses limit frequencies to hundreds of MHz and thus limit their usable bandwidth, while semiconductor film convolvers still fail to break over 1 GHz and are much more challenging to process [2]. The mass effect due to the metal film limits the highest operational frequency and the electromechanical coupling of devices, in particular when the piezoelectric film thickness is highly reduced. To improve performance, two-dimensional mass-free nonlinear conductors, such as graphene, offer a great opportunity. Recently, graphene transfer on piezoelectric substrates has been studied for acoustoelectronic transport measurements [3]. However, the electrical characterization of graphene transferred onto lithium niobate (LN) piezoelectric substrates is weakly documented (effect of orientation of LN substrate, contamination, processing).

In this work, the presence of a graphene monolayer on (YXlt)/128°/90° $LiNbO_3$ was confirmed by Raman scattering (see Fig 1). Room temperature transmission line measurement presents a sheet resistivity in the range 640-720 Ω/□ for the processed graphene and contact resistivity in the range 225-390 Ω·µm for graphene-gold all-around contacts. Fig 2 presents the quantum Hall effect on a Hall bar at 2K. Hall measurements will be presented and discussed for different temperatures in the 2-295 K range.

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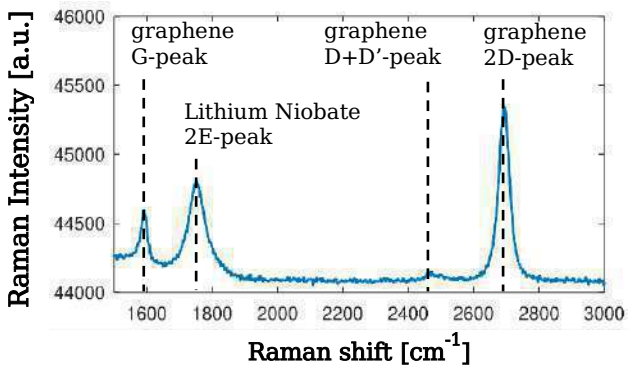

Figure 1: Raman spectrum of graphene on LN

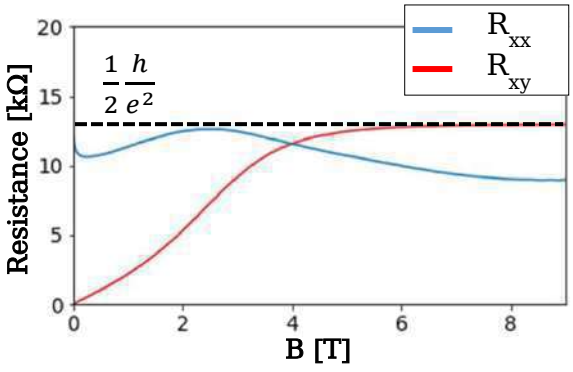

Figure 2: Transverse R_{xx} and longitudinal R_{xy} resistances vs applied magnetic field B at 2K for graphene on LN.

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DESIGN AND OPTIMIZATION OF GRAPHENE PHOTOTHERMOELECTRIC DETECTORS

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Owing to its unique properties, graphene is a promising material for a wide range of applications [1]. Particularly promising are applications that utilize several of graphene's unique properties in a single system or device. A perfect example of such devices are photodetectors based on the photothermoelectric effect (PTE) in graphene, which combine a broadband and fast photoresponse with high signal-to-noise ratio and minimal power consumption [2-5]. There are many design parameters impacting the performance of these devices, including the light profile, the device geometry, and the material quality.

In this talk, I will discuss the impact that these design parameters have on the performance of PTE-based graphene photodetectors, and I will demonstrate how their performance may be optimized. Careful tuning of the light profile and device geometry can improve the photoresponse by more than one order of magnitude. Detector performance can also be improved with higher graphene material quality, but only to a point. When material quality is too high the photoresponse can actually degrade, indicating an upper bound on device performance and suggesting that ultraclean graphene may be unnecessary for, and actually detrimental to, the performance of these detectors [6]. Time permitting, I will also discuss efforts to induce optical anisotropy in graphene [7], expanding its functionality in photodetection and sensing.

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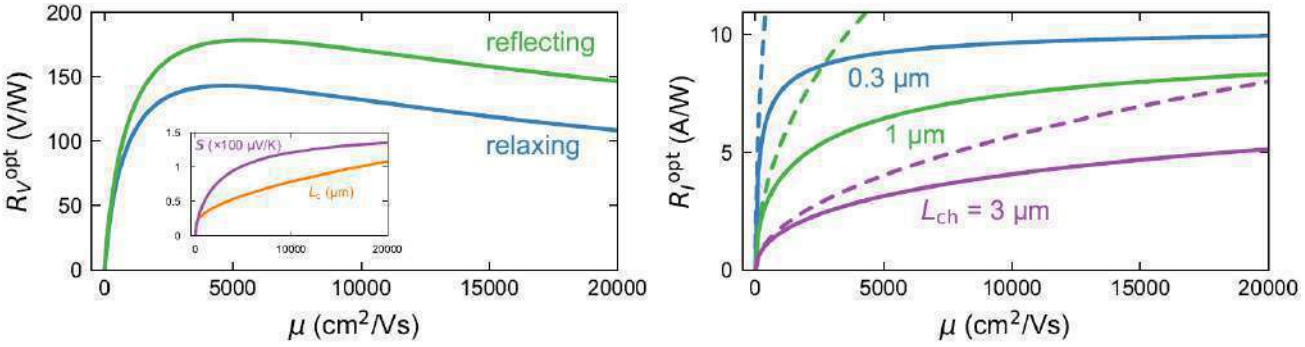

Figure 1: Optimal photovoltage (left) and photocurrent (right) as a function of graphene carrier mobility. In both cases, the photoresponse saturates for a mobility around 5000 cm²/Vs.

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WET-CHEMICAL NON-COVALENT FUNCTIONALIZATION OF CVD-GRAPHENE: MOLECULAR DOPING AND ITS EFFECT ON ELECTROLYTE-GATED GRAPHENE FIELD-EFFECT TRANSISTOR CHARACTERISTICS

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Graphene has attracted considerable attention in many areas of nanoscience and nanotechnology due to its exceptional electrical, mechanical, and chemical properties [1-2]. However, graphene is a semimetal with zero band gap. This character limit its use in some applications that exploit its semiconducting behavior. Chemical modification of graphene sheets with small organic molecules represents a viable approach for tailoring electronic properties such as band gap opening, majority carrier type, and improving its dispersing ability and compatibility. In this study, graphene was synthesized by chemical vapor deposition and functionalized with Fe-/Co-porphyrin and Fe-phthalocyanine through π-π interactions. The resulting nano-hybrid materials were characterized by Raman spectroscopy (RS), X-ray photoelectron spectroscopy, scanning electron microscopy, and high-angle annular dark-field scanning transmission electron microscopy techniques. The presence of physi-adsorbed molecules on the graphene sheet surface is evidenced by spectroscopic and microscopic analysis, which confirm that these molecules are immobilized through electrostatic and π-π interactions. RS confirmed the n- or p-type doping of graphene, according to the chemical nature of those physi-adsorbed molecules. The electrical characteristics of electrolyte-gated graphene field-effect transistors based on nano-hybrid materials were subsequently evaluated and demonstrated a charge transfer between the physi-adsorbed molecules and the graphene. All these results suggest that the electronic structure of graphene can be tailored by doping with aromatic molecules. Density Functional Theory calculations were performed to confirm these observations.

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OPTICAL SPECTROSCOPY OF NONPLANAR GRAPHENE NANORIBBONS WITH FJORD EDGES

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The band structure of graphene and its zero-gap at the K point of the first Brillouin zone lead to unique physical and electronic properties owing it to be used as an emerging material for many applications such as fast electronics, ultra-sensitive sensors, etc.. Nevertheless, the semimetal property in graphene constitutes a severe limitation for this material to be used in light harvesting devices. For that, various strategies have been investigated in order to open a gap in the electronic structure of graphene.

The carbon atoms in graphene are assembled in a 2D network of honeycombed hexagons. The reduction of the dimensionality of a single graphene layer in the form of a 1D graphene nanoribbons (GNR) or 0D graphene quantum dots (GQD) is a very promising method in order to open a significant gap (up to 1 eV). In this perspective, the electronic, optical, and spin properties can be controlled by designing the size, shape and edges of GNRs and GQDs. The fabrication of such nano-objects can be achieved for instance by the so called bottom-up chemistry approach, allowing to obtain a variety of desired structures with an atomic precision.

Bottom-up synthesized GNRs have been largely studied in order to understand their electronic and transport properties [1], while their fundamental optical properties are still unexplored. Here, we are interested by the study of intrinsic optical properties of GNRs. Recently, the synthesis of Fjord-GNRs, whose Fjord-edges are highly twisted, have been reported [2].

The photoluminescence spectra measured on ensemble of Fjord-GNRs in solution shows a broad band emission centered around 680 nm, which is interesting for optoelectronic devices. In order to investigate close-to intrinsic properties of Fjord-GNRs, we performed experiments at the single particle level using a confocal microscopy setup allowing us to study the emission process of a single Fjord-GNR (Figures 1 & 2 below). In this presentation we will show aspects of the photo-physics of a single Fjord-GNR [3].

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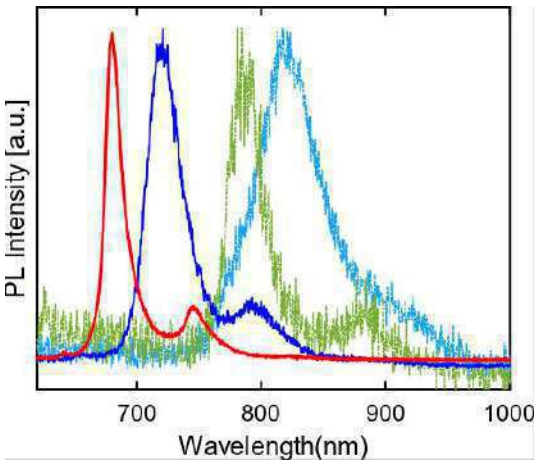

Figure 1: Photoluminescence spectra measured on different single F-GNRs at room temperature.

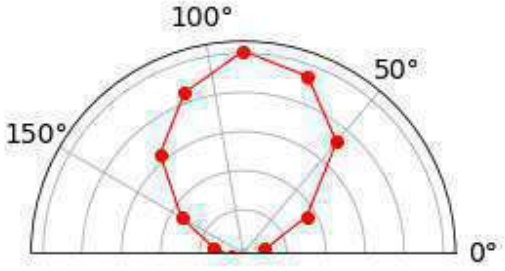

Figure 2: Polar plot showing the polarization of PL excitation for a single F-GNR at room temperature.

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PHOTOSWITCHING MOLECULAR CONJUGATION ON SINGLE-WALLED CARBON NANOTUBES

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Enhanced emission from the functionalization of carbon nanotubes has been utilized in optoelectronics, biosensing, bioimaging, etc. In our previous work, we presented a non-destructive covalent approach to tailor luminescent SWNTs using photoswitching spiropyran [1]. This hybrid nanomaterial was used in the control of the SWNTs intrinsic luminescence in the NIR region (beyond 1μm) [2]. However, the synthetic approach used to obtain this nanomaterial was based on a single reaction step, which makes challenging controlling the number of groups attached to the nanomaterials as well as the reaction outcome. Herein we present the structural, electronic and vibrational properties of this hybrid nanomaterial designed using a stepwise synthetic approach.

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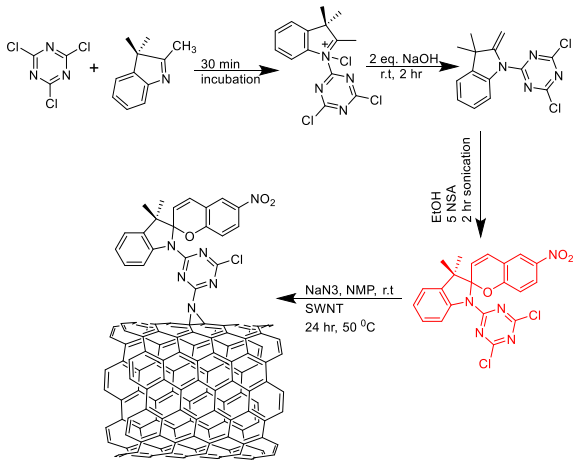

Figure 1: Multistep synthetic route for the NCF of photoswitchable spiropyran onto SWNT.

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ELECTRICAL CONTROL OF DETERMINISTICALLY-POSITIONNED QUANTUM EMITTERS IN HBN

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Single photon emitters (SPEs) constitute a fundamental resource for quantum technologies. Among single photon sources, optically active point defects known as colour centres are promising candidates. Such colour centres have been discovered in the 2D material hexagonal boron nitride (hBN) [1, 2]. They are actively studied because of their appealing optical properties such as bright and stable emission, and a narrow individual linewidth. But they have two major drawbacks: they appear at random spatial locations and their emission wavelength is not reproducible.

We recently identified a new family of colour centres in hBN [3] that can be activated at pre-selected locations through irradiation with an electron beam. From a technological point of view, this represents a clear advantage for their integration in heterostructures. Additionally, the ensemble inhomogeneous linewidth is strongly reduced ($\Delta\lambda < 1$ nm). This property is valuable because a number of applications need indistinguishable photons, which implies an identical wavelength.

In this context, we have realised van der Waals heterostructures made of graphene/hBN/graphene (fig. 1). The hBN flake contains electron beam-activated colour centres and the two graphene flakes serve as electrodes to apply a static electric field to the SPEs. Based on spectroscopic measurements of individual SPEs, we observe a voltage-dependent shift of the emission wavelength that originates from Stark effect (fig. 2). This new degree of freedom could be used to compensate for small wavelength differences, thus taking us a step closer to the goal of integrated sources of indistinguishable single photons.

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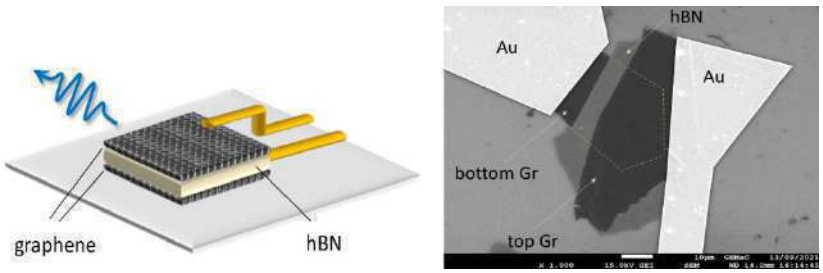

Figure 1: Left, a schematic illustration of the heterostructure. Right, a scanning electron microscope image of the heterostructure.

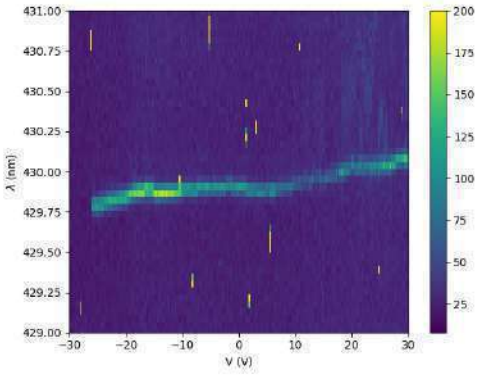

Figure 2: Low temperature spectrum as a function of gate voltage, showing a shift in the emission wavelength.

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GDR HOWDI 2022 MEETING

Novel spectroscopic detection of reversible collapse of single walled carbon nanotubes at high pressure

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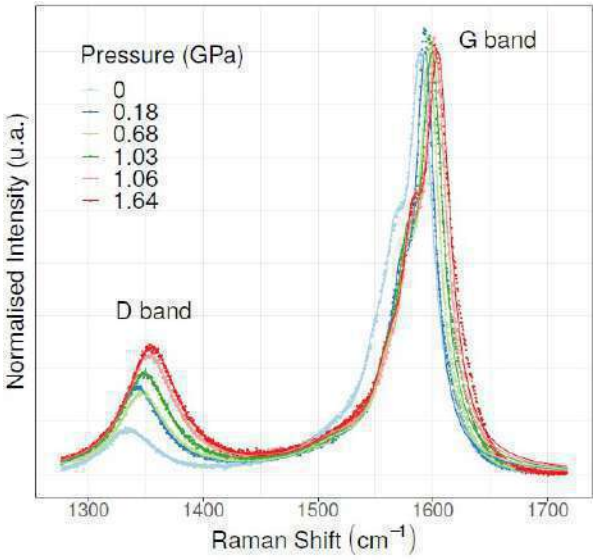

Fig. 1. *In situ Raman signature of the pressure evolution of SWCNTs through their collapse pressure using a sapphire anvil cell.*

The radially collapsed structure of carbon nanotubes [1] constitutes an intermediate geometry between the 1D-tube and 2D ribbon-like structure which offers opportunities in the optimization of electrically conductive composites [2] or reinforcing fibers [3] for instance. The pressure induced radial collapse of carbon nanotubes [4] has been shown to exhibit characteristic signatures in the Raman spectrum as changes in the evolution of the G-mode associated to the attenuation of the associated radial breathing mode (RBM) [5,6].

It has been recently shown that the symmetry reduction introduced by the radial collapse leads to the formation of a characteristic D-band in the Raman spectrum without disorder [7]. In this work, we have successfully shown the use of this signature as a probe for the high-pressure evolution between the circular and the collapsed structure of single-walled carbon nanotubes.

The study of the D-band is not possible in Raman high-pressure experiments using the diamond anvil cell pressure apparatus at pressures below ~10 GPa [8]. In fact, diamond most intense Raman peak overlaps the D-band, hence preventing its detection. In order to avoid such problem, we used a sapphire anvil cell, which provides an optical window for the detection of both the D-band and the G-band. Our study allowed us to observe the D-band development at the expected nanotube collapse pressure as well as its reduction after pressure release, confirming its link to the collapse process.

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EXCITON DYNAMICS STUDY OF hBN BY TIME-RESOLVED CATHODOLUMINESCENCE

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Hexagonal boron nitride (hBN) is identified as a strategic material for the integration of graphene and 2D semiconductors in optoelectronic devices based on van der Waals heterostructures [1-2]. Due to its strong binding energy (~300 meV) [3], exciton plays an important role in the electrical and optical characteristics of hBN, even at ambient temperature. The optimization of hBN-based optoelectronic devices requires a better understanding of the exciton recombination mechanisms and sources of non-radiative losses. Some of these losses depend on the quality of hBN and some others are intrinsic to the material, like exciton-exciton annihilation (EEA). The EEA can turn out to be an efficient nonradiative recombination channel at high excitation densities as it has been shown in low-dimensional materials such as carbon nanotubes, quantum dots, nanowires, and 2D and TMDs [1, 4-7].

Much information on these non-radiative channels can be deduced by studying the dynamics of excitons recombination, unfortunately the deep-UV luminescence of excitons in hBN complicates the measurements by photoexcitation. Here, we present our results on the exciton dynamic in hBN using our recently developed time-resolved cathodoluminescence (TRCL) setup. Measurements have been carried out on high quality hBN single crystal fabricated at GEMaC using atmospheric pressure high temperature (APHT) method. hBN quality is assessed from the free exciton lifetime by sampling the crystal at centimeter scale at room temperature and lifetime is found to be 3.2 ns (std. dev. 12%). These results are close to the reported values of best HPHT crystals (4.2 ns) [8]. We have also investigated the exciton dynamic at low-temperature (5 K) over a wide range of excitation densities (almost three orders of magnitudes). We observed that at low excitation densities, the exciton dynamics shows mono-exponential decay (lifetime ~ 0.75 ns). Interestingly, with increasing exciton current density, a fast, non-exponential component develops, pointing the exciton-exciton annihilation as the dominant recombination mechanism under high excitation densities. The EEA rate is estimated by considering a bimolecular recombination model involving exciton-exciton annihilation term. Such exciton recombination studies at high excitation densities could have important implications for the optimization of hBN based advanced optoelectronic devices.

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MAGNON-EXCITON PROXIMITY COUPLING AT A VAN DER WAALS HETEROINTERFACE

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Spin and photonic systems are at the heart of modern information devices and emerging quantum technologies. An interplay between electron-hole pairs (excitons) in semiconductors and collective spin excitations (magnons) in magnetic crystals would bridge these heterogeneous systems, leveraging their individual assets in novel interconnected devices. We report the magnon-exciton coupling at the interface between a magnetic thin film and an atomically-thin semiconductor [1]. Our approach allies the long-lived magnons hosted in a film of yttrium iron garnet (YIG) to strongly-bound excitons in a flake of a transition metal dichalcogenide, $MoSe_2$. The magnons induce on the excitons a dynamical valley Zeeman effect ruled by interfacial exchange interactions. This nascent class of hybrid system suggests new opportunities for information transduction between microwave and optical regions.

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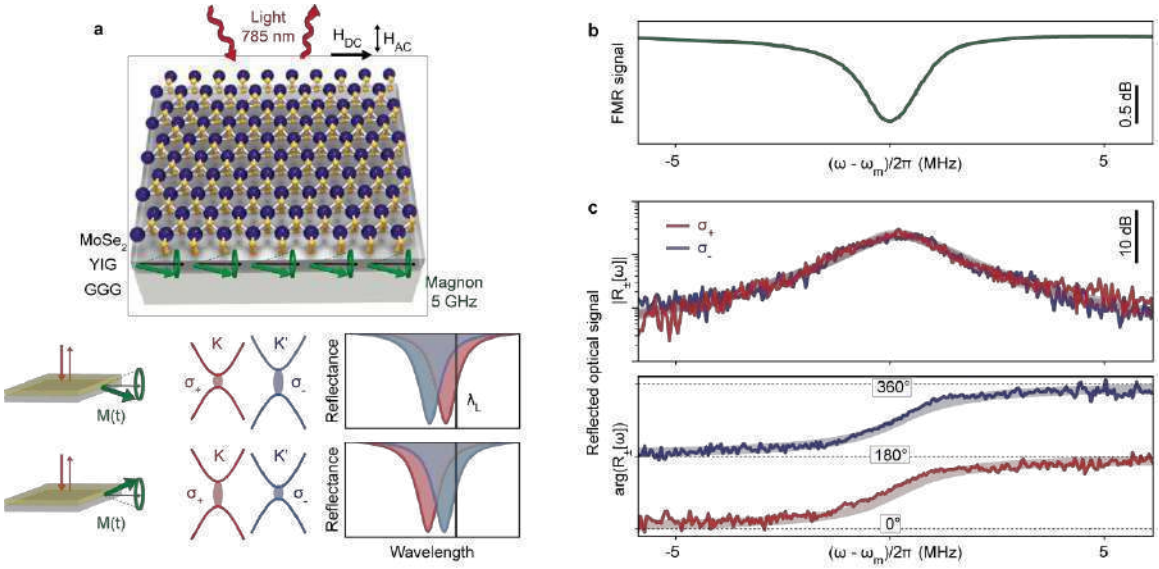

Figure 1: a) Atomically-thin flakes of $MoSe_2$ are stacked on a magnetic YIG film grown on gadolinium gallium garnet. A microwave antenna excites magnons of the fundamental magnetostatic mode of frequency $\omega_m/2\pi$. The magnons support a coherent oscillation of the magnetization vector, responsible for an effective magnetic field modulating the excitonic resonances of the $MoSe_2$ flakes through a dynamical valley Zeeman effect. b) Microwave absorption signal revealing the ferromagnetic resonance (FMR) at $\omega_m/2\pi$ = 5.64 GHz. c) Magnitude and relative phase of the optically-probed FMR spectra $R_\pm[\omega]$ with left-handed σ_+ and right-handed σ_- circularly polarized light to address respectively the K and K' valleys of the $MoSe_2$ flake.

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GDR HOWDI 2022 MEETING: AB-INITIO INVESTIGATION ON THE EVOLUTION OF THE ELECTRONIC AND OPTICAL PROPERTIES OF META-STABLE ALLOTROPIC FORMS OF 2D TELLURIUM FOR INCREASING NUMBER OF LAYERS

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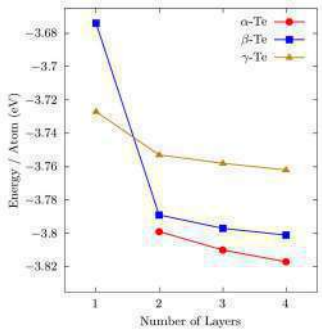
Tellurene is an emerging 2D anisotropic semiconductor, with fascinating electronic and optical properties that differ dramatically from its bulk counterpart, which has come to us owing to its unique chained structures. Tellurene is the 2D form of Tellurium and it was proposed by theoretical calculations - and then verified by experiments - in 2017 [1].
In this work, by means of ab-initio calculations, using Density Functional Theory, the evolution of the physical properties of Tellurene has been studied for increasing number of layers (from 1 to 4). Structural relaxations, electronic bandstructures and optical properties calculations have been carried out, for different allotropic forms (α-, β- and γ-Te), using the Quantum ESPRESSO integrated suite [2]. Also, the nature of the interaction between the helical chains of Tellurium atoms (characteristic of the bulk and α-phase crystal structures) has been carefully investigated. Finally, the exciton binding energies and radii have been evaluated, using an analytical model [3-6], for some of the studied systems, and then verified at the GW-BSE level, using the YAMBO code [7].



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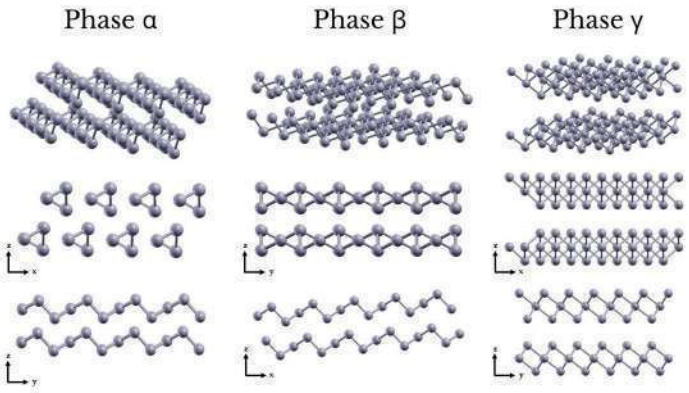

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GDR HOWDI
2022 MEETING: ULTRAFAST TERAHERTZ PHOTOCURRENTS IN SEMI-METAL AND SEMICONDUCTOR FEW LAYER $PTSE_2$

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A breadth of 2D transition metal dichalcogenides (TMD) semiconductors has been investigated in recent years, each with unique bandstructures that are distinctly different from the bulk. Some of the most commonly studied materials include MoS_2, WS_2, $MoSe_2$, and WSe_2, and key features include tuneable bandgap energies in the optical region. On the other hand, the recently discovered TMD $PtSe_2$ has garnered considerable interest owing to its relatively high electron mobilities [1]. Further the layered controlled bandgap can tuned from an indirect semiconductor to a semi-metal, covering a vast energy scale, from the near-infrared for monolayers to the terahertz (THz) region for multiple layers. This has permitted, for example, the recent demonstration of atmospheric stable mid-infrared detectors based on 2D materials [2].
The present contribution investigates THz intra- and inter- layer carrier dynamics and transport mechanisms in $PtSe_2$, where a femtosecond optical excitation permits to generate photocurrents that are probed using terahertz time domain spectroscopy (THz-TDS). Here, the $PtSe_2$ is excited with a 100fs, 800nm Ti:Sapphire laser (Fig. 1a) for the ultrafast generation of interband carriers, generating a time varying current that radiates as a THz single cycle pulse. Fig. 1b shows the typical THz pulse generated from a 36nm thick semi-metal $PtSe_2$ layer, with the inset the corresponding THz spectrum, which constitutes the first experimental demonstration of such THz emission in $PtSe_2$. This THz pulse permits to access the processes of current generation (in a non-contact, geometry), and determine the underlying second-order processes such as 'photon drag' (PD) and 'photogalvanique' (PDG) effects, which each contribute to the nonlinear processes. Finally, we present the strong effect of $PtSe_2$ thickness and hence the bandstructure on the THz emission. Fig. 2 compares the THz emission from 6 nm thick $PtSe_2$ (semiconductor) and the 36 nm semi-metal $PtSe_2$ under circular right and left polarised femtosecond excitation. A clear change in phase is seen in the thick $PtSe_2$ between polarisations, corresponding to an ultrafast current generated in opposite directions, whilst no change is seen in the thin sample. (The effect of linear polarisation is also shown). These results are signatures that $PtSe_2$ can be potentially exploited in THz optoelectronic applications, as well as understanding transport phenomena in 2D materials.

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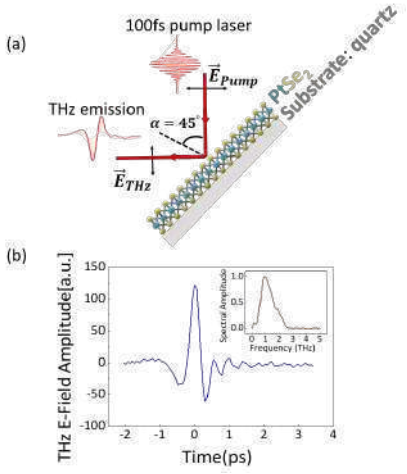

Figure 1: THz emission of 36nm PtSe2 sample: a) Measurement geometry. b) THz electric field showing a single cycle pulse. The Fourier transform for the spectrum is shown in the inset.

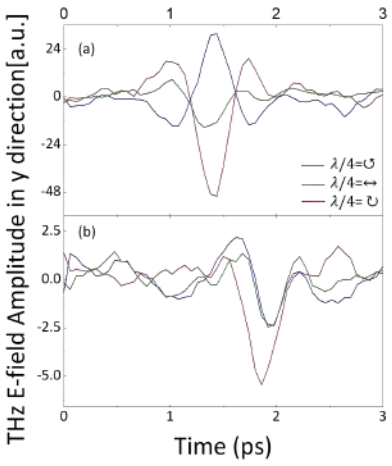

Figure 2: THz electric field dependency of PtSe2 on the circular polarization of the optical pump laser for a) thick (36nm) and b) thin (6nm) PtSe2 layer .

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OPTICAL RESPONSE OF CORRUGATED 2D MATERIALS AND HETEROSTRUCTURES

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The optical properties of 2D materials can be modeled in classical electrodynamics by a strictly 2D surface susceptibility or by a thin film of finite thickness. Both approaches have their drawbacks and they are based on an idealization of the materials since no materials are neither strictly bidimensional, nor can be considered as homogeneous perpendicular to the layer. However, the role of the intrinsic anisotropy is prime importance [1] and could be associated to a modification of the optical response as demonstrated by the investigation of the change of the Brewster angle of a substrate coated by graphene [2].

The detailed understanding of the above description is important if we want to extend it to heterostructures or to nanostructured 2D layers. We have investigated the conditions at which the optical response of an heterostructure of several 2D materials can be described by a stacking of independent 2D sheet or by layers of finite thicknesses. We also investigate the structuring within the layer, as for nanoribbon, can be described by an effective medium approach.

Corrugation of 2D materials is another way to tune their optical properties. SERS measurements on corrugated graphene show a strong enhancement for visible laser (figure). Atomistic quantum simulations evidence the appearance of optical response of corrugated graphene related to plasmon excitations in the IR/Visible related to such corrugation. Further SNOM measurements support the presence of propagating plasmon in the visible range. The fact that nanocorrugated graphene can host localized and propagating visible plasmons provides evidence for its unique potential as a versatile material platform for graphene plasmonics at the visible range [3]

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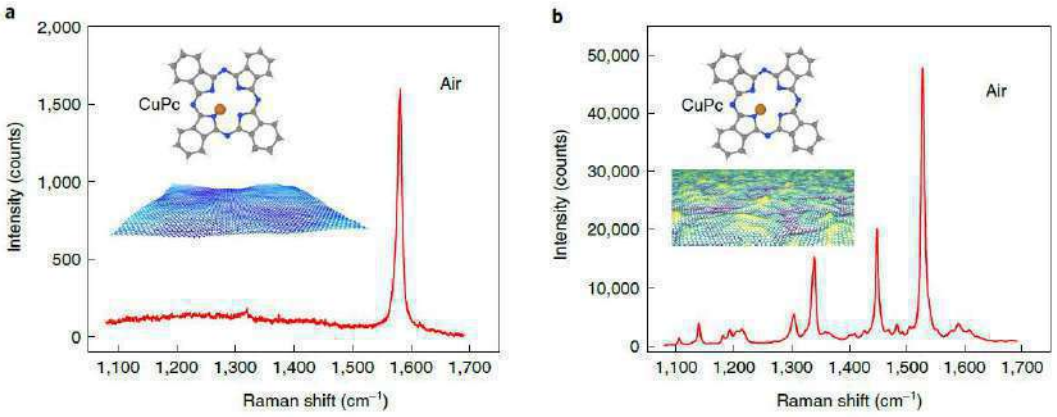

Figure : Illustration of the Raman enhancement of nanocorrugated graphene (b) compared to flat layer (a) . From [3]

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PHONON DRAG-ELECTRIC CURRENT GENERATION AT THE LIQUID-GRAPHENE INTERFACE

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Fluid transport at the nanoscale is essentially an interfacial phenomenon governed by the interaction of fluid molecules with the solid interface. While it is generally accepted that the structural properties and the chemistry of the liquid-solid interface is a key element for fluid-solid interaction at the nanoscale, the effect of the solid-state electronic properties of the interface has been broadly overlooked up to now. In this context, it has been demonstrated that water flowing against the surface of carbon-based nanomaterials, such as carbon nanotubes or graphene sheets [2, 3] , induces an electrical potential difference between the downstream and the upstream side of the material, but the exact mechanism at stake remains controversial [1]. Here, we use a tuning fork-Atomic Force Microscope (AFM) to deposit a micrometric droplet of viscous liquid on a thin graphite sample. We then induce an oscillatory motion of the droplet while recording the electrical current through the graphite flake. We report measurements of an oscillation-induced current of the order of a few nanoamperes for droplet motion velocities of the order of 1 μm/s. Extrapolating to the same contact area between the liquid and solid and to the same droplet velocity yields a generated current several orders of magnitude larger than previously reported for water-salt solutions on graphite [4]. We fully characterize the mechanism by measuring the dependency of the generated current on oscillation amplitude, on the applied bias between the electrodes and on the surface topography of the graphite flakes.
Our results point out a peculiar interaction between the molecules in the liquid and the charge carriers in the graphene mediated by momentum-transfert from the liquid molecules to the phonons in the solid [2]. Our finding pave the way for active control of fluid transfer at the nanoscale by harnessing the complex interplay between collective excitations in the solid and the molecules in the fluid.

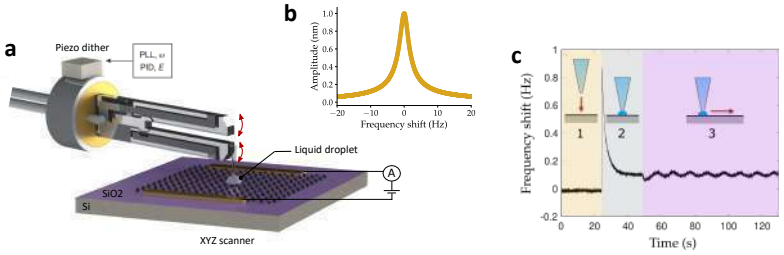

Figure 1: Experimental setup: asingle micrometric liquid droplet is moved on a graphene sheet

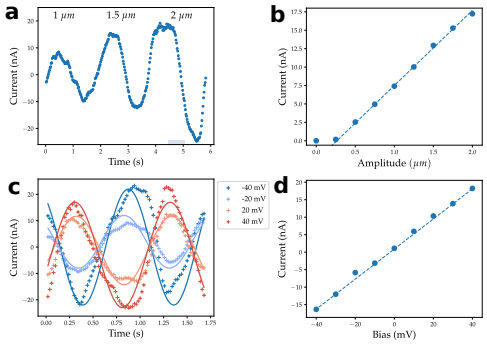

Figure 2: Generated current vs amplitude and bias.

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GDR HOWDI 2022 MEETING:
SAMPLE ABSTRACT AND PREPARATION INSTRUCTIONS

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The polarized fluorescence emission of organic fluorophores has been extensively studied in photonics for bio-imaging [1], solar energy harvesting [2,3] and quantum photonics[4] applications. The unique polarization properties and bright emission of a single molecule is hard to translate to larger assemblies of that molecule because the self-assembly process generally prevents extended alignment of the molecular dipoles which induces quenching effects and hence lowers its emissivity. Here we demonstrate that Boron Nitride Nanotubes (BNNTs) can act as a 1D host-template for the alignment of encapsulated a-sexithiophene (6T) inside BNNTs. We show that the fluorescence from the nanohybrid (6T@BNNT) is strongly polarized with extinction ratios as high as 700 at room temperature. A statistical analysis of the 6T orientation inside BNNTs with inner diameter up to 1.5 nm shows that at least 80% of the encapsulated 6Ts exhibit a maximum deviation angle of less than 10° with respect to the BNNT axis. Our results also highlight the presence of an adsorption competition between 6T-6T and 6T-BNNT with preferential stacking of the molecules on the BNNT sidewall. We also dispersed these polarized emitters inside a thin PMMA matrix and we show, by using confocal 3D fluorescence imaging, that a stretching of the matrix induces a significant alignment of these nanohybrids. As a result we observed that this alignment of the 6T@BNNT lead to polarized optical properties of the thin film.

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Figure 1: Conference logo.

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LASER HEATING OF SUSPENDED GRAPHENE

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Fourier law of heat transport seems to be no more applicable in 2D materials due to their extremely low thickness [1]. Thermal physics of graphene is predicted to reach hydrodynamic to ballistic regimes of thermal transport [2,3]. Optothermal Raman spectroscopy has allowed estimating an effective thermal conductivity of graphene [4] and proven to be a promising technique for thermal measurements. However, so far, the extraction of the thermal coefficients from the actual measurements is not a direct procedure and the values reported in literature heavily depend on some assumptions in the models used. In this context, a direct detection of the spatial dependence of the temperature profile on the heated graphene membrane would bring important information.

We suspend CVD grown graphene over holes of different size to study the thermal transport by using 2 laser Raman thermometry (Figure 1) [5]. A temperature calibration of the G mode shift (-0.018 +0.001 cm^{-1}/K) allows us to convert Raman maps into in spatially resolved temperature maps. We will discuss our results in the framework of thermal transport.

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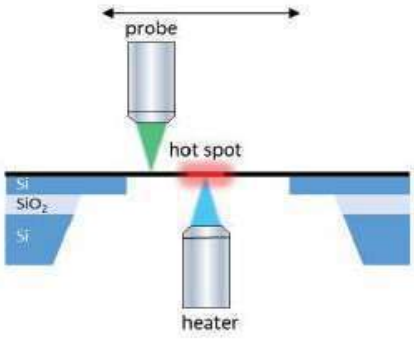

Figure 1: Principle of the 2-laser Raman thermometry: the probe laser can scan the suspended graphene while the heating laser is focused on a fixed spot of the membrane.

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UNIFORM CVD OF GRAPHENE ON 2" SIC WAFER

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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. The presence of hydrogen during growth, beyond strongly changing the chemistry during growth, allows to tune graphene properties from p-type multilayer to n-type monolayer. The quality of graphene monolayers prepared by hydrogen CVD is appealing for electronics applications, such as electrical metrology [3]. Graphene is also seen as a surface of choice for van der Waals epitaxy of nitrides [4] or 2D materials. For both applications, the growth of uniform high quality graphene films remains a crucial issue. This contribution focusses on the growth of graphene on 2" SiC wafers using propane/hydrogen CVD.

Graphene films were prepared on the Si-face of 2" SiC wafers in a horizontal hot-wall CVD reactor with a rotating substrate holder under the same growth conditions: a 9% H_2 / 91% Ar growth atmosphere under 800 mbar, plus 0.1% C_3H_8 during a 15' plateau at 1550°C for graphene growth. All graphene films are characterized using atomic force microscopy (AFM), and some are additionally studied using Raman spectroscopy and X-ray photoemission (XPS). Overall, the properties and the quality of the graphene films depend on the SiC polytype and on the wafer residual offcut. Representative XPS spectra from four samples grown on 6H-SiC are shown in Fig. 1. The two spectra from graphene grown on two wafers from the same series appear almost superimposed (red and green curves), while graphene grown on other series presents only small differences. Best graphene films are obtained on 6H-SiC wafers with a residual offcut of the order of 0.1 to 0.2°. For these optimized graphene films, morphology appears very uniform at the wafer scale, as shown by two representative images in the center and 200 mm away (Fig. 2). Our contribution will present these results with further characterizations and will discuss the key parameters to obtain uniform films at the wafer scale.

This work, supported in part by the Joint Research Project GIQS (18SIB07), received funding from the EMPIR and from the European Unions' Horizon 2020 research and innovation programme. This work was funded in part by MUR in the framework of the FlagERA-JTC 2019 project ETMOS.

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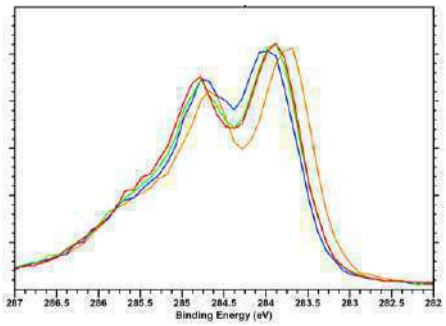

Figure 1: C1s XPS spectra on four different 2" 6H-SiC wafer covered by graphene.

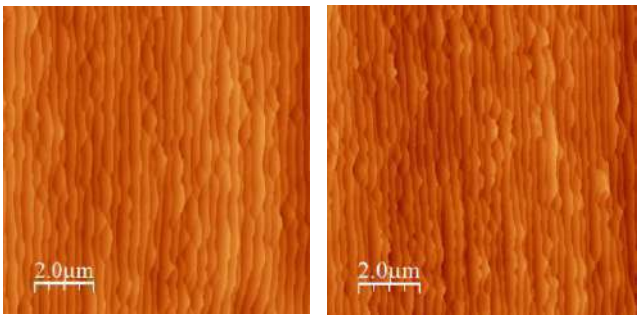

Figure 2: AFM images of graphene film in the center of a 2" 6H-SiC wafer and 20 mm away.

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GDR HOWDI 2022 MEETING:

ROLE OF HETEROATOM DOMAINS ON VOCs RECOGNITON ON B/N CO-DOPED GRAPHENE

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The recent collapse in economy of most developing countries due to the prevailing pandemic has led to an exponential illegal use of volatile organic compounds (VOCs) such as methanol and ethanol. This is mainly driven by the need to earn income from the illegal production of home-made hand sanitizers and backyard alcoholic beverages [1], [2]. As such, it is of great importance that faster and easy detection of these VOCs is of great importance, especially the detection of methanol so as to lower the lethal health effects associated with methanol contamination. Despite the use of numerous materials for the selective detection of VOCs, the fascinating properties of graphene and its derivatives are known to provide new avenue for improving sensitivity and selectivity of methanol and/or ethanol detection at room temperature. Moreover, co-doping with boron (B) and nitrogen (N) heteroatoms endows graphene with inter-changeable *p*- and *n*-type semiconducting properties, thereby tuning its chemical reactivity and electronic conductivity. Therefore, for this work, role of heteroatom domains on the VOCs detection properties of B/N co-doped graphene oxide nanostructures was investigated by using different B and N sources, in the form of ammonia borane (AB), and tetramethylammonium borohydride (TMABH). The study showed strong dependance of the type of heteroatom domains to the precursor material, and the influence of the domains to the sensing properties. In particular, the BN-rGO$_{AB}$ exhibited predominantly *h*BN domains with 0.5 B: N ratio as well as more pyridinic-N and NO$_x$ configurations ; thus promoting better stability of up to ~3 weeks with improved room temperature selectivity to methanol and/or ethanol.

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Figure 1: Conference logo.

Figure 2: Microwave-assisted synthesis of B/N-rGO for selective detection of VOCs

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GDR HOWDI 2022 MEETING: COPROPAGATING EDGE STATES PRODUCED BY THE INTERACTION BETWEEN ELECTRONS AND CHIRAL PHONONS IN TWO-DIMENSIONAL MATERIALS [1]

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Unlike the chirality of electrons, the intrinsic chirality of phonons has only surfaced in recent years [2, 3]. Here, we report on the effects of the interaction between electrons and chiral phonons in two-dimensional materials by using a non-perturbative and non-adiabatic Fock space solution. We show that chiral phonons introduce inelastic *Umklapp* processes resulting in a valley-selective pseudogap (as shown in Fig. 1), bridged by copropagating edge states that coexist with a continuum. Transport simulations further reveal the robustness of the edge states. Our results hint on the possibility of having a metal embedded with hybrid electron-phonon states of matter.

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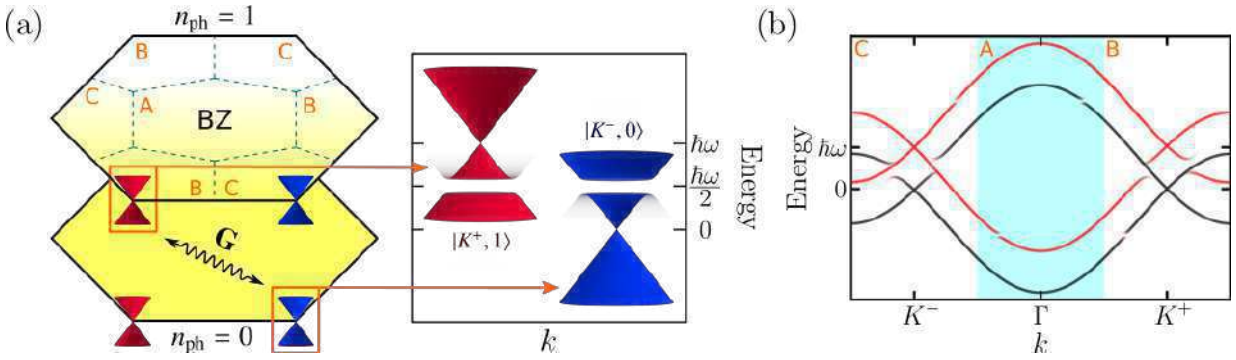

*Figure 1: We consider the interaction between electrons and a single chiral phonon mode of frequency ω, and momentum **G** corresponding to valley K^+. Considering the phonon Fock space, the system can be viewed as a semi-infinite series of pure electronic replicas centred at energies $\hbar\omega n_{ph}$, with n_{ph} the phonon population. Electron-phonon interactions generate transitions between momentum **k** in replica $n_{ph}=0$ and **k** - **G** in replica $n_{ph}=2$, opening a valley-selective pseudogap. A scheme of the mechanism is shown in panel (a), while the bulk band structure of the system is shown in panel (b), truncated to $n_{ph}=1, 2$.*

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TOWARDS MODELLING REALISTIC $WS_2/H_2O/SIO_2$ INTERFACES

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Transition metal dichalcogenides (TMDs) are studied extensively for use in electronic devices due to their 2D nature and semi-conducting properties. Films are often transferred using mechanical exfoliation onto substrates, such as SiO_2. However, little is known how substrate affects film properties. In the case SiO_2, it is well known that water layers are present at the surface under ambient conditions. This adds complexity to the interface and the interactions between the TMD and substrate. In this work we investigate the interface SiO_2/WS_2 with different thickness of water trapped between the two materials using density functional theory (DFT). We have produced different interfaces to capture the geometry of the interface and a type I band alignment was observed at the interface. The amount of water at the interface has been found to change the band offset. The interface structures of silica surfaces with water layers were created using classical molecular dynamics (MD)[1,2]. Several equilibrated water layers on the surface of silica were then truncated based on Radial Distribution Functions to 1, 2 and 3 water layers corresponding to different humidity and anneal conditions. These SiO_2/H_2O interfaces were then capped with WS2 and their geometries system optimised using DFT with PBE XC functional[3] and Grimme D3 VdW correction[4].

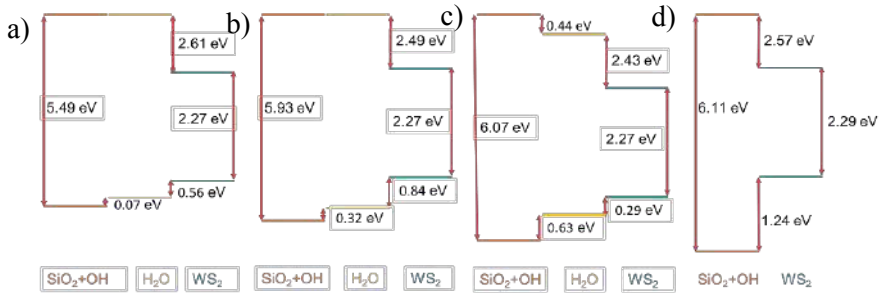

Figure 1: Band alignment diagrams of the $SiO_2/H_2O/WS_2$ interface. a) 1 layer of water, b) 2 layers, c) 3 layers and d) no water, hydroxylated surface.

In Figure 1, calculated band offsets are seen to fluctuate with amount of water present. This highlights the importance of experimental conditions during the synthesis of these 2D materials. The calculated band offset between SiO_2 CBM and WS_2 VBM of 4.79-5.14 eV is similar to values for exfoliated TMDs on SiO_2[5,6]. Further work using ab initio MD has been conducted to understand the structure of the interface. This shows a structured water layer near the SiO_2 surface with minimal interaction with the pristine WS_2 layer. Further analysis of structure and dipole moments of the materials will be analysed to understand the change in band offset at the interface. Overall, this work sheds a light on the interactions at the interface of SiO2/WS2 in realistic systems. The effect of water has been explored and indicates a large effect on the band alignment of the interface. This area is still being investigated and will be critical in understanding the functioning of 2D materials in electronic devices

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EXPERIMENTAL METHODS FOR NANOFLUIDICS: FOCUS ON SEALING TECHNOLOGY FOR DELICATE NANOMATERIALS

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Being the primordial solvent of life, water is essential to living organisms and human societies. The primordial role of water can be related to its unique physical properties particularly due to the structure of its hydrogen bond network or its dipolar moment. In extreme confinement situation, such as inside nanoscale channels, important modifications of these features are expected. Thus, many theoretical predicted that confined water in extremely small diameter pores exhibits unusual phase behavior[1] and structure compared to bulk water. Thanks to their stiffness, hydrophobic smooth surface and high aspect ratio, Single Wall Carbon Nanotubes (SWCNT) can be considered as a model nanochannel to get insight into the confinement of water molecules. As for instance, it was calculated that the phase of confined water in SWCNT which diameter is smaller than 1.4nm, behaves as ice-like water with structures from single file water chain to pentagonal or hexagonal structure depending on the SWCNT diameter [2]. On the other hand, it has been shown from experimental [3] and theoretical [4] calculations that water diffusion in SWCNT is significantly enhanced. Expanding our fundamental understanding of water properties when it is confined in SWCNTs can yield to substantial progress in desalination, drug delivery, energy harvesting, etc. applications. Although there are many numerical simulations reported on this system, only a few experimental works have been achieved and it remains a challenging task to get experimental proof on water behavior in such confined environment.

One of the main challenges to experimentally measure the properties of nanoconfined water is to be able to fabricate fully sealed microchips. Sealing is a central process for micro and nanofluidic chip fabrication, yet only a few materials can be used as they must be chemically inert, vacuum compatible, resistant to temperature change and must have no electrical effect.

In this poster, we will present a new sealing technology based on SU8 epoxy resist. We show that our bonding method is reliable and versatile for microfluidic, as it can be patterned by photolithography down to micrometric dimensions. It is thus found that a 30 µm high and 20 µm thick wall made of SU8 can sustain relatively pressures up to ~5 bars. We also measured ions permeation through the SU8 walls and found that it is similar or even better to PDMS. Electrical test shows no significant perturbation of electrical devices down to the sensitivity of our measurement set-up, i.e. pA, which makes the SU8 wall resistivity several orders of magnitude higher than that of carbon nanotubes. In addition, our sealing technology turned out to be chemically stable even at high temperature or under energy plasma. It is therefore perfectly suited for the fabrication of such as nanomaterials.

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High pressure tuning of the magnon-polaron resonance in the layered antiferromagnet $FePS_3$

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Iron thiophosphate ($FePS_3$) belongs to the family of van der Waals layered materials and has recently attracted much attention due to its remarkable magnetic properties. $FePS_3$ becomes antiferromagnetic below a Neel temperature of about 120 K with an unusually high magnon energy close to 120 cm^{-1}. We have applied high pressures to a bulk $FePS_3$ to tune the collective lattice excitations (phonons) in resonance with magnetic excitations (magnons). For pressures close to P~3 GPa, the magnon-phonon resonance is achieved and the strong coupling between the collective modes leads to the formation of new quasi-particles, the magnon-polarons, evidenced in our low temperature Raman scattering experiments by a particular avoided crossing behavior between the phonon and the doubly degenerate antiferromagnetic magnon. At the pressure-induced magnon-phonon resonance, three distinct coupled modes emerge that can be identified by applying a magnetic field. Up to P ~ 8 GPa, low temperature magneto-Raman scattering experiments allow for the identification of the magnon excitations which energy appears as nearly pressure independent and we can explore the different magnon-polaron regimes for which the phonon has an energy lower, equal to, or higher than the magnon energy. This results open new way to tune magnon-phonon interaction.

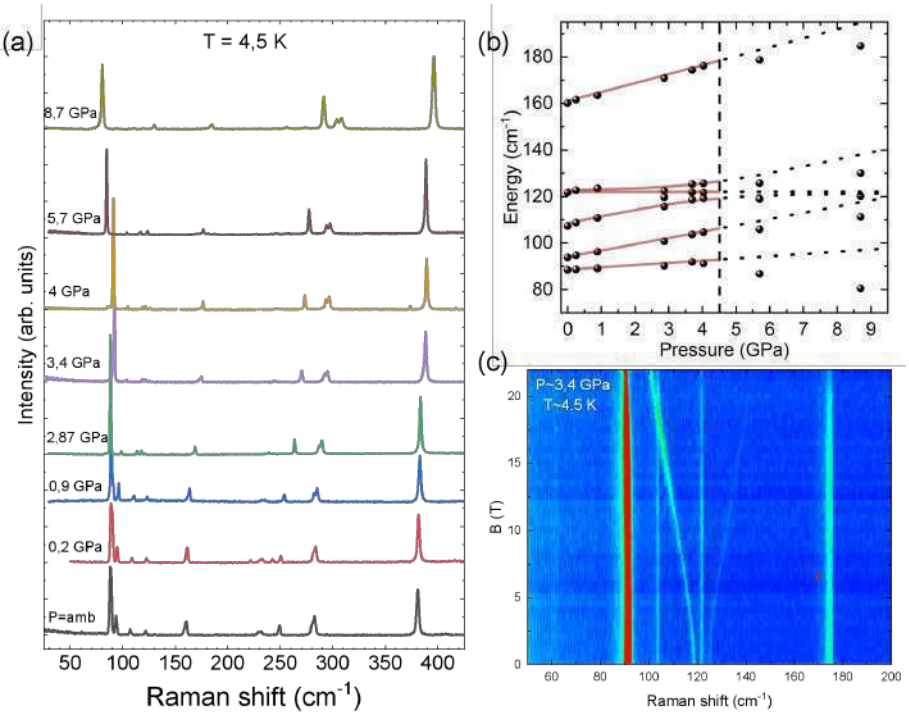

Fig. 1: (a) Low temperature Raman scattering spectra measured at different hydrostatic pressures up to P = 8.7 GPa. (b) evolution of the maxima of the peaks of the Raman scattering response as a function of the applied pressure. Solid lines are the results of a calculation using a coupling constant L3 = 2.8±0:3 cm^{-1}. The vertical dashed line indicates P= 4,6 GPa, the pressure induced structural phase transition. (c) False color maps of the magneto-Raman scattering response of bulk $FePS_3$ measured at T = 4.5 K and P = 3.4 GPa.

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DIELECTRIC PERMITTIVITY, CONDUCTIVITY AND BREAKDOWN FIELD OF HEXAGONAL BORON NITRIDE

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Hexagonal boron nitride (hBN) is a van der Waals insulator extensively used as gate dielectric in 2D material heterostructures. It is important to improve its characterization in terms of low-field permittivity and high-field strength up to the breakdown voltage. The present study, based on DC and RF transport in Au-hBN-Au capacitors aims at filling this gap. We benchmark two capacitor series: one with high-pressure, high-temperature crystals (from NIMS lab) and one with crystals obtained by the polymeric route (from LMI lab) [1].
From RF measurements in hBN crystals of thickness 10-100 µm, we extract a recommended value for the dielectric constant $\epsilon = 3.4 \pm 0.2$, which narrows down the commonly used estimate $\epsilon = [3 - 4]$.
Dielectric strength is characterized by monitoring the leakage current as function of DC bias. We find a breakdown electric field E_{BD} around 5MV/cm. The phenomenon is well described in terms of a non-linear dielectric conductivity with turns out to obey the Frenkel-Pool trap-assisted, thermally activated, Schottky transport law [2,3]:

$$\frac{J}{E} = \sigma_{BD} \times Exp\left[-e\frac{\Phi_B - \sqrt{eE/\pi\epsilon_0\epsilon}}{kT}\right] \quad (1)$$

where Φ_B is the deep-level trap energy and σ_{BD} the conductivity for fully ionized traps. Figure 2 illustrates the characteristic $\sqrt{E}$ lowering of the trapping barrier, and the thermally activated nature of conductivity (inset). We find a small variability of the trap energy, $\Phi_B = 1.27 \pm 0.03$ *eV* for the best samples and $\Phi_B \leq 1$ *eV* for defective samples. The largest value is quite comparable with literature measurements in SiO_2 [4] and Si_3N_4 [5].

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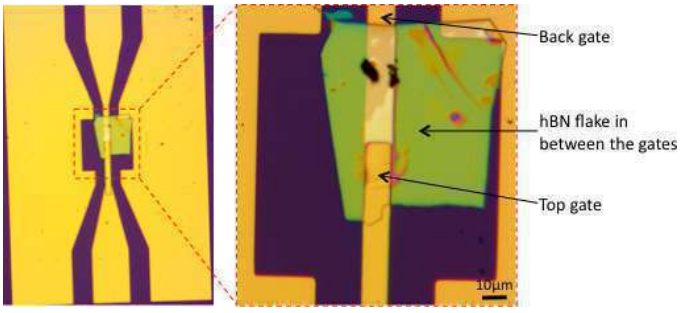

Figure 1: Metal-hBN-metal capacitor with zoom-in on the active flow

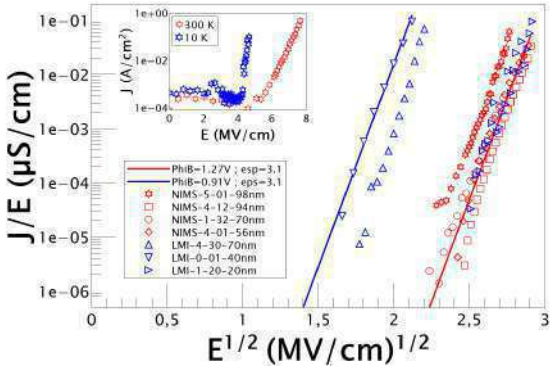

Figure 2: Frenkel-Pool plot of high-field hBN conductivity. Red symbols correspond to NIMS crystals and blue symbols to LMI crystals. Solid lines correspond to theoretical fits to the Frenkel-Pool law (1) taking $\sigma_{BD} = 0.1$ µS/cm, $\Phi_B = 1.27$ eV (red line) and $\Phi_B = 0.9$ eV (blue line)

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GDR HOWDI 2022 MEETING:
PHONON SIGNATURES OF GRAPHENE BASED SYSTEMS UNDER HIGH-PRESSURE CONDITIONS: SUSPENDED VERSUS SUPPORTED GEOMETRIES

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Graphene is a two-dimensional (2D) van der Waals (vdW) system that has created tremendous fundamental and technological interests mainly due to its 2D layered structure and unique electronic properties of massless relativistic fermions in condensed matter systems [1-2]. Highly-crystalline graphene may be obtained by exfoliation from graphite and transferred to SiO_2/Si substrates. Therefore, the application of hydrostatic pressure (3D effect) using Diamond Anvil Cell (DAC) in supported graphene creates a biaxial compression (2D effect) on the substrate. Hence, the study of supported 2D-vdW systems complicates the accurate estimation of elastic constants and other mechanical properties [3-6]. To overcome such limitation, we have designed a suspended geometry, which ensures the pure hydrostatic pressure in the multi-GPa domain on 2D-vdW systems. We will present our recent experimental high-pressure comparative study of bilayer graphene in suspended and supported geometries using different pressure transmitting media (PTMs). In particular, using in situ Raman spectroscopy as a probe, we identify a different pressure evolution between the two geometries when using methanol: ethanol (4:1) PTM. We followed the G and 2D phonons' pressure evolution and observe distinct responses related to delamination (pressure-induced wrinkle formation in SiO_2/Si substrates [7]). Moreover, we have investigated the possibility of pressure-induced bonding modification (i.e., sp^2 to sp^3) in our n-graphene samples using water as PTM [8] both in suspended and supported configurations.

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First observation of bernal boron nitride single crystals

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Hexagonal boron nitride is a wide band gap semiconductor which differs from the other nitrides because of its sp2 hybridized bonds forming honeycomb atomic planes weakly stacked through van-der-Waals interactions [1]. Since the first synthesis of large hBN single crystal by Watanabe and Tanigushi in 2004 [2], hBN has become a pivotal crystal in a wide variety of applications [1]. However, even though the hBN polytype (namely the AA' stacking) is the most commonly observed in high quality crystals, other boron nitride sp2 polytypes with different stacking can be formed [3, 4]. The calculations made on these polytypes predict changes of the band gap properties [5, 6]. Until now, no boron nitride sp2 polytypes single crystal other than hBN has been observed and little is known about their properties.

In this work we report the first observation of a bernal boron nitride high quality single crystal. In contrast to hBN which is centrosymmetric prohibiting second harmonic generation (SHG), the bernal polytype is non-centrosymmetric and SHG can be observed. By combining hyperspectral photoluminescence and SHG spectroscopy and photoluminescence excitation (PLE) spectroscopy on carbon-doped sp2 boron nitride crystals synthetized by the Ni-Cr flux method we identify a 10um size bernal boron nitride single crystal between two hBN single crystals. We then unravel the optical properties in correlation with calculations, where indirect and direct bandgaps are quasi-degenerate. This work paves the way for research on sp2 boron nitride polytype and their potential applications in optoelectronics.

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SELF-TRAPPED EXCITONS IN TWISTED hBN HETEROSTRUCTURES

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A new luminescence was recently discovered at the interface between two disoriented hBN, revealing the existence of a bright exciton at the interface [1], [2]. The luminescence of the interface is characterized by a large linewidth (~2 eV) and a maximum arising at 4 eV, i.e. 2 eV under the hBN gap. These properties are unexpected since the interface potential is estimated to be only a few 0.1 eV [3]. Their origin remains to elucidate.

In this work, I will present continuous cathodoluminescence (CL) and time-resolved CL (TRCL) study performed on a set of 30 hBN-hBN heterostructures. They are composed of hBN flakes obtained by mechanical exfoliation from different kind of hBN crystals (HPHT, APHT, PDC). An example of hBN-hBN heterostructure from HPHT crystal is illustrated in Fig. (a). The twist angle between top and bottom hBN was measured by electron backscattered diffraction (EBSD) in a scanning electron microscope. All fabricated heterostructures exhibit this new luminescence signal, as shown in Fig. (c) from 250 to 400 nm, with a particularly high intensity for twist angles larger than 5°. The map of its luminescence shown in Fig. (b) is clearly correlated to the presence of the hBN-hBN interface in Fig. (a). The exciton properties are investigated by exploring their luminescence dynamics in TRCL as a function of twist angle and temperature. Analysing the temporal decay of free excitons emitting at 215 nm reveal their trapping and detrapping from the interface, which is shown to be thermally activated on the 5K-300K range. The results suggest a self-trapping of free excitons at the hBN-hBN twisted interface, that will be discussed.

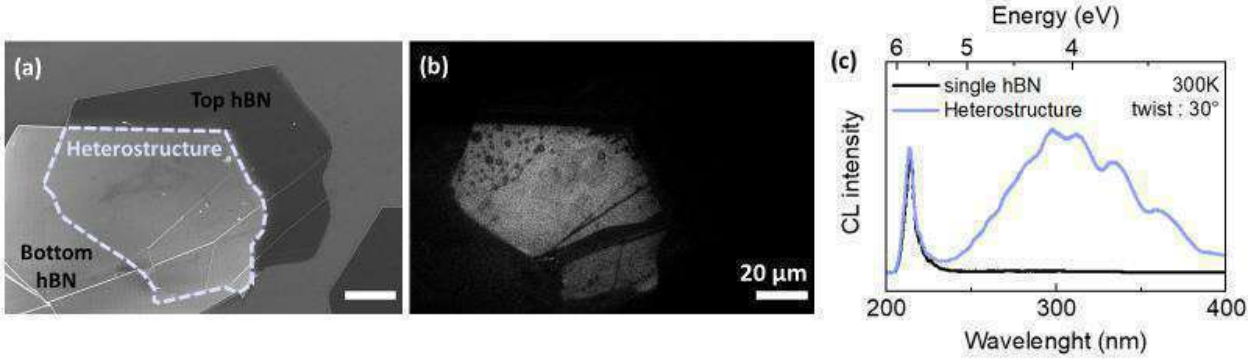

Figure (a) SEM image of a hBN-hBN heterostructure composed of two hBN crystals twisted by 10°. (b) Image of the cathodoluminescence signal at 300 nm. (c) Cathodoluminescence spectra from a single hBN and from a 30° twisted heterostructure. The free exciton luminescence occurs at 215 nm in hBN crystals, while the new luminescence appears between 250 and 400 nm in the heterostructure.

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GROWTH OF hBN SINGLE CRYSTALS AT ATMOSPHERIC PRESSURE

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High quality hBN single crystals are needed for the assembly of van der Waals heterostructures. Today graphene and TMDs devices are mostly assembled using hBN grown at high pressure high temperature (HPHT) provided worlwide by a single japanese lab [1]. The high quality HPHT crystals are though submillimiter, their size being limited by the anvil cells needed to reach high pressures. The atmospheric pressure high temperature (APHT) method [2,3] is an alternative and potentially up-scalable method which has already proven to give hBN single crystals of sufficiently high quality for graphene electronics [4].

In this work, we implemented the APHT method using NiCr metallic solvent for hBN growth. We fabricated centimeter scale hBN crystals, almost single crystalline as shown by electron backscattered diffraction. The hBN crystal quality is assessed from the free exciton lifetime measured by time-resolved cathodoluminescence at room temperature according to ref. [5]. The lifetime is found equal to 3.2 ns in average with a 12% standard deviation by sampling the crystal at the centimeter scale. These results are close to the best HPHT crystals reported (4.2 ns). It makes the APHT method very promising for the growth of hBN single crystals, with dimensions closer to microelectronic standards.

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CVD-GRAPHENE BASED TRANSISTOR MICROARRAYS FOR BIODETECTION OF NUCLEIC ACID SEQUENCES

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Graphene is a very promising 2D material which receives massive scientific interest. Label-free detection of bio-molecules, like DNA, by graphene field effect transistors (GFETs) with excellent sensitivities up to a few femto molar has been demonstrated by our group previously [1]. The detection principle is based on the electric field effect induced on graphene by the intrinsic charge of nucleic acid molecules.

We demonstrate the fabrication and characterization of 48 high quality GFETs arrayed in a single line with a common source and individual drain contacts. This arrangement requires homogeneous and defect free graphene sheets over a few square millimeters. Therefore, CVD-grown graphene was wet-transferred onto a regular silicon wafer piece. The graphene was covered with Al_2O_3 and SiO_2, respectively deposited by ALD and PECVD, to stabilize the electric characteristics of the devices. Conventional photolithography with UV illumination and lithographic masks was used for channel and contact patterning. Drain and source contacts were done by consecutive e-beam evaporation of titanium and gold.

The GFETs were characterized in a backgate setup and we report electron and hole carrier mobilities of around 4000 $cm^2\ V^{-1}\ s^{-1}$ with the Dirac peak location close to zero voltage. Typically, 95% of all GFETs on a given chip display high quality and homogeneous characteristics.

The outstanding charge carrier mobility of graphene devices at room temperature makes them a prime candidate for sensing weak electric fields. Negatively charged DNA can be accumulated on the device surface by hybridization. The resulting electric field of the surface-immobilized DNA induces a shift of the graphene's Dirac peak. We aim to use this technology to perform sensitive and label-free multiplex microarray experiments. Microarrays based on GFETs represent a promising novel method, ready to overcome the obstacles of conventional fluorophore based microarrays.

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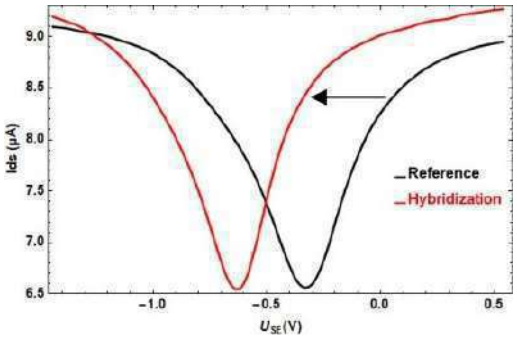

Figure 1: Dirac peak shift upon surface hybridization of nucleic acid molecules. From [1].

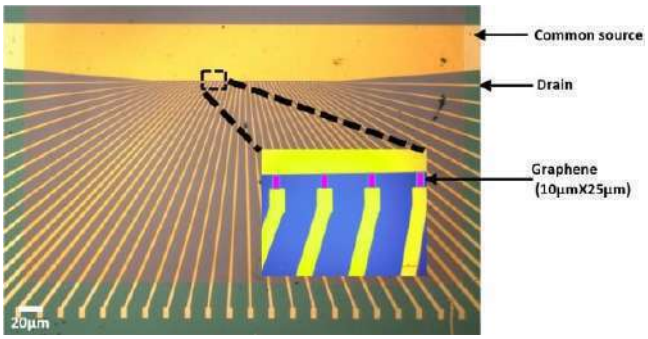

Figure 2: Microscopic image of the CVD-graphene transistor array device layout. From [1].

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HOWDI Low dimensional van der Waals heterostructures

MODELLING ELECTRONIC AND OPTICAL PROPERTIES OF GRAPHENE AND BORON-NITRIDE NANORIBBONS

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In recent decades, graphene and hexagonal boron nitride (hBN) have attracted a great deal of interest as other 2D materials, with their high conductivity and optical properties, respectively, being of particular interest. Introducing a confinement in one direction produces interesting changes in their properties, for the study of these structures (nanoribbons), it is necessary to take into account their morphology since their properties are very sensitive to it [1-3]. As far as the shape of the edge of the nanoribbons is concerned, two types can be distinguished: zig-zag and armchair [2,3]. The latter have a gap at Γ, both for graphene (AGNR) and hBN (ABNNR) nanoribbons. The gap value depends on the system size and there is three different gap families dependences [4,5], which tend to the gap value of their respective 2D material, if the nanoribbon is large enough.
This peculiar dependence allow us to tune the gap of both nanoribbons and also their optical properties, changing minimally their size. First, we present a study of AGNR and ABNNR electronic structure as a function of their width, for that simulations have been carried out with density functional theory and a ladder tight-binding model proposed in other works [5,6]. And also, optical spectrum calculated by time-dependent density functional theory.

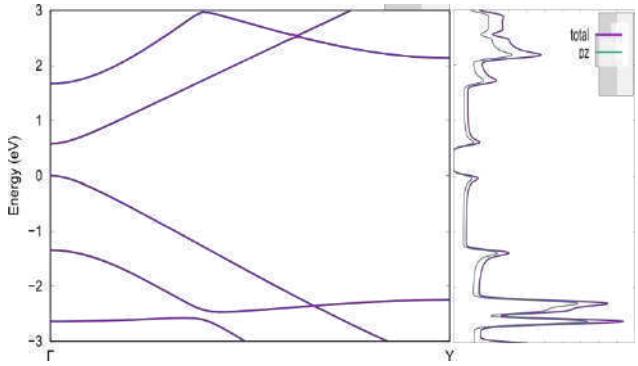

Figure 1: Band structure of AGNR with width = 4.87Å and passivated with hydrogens on the left panel and density of states total and projected on p_z orbitals on right panel. Calculations have been carried out with density functional theory.

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MOBILITY
OF GATED TMDS AS A FUNCTION OF VALLEY PROFILE

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Monolayer semiconducting transition metal dichalcogenides (TMDs) are some of the most intensively studied 2D materials. Their rich transport and optical properties are dictated by a multi-valley band structure and a spin texture induced by spin-orbit interactions. Experiments and ab initio simulations suggest that those features are quite sensitive to the environment, meaning that integrating TMDs in van der Waals heterostructures will change their properties. This is particularly true of the valley profile, i.e. the relative energy of the different valleys. Indeed, in conjunction with gate-induced changes in the carrier density, the valley profile has a significant impact on the electron-phonon scattering, by changing the electronic states involved and the strength of the coupling itself.

We develop an ab initio model of electron-phonon scattering and the room-temperature mobility of semiconducting TMDs (MoS2, WS2, WSe2, MoSe2) where valley profile and electrostatic doping are treated as parameters. We start from state-of-the-art transport simulations [1] in electron- and hole-doped TMDs and model the consequences of shifting the valley and changing doping. We account for standard free-carrier screening as well as the enhancement of electron-phonon interactions in case of multivalley occupation [2]. The results provide a unified understanding of phonon-limited transport in the conduction and valence bands of all semiconducting TMDs. Due to free-carrier screening, the doping-dependent mobility consistently peaks around $n/p \approx 8\ 10^{12}$ cm^{-2}. Multivalley profiles (i.e. second valley close to the band edge) reduce the maximum mobility significantly. This work [3] gives clear guidelines to the experimental community on how to optimize the transport properties, and suggests ways to characterize the valley profile from doping-dependent transport.

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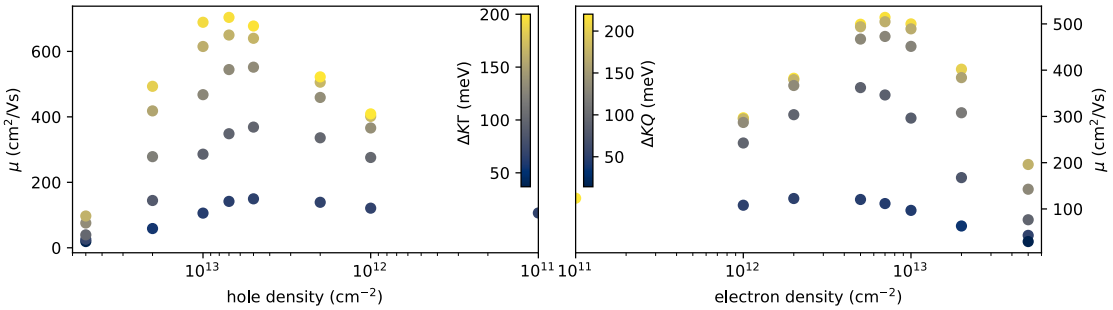

Figure 1: Mobility of MoS2 as a function of carrier density and valley profile. The colorscale represents the valley profile, via the parameters ΔKQ and $\Delta K\Gamma$, i.e. the energy difference between the K and Q or Γ valleys, respectively.

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X-RAY EXCITED OPTICAL LUMINESCENCE OF BORON NITRIDE MATERIALS

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Hexagonal boron nitride (h-BN) is a 2D wide-bandgap semiconductor that, in the last years, is emerging as a novel optical material with strong luminescence in the far-UV. Besides the intrinsic luminescence of the perfect crystals, h-BN hosts a number of luminescence centers which has been identified as bright and stable single photon sources in the visible and far-UV spectral range. Despite a large number of recent works, the structure and chemical origin of these optical centers are still controversial. The possibility of correlating optical features and elemental information at the relevant atomic scale could provide fundamental insights for it. This goal can be achieved by combining cathodoluminescence and core-eels spectroscopy within a spherical aberration corrected scanning transmission electron microscopes (STEM) which allows high space selectivity through sub-angstrom electron probe. Complementary information can be obtained by using the element selectivity of X-rays when tuned at a resonance of the elements present in the sample, through the so-called X-ray excited optical luminescence (XEOL).

This technique allows to acquire full luminescence spectra in the visible-far UV range while scanning the energy of the incident radiation across the core absorption edge. State of the art XEOL has been applied to the study of the luminescence of high quality pristine and doped hexagonal and cubic BN crystals by using a novel experimental setup we implemented at the SEXTANTS beamline of the Synchrotron SOLEIL. Several absorption edges (B, C, N, O) have been investigated demonstrating the correlation between specific luminescence features and the presence of O-B bonds.

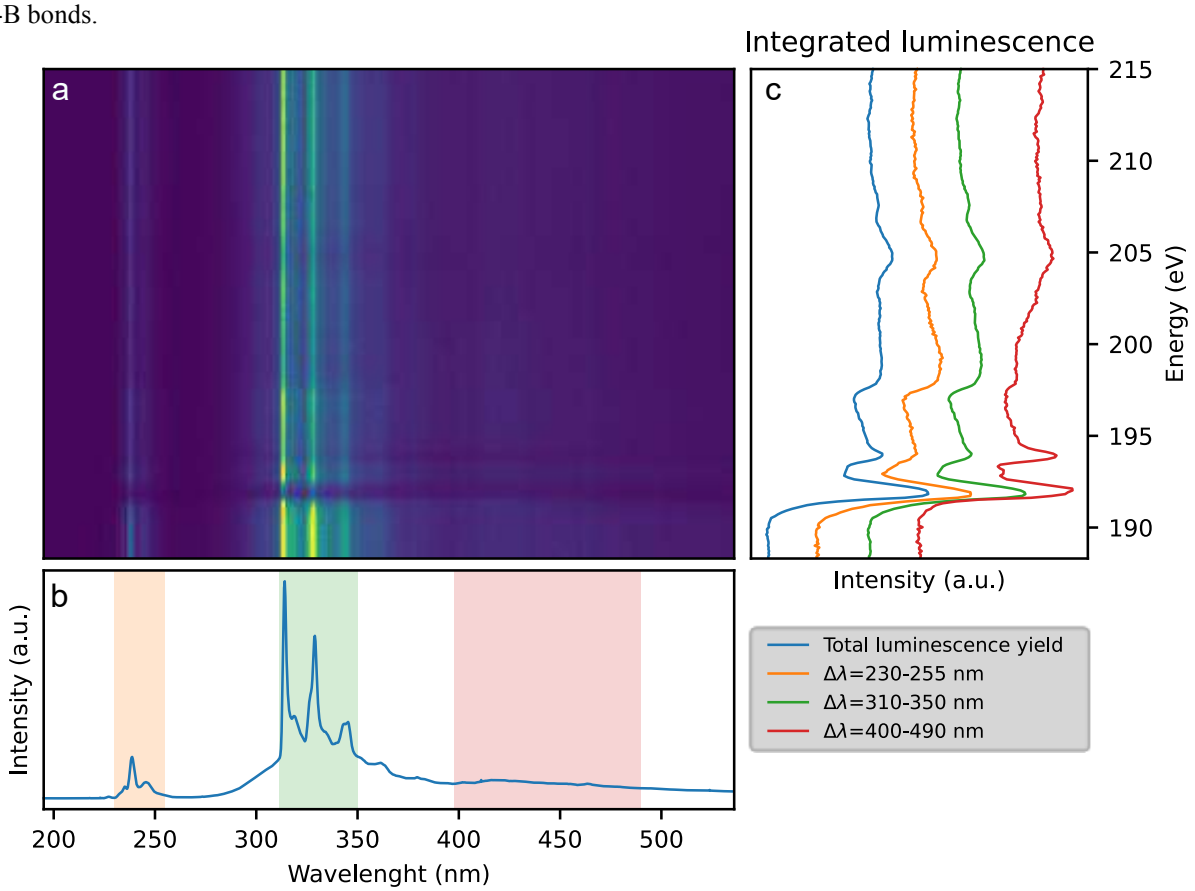

Figure 1: (a) Luminescence spectra of high purity h-BN crystal acquired while scanning the incident beam across the boron K edge. (b) Luminescence spectrum integrated over all the X-ray beam energies. (c) Total luminescence yield (blue line) and partial luminescence yield integrated at different wavelength windows.

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GDR HOWDI 2022 MEETING:

ULTRA WIDE-BAND NIR-VIS MICRO-ABSORPTION CHARACTERIZATION OF PTSE2 THIN FILMS

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Among transition metal dichalcogeniodes, few layer PtSe2 stands out for its potential in high frequency optoelectronic properties in the telecom band (around 1.55 µm) thanks to a tunable bandgap and large electronic mobility [1] . First synthesized in 2015, this material has attracted much attention, and several growth methods have been developed with various success. For example, thermally assisted conversion (TAC) of Pt provides continuous polycrystalline films but with sizeable Se vacancies which can affect the optical and electronic properties of the material. In this work, we compare the light absorption properties of several PtSe2 sources (CVT/exfoliated, MBE, TAC, ion implantation).

To this aim we have developed a micro-absorption setup enabling to study both continuous films and micro-metric samples obtained by exfoliation, and to resolve inhomogeneities. This setup covers both the visible and near infrared range 0.4 – 1.6 µm using both of Si and InGaAs detectors (see Fig. 1). The performance and accuracy of the experimental setup is assessed by studying graphene and SiO2 on Si calibres.

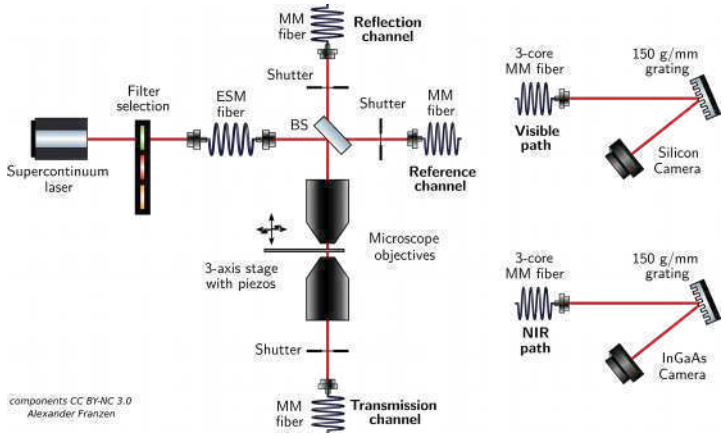

Figure 1: micro-absorption NIR-VIS setup experimental scheme

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CVD synthesis of sp2-hybridized multilayer boron nitride films

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Since graphene isolation in 2004, the 2D materials is a blooming research field. Due to its unique properties, sp² hybridized boron nitride (BN) has been acknowledge as a key towards integration of other 2D materials in devices. Indeed, it is structurally very close to graphene – their lattice mismatch is only 1.7%- a semiconductor, atomically flat and thermally and chemically inert. It is therefore a choice material to be used in the van der Waals heterostructures with other 2D materials either as a top layer to protect another 2D material from its environment [1], or as a dielectric interlayer [2] and mostly, as a flat substrate [3]. However, these applications have been demonstrated using mechanically exfoliated BN from low defective and highly crystalline single crystals. Yet, this process limits the size of the devices that can be created to sub millimeter scale. In order to develop devices at a wafer scale, it is therefore critical to master the synthesis sp² hybridized BN layers at low cost, large scale and high quality.

In that respect, the goal of the researches we have undertaken is to develop the synthesis of sp²-hybridized multilayer BN films with structural specifications fitting these requirements. We have already successfully obtained heteroepitaxial growth of a few nanometer-thick sp2 hybridized BN film of well-stacked and flat layers on Ni (111) surface of polycrystalline substrate [4]. Here, we will present our work on Rapid Thermal CVD from Annealsys (www.annealsys.com). We will show how we successfully adapt our growth process to this new reactor on centimeter monocrystalline nickel substrates. We will detail the crucial step of nickel surface preparation before the synthesis for these Ni(111)/YSZ/Si(111) pseudosubstrate, and how it can impact the quality of the synthetized BN. We will present the results of the structural and quality characterization of the BN films from the macroscale to the nanoscale (OM, SEM, TEM, AFM, LEED, Raman and luminescence spectroscopies) on the growth substrate and after transfer onto dedicated substrate.

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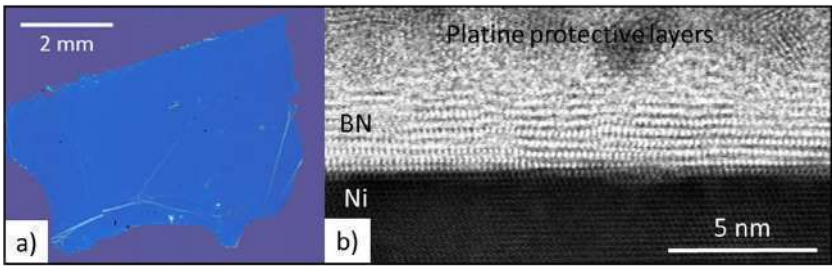

Figure 1: All the results present here are obtained on the Annealsys RTCVD (a) Optical microscopy image of a BN film grown on Ni(111)/YSZ/Si(111) pseudosubstrate and transferred on SiO2/Si, showing the large scale transfer.(b) HRTEM image of multilayers BN film grown on nickel (111) showing the thickness and the regular stacking of the BN layer (MATMECA, Titan G2 Centrale Supelec, 300 kV).

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THEORETICAL STUDIES OF NOVEL GRAPHENE BASED NANOSTRUCTURES

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The outstanding electronic, optical and mechanical properties of graphene have inspired the scientific community at both the fundamental and application levels. However, along the way several key scientific issues have to be addressed and one of the main challenges is the control and the modification of graphene electronic properties. This concerns notably the controlled opening of a sizable bandgap (of a few hundreds of meV). Indeed, despite its exceptional carrier mobility of high interest for future applications, graphene is a zero-bandgap semiconductor. Therefore, a graphene layer in itself is not appropriate for most applications in electronics or in optoelectronics like diodes or transistors for example.

Some very appealing methods to open a sizable bandgap in graphene consist in reducing nanoscale dimensions or in forming an ordered array of holes in its honeycomb lattice. Indeed, the reduction of one dimension of graphene leads to graphene nanoribbons (GNRs) [1] while the reduction of the two dimensions leads to graphene quantum dots (GQDs) [2]. As forementioned, a gap can be opened via ordering an array of holes in a graphene lattice as shown in a first theoretical study in 2008. It is called a Graphene Nanomesh (GNM) or a Graphene Anti-dot Lattice (GAL) [3]. First, experimental realizations of GNMs started in 2010 at UCLA [4] and LBNL [5] through the use of a combination of di-block copolymer organization or nanoprinting and selective etching (top-down approach).

In the context of two very close projects in the Saclay area namely **BOGART** and **GANESH**, we study theoretically electronic, optic and transport properties of novel graphene based nanostructures as a function of their size (see Fig. 1a). To this end, we perform Density Functional Theory (DFT) and Tight-binding (TB) calculations in order to compare with experimental results. These new 2D-materials can be graphene nanoribbons (GNRs), graphene flakes and graphene Nanomesh (GNMs) (see Fig. 1). The synthesis of those is achieved by assembly of molecular precursors on a metal surface (Au(111) or Cu(111)) via the Ullmann coupling and after annealing at high temperature thanks to our collaboration teams.

In this poster, we will explore their property dependence with on the system size and symmetry. Besides, different theorectical methods to control a gap will explored. We will show our TB and *ab initio* calculated results on their electronic strutures and optical absorptions from a starting molecule to its infinite structure. In addition, the transport properties will be exhibited by *ab initio* simulated Scanning tunneling microscopy (STM) images as well as tunnel current spectroscopies (STS). In Fig. 1, it's possible to obtain a GNMs from a starting C_{42} molecule (a derivative of Hexa-benzocoronene) by increasing its mass (called M) with lattice vectors $\{\mathbf{b}_1,\mathbf{b}_2\}$ in (a), this network is a centered rectangular 2D crystal, where a semiconductor behavior is predicted, as it is shown in (d). Valence and conduction bands are pure $2p_z$ delocalized states. A direct gap is located at the gamma point, while the valence and conduction bands are no longer degenerate due to the loss of hexagonal symmetry compared to the complete graphene lattice. On the other hand, following the idea in [2], we predict the properties of some graphene quantum dots (GQDs) as C_{78}, C_{96}, C_{132}, C_{162} in (b). Especially, in (c), we found out to break down their symmetry by adding another layer below translated or rotated.

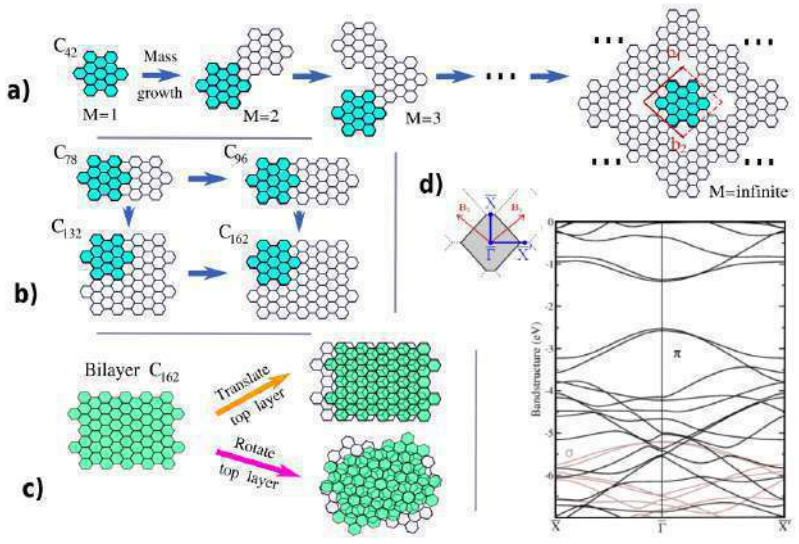

Figure 1: a) GNMs built up from a C_{42} molecule. b) Amount of examples of studied big molecules. c) Some studied bilayer structures from C_{162}. d) DFT result of GNMs in a).

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NANO-OPTOMECHANICS OF A FEW-LAYER $FePS_3$ SUSPENDED MEMBRANE

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The persistence of a magnetic order in a monolayer of van der Waals magnetic material has been established in 2016, offering the perspective to embed a magnetic degree of freedom in heterostructures made of other bidimensional materials such as graphene or transition metal dichalcogenides. The physical properties of van der Waals materials can be easily tuned by perturbations like strain or doping, inviting to the exploration of magnetism in two dimensions and its exploitation in novel ultrathin devices [1]. Our approach is to suspend these magnetic materials forming drum-like resonators in order to investigate the influence of the strain on their magnetic order (Fig. 1 **a**,**b**). We probe the phase transition of $FePS_3$, an Ising zigzag antiferromagnet, combining two complementary methods on the same experimental setup: Raman spectroscopy and nano-optomechanics [2, 3]. The magnetic phase transition of the membrane is attested by a modification of its Raman signature arising from the vibrational modes of the iron atom in the crystal (Fig. 1 **c**), concomitant with changes in the drumhead mechanical resonance frequencies around its Néel temperature, monitored through the spectra of their Brownian and laser-actuated motions (Fig. 1 **d**). These results are enriched by a reconstruction of the membrane vibrational modes spatial profiles and a preliminary study of the light-induced measurement backaction. Further experiments on more elaborated samples will explore the phase transitions of magnetic van der Waals heterostructures and their control by strain.

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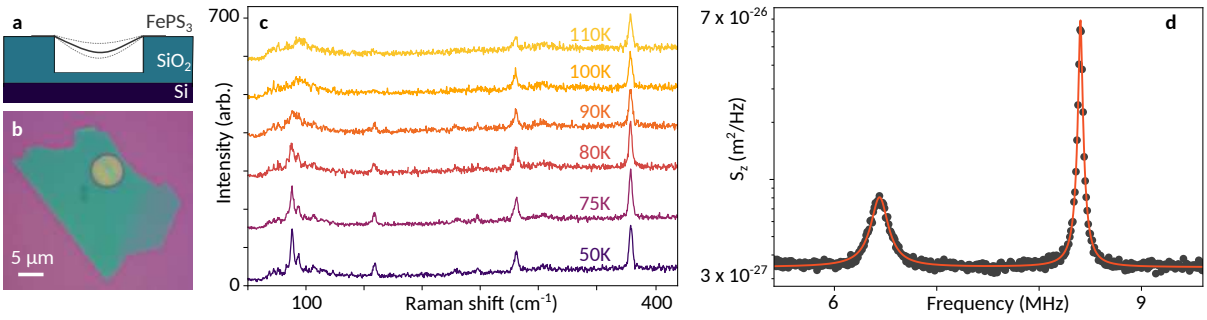

Figure 1: **a**. Schematic representation of a nanoresonator made of few-layer $FePS_3$ suspended over a hole etched in a Si/SiO_2 substrate. **b**. Optical picture of the studied sample constituted of a $FePS_3$ suspended membrane with an estimated thickness of 10 nm (appearing in yellow) over a hole of 6 µm in diameter and 400 nm in depth. **c**. Raman spectra recorded around the Néel temperature of our sample. The spectra are vertically offset for clarity. **d**. Displacement spectral density of noise of the $FePS_3$ membrane at room temperature (black dots: data, orange line: Lorentzian fits).

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GDR HOWDI 2022 MEETING:
SAMPLE ABSTRACT AND PREPARATION INSTRUCTIONS

Revealing low frequency magnetic moment fluctuations of TbPc2 single-molecule magnets grafted on graphene.

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In this work, we explore low temperature transport in graphene field effect transistors decorated with TbPc2 single-molecular magnets (SMM)[1].
The low temperature magnetoresistance features typical universal conductance fluctuations (UCF) of a phase-coherent sample. However, these UCF also display a magnetic field-dependent noise, which is highest at low temperature and low field. We find a noise spectrum with a 1/f dependence that suggests the existence of magnetic two-level systems with a wide distribution of field-dependent relaxation times. This points to anisotropic Ising-like fluctuating magnetic moments whose characteristic energy barrier decreases with out-of-plane magnetic field.

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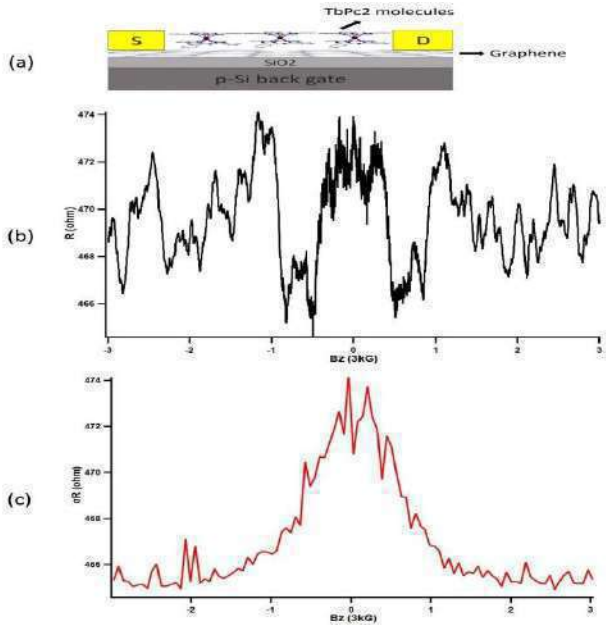

Figure 1: (a) The graphene monolayer connected to source and drain electrodes. TbPc2 deposited on top of device. (b) Out of plane field sweep in between ±3000 gauss. The magnetoresistance reveals low frequency magnetic noise when the applied field is close to zero. (c) The variance of the low frequency noise from Fig. 1b.

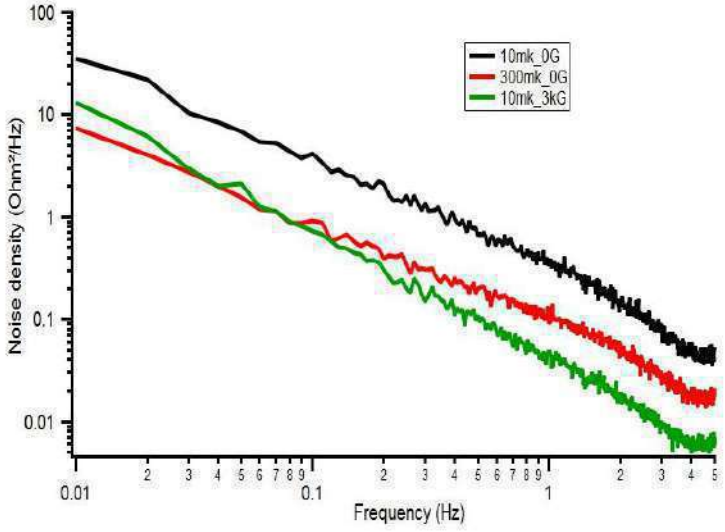

Figure 2: Noise spectral density as a function of frequency, at zero field and 10 mK (black curve), at zero field and 300 mK (red curve), and at 10 mK in a 3000 G magnetic field. The noise has a 1/f dependence between 10 mHz and 1 Hz. The noise amplitude decreases with increasing temperature and magnetic field.

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THERMODYNAMIC CALCULATIONS OF CVD GRAPHENE GROWTH FROM SOLID AND GASEOUS PRECURSORS

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Chemical vapor deposition (CVD) is generally limited to the use of gaseous raw materials, making it difficult to apply such technology to a wider variety of available carbon feedstocks. Nevertheless, it was already demonstrated that large area, high quality graphene with controllable thickness can be grown from different solid carbon sources such as polymers, green biosources or waste materials, deposited on a metal catalyst substrates [1,2]. Till now, the design of these processes and the choice of their operating conditions have been performed quite exclusively by long, tedious and expensive series of experiments. To improve the process, it is interesting to provide a more comprehensive understanding of the growth precursors through modeling. Hence, this work aims to compare the growth precursors of graphene issued from solid precursor's vaporization with those obtained by direct methane thermal decomposition [3]. In our approach, poly methyl methacrylate (PMMA) obtained by polymerization of methyl methacrylate monomer $C_5H_8O_2$, is token as model for solid carbon source and compared to CH_4 decomposition. So, for a chemical system, the set of existing gaseous molecules must be well-known for the understanding of the CVD process. This could be described by the species molar fractions as determined using extended chemical model with 134 species, including radicals, cycles and polycyclic aromatic hydrocarbons (PAHs). Thermodynamic equilibrium calculations shown in Figure 1 were performed by varying the carbon source precursor from gaseous CH_4 (a) to solid pmma (b) with the idea of finding working windows allowing the synthesis of graphene without defects and with a large grain size from solid sources. We also estimated the minor species which have not been completely studied such as PAHs issued from pmma Figure 1 (c). If these PAHs are present in small mole fraction < 3 10^{-2}, they are thought to play a role in graphene nucleation

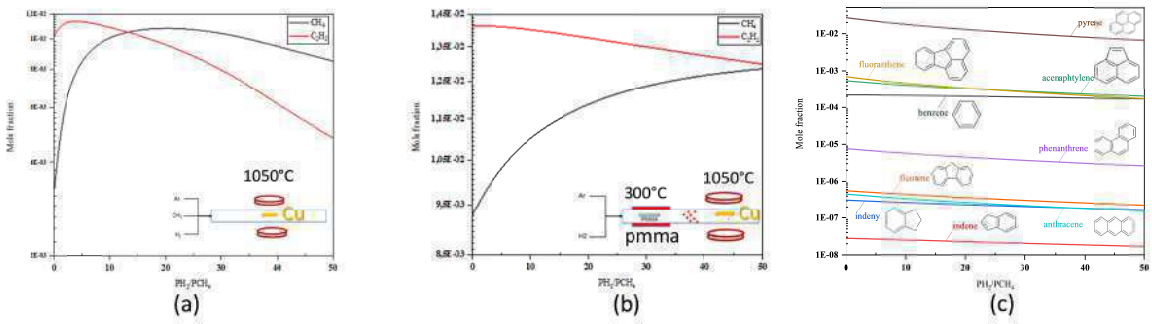

Figure 1: Methane and acetylene flow rates versus the ratio of hydrogen and methane partial pressure calculated at T=1050°C - P=20 mbar and 25 sccm of argon for two classes of precursors in the inlet. (a) 10 sccm of gaseous methane (b) solid PMMA decomposed at 300°C upstream the growth zone. (c) polycyclic aromatic hydrocarbons (PAHs)

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NANOSCALE WETTING FILMS ON 2D MATERIALS

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Transport studies (ionic/chemical/mass/thermal transport) in a liquid confined at the nanoscale is an emerging field referred to as nanofluidics with many applications such as osmotic power generation, desalination or molecular separation. Unconventional behaviors have been demonstrated when ultra-confinement is reached in a channel, below 10 nm and essentially near the liquid molecular scale. Electrical conductivity, wettability, surface charge and polarity of the confining walls are then key parameters to consider. The field benefited from the recent developments of nanofabrication techniques and the implementation of original nanofluidic devices, many of those based on 2D materials (graphene, MoS_2, hBN) in geometries such as nanotubes, nanopores drilled membranes or lithographed slits [1,2]. Yet they all rely on many steps of complex nanofabrication, show limited *in-situ* control and are subject to fouling [3].

Here we propose a new class of versatile nanofluidic devices based on wetting films, which simply originate from the condensation of water humidity on a surface, using an original environmental cell developed in the group. The condensed water film is controlled in thickness in the nanoscale range. Far-field optical characterization through a window and electronic transport measurements with pre-patterned electrodes can be performed. Preliminary work has been done on hydrophilic SiO_2 substrate, correlating film thickness and electrical conductivity. Condensation on 2D materials is under study with the aim to better understand the controversial wetting mechanisms [4], and to take full advantage of their defect-free flat surface and their *in-situ* electrostatic or optical actuation for advanced nanofluidics experiments.

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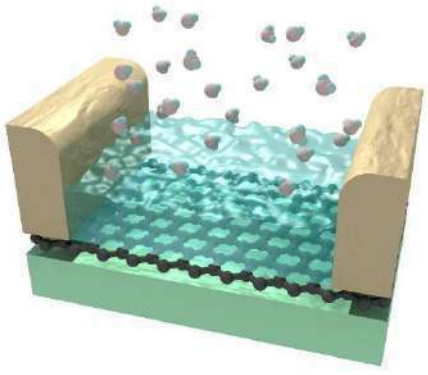

Figure 1: Schematic visualization of the targeted device, with a condensed water wetting layer on top of a contacted graphene layer.

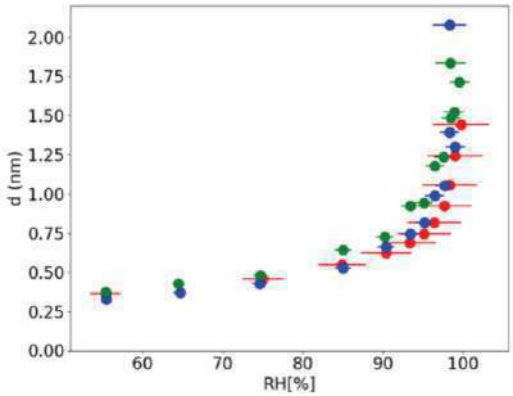

Figure 2: Thickness of the water wetting layer on top of SiO_2 measured by ellipsometry, as function of the cell atmosphere humidity.

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GDR HOWDI 2022 MEETING:
VAN DER WAALS HETEROSTRUCTURE FERROELECTRIC SYNAPSE

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Saturation of CMOS technology while increasing demand for powerful computers, accompanied by the massive progress in AI on the programing side which is unmatched by the hardware side forms the biggest technological challenge in the computer science domain at the moment. Inspired by the human brain, massive efforts are being spent addressing that challenge. Two components are needed to mimic the human brain architecture: Neurons and Synapses. Many device concepts have been proposed to mimic the behavior of both the biological neurons and synapses. One of these devices is the ferroelectric Field-effect-transistor as a possible electronic synapse. Here we demonstrate the synaptic functionality of a full 2D Van der Waals heterostructure ferroelectric FET. Multistate Ferroelectric memory effect was demonstrated with high on/off ratio (~ 6 orders of magnitudes). Synaptic functionality was demonstrated and characterized (ex. LTP/LTD, SRDP) showing a high dynamic range (up to 100 states) and Excellent cycle to cycle reproducibility (less than 1% variation). Furthermore, extracted parameters were used to emulate a neural network and very good accuracy (~91%) has been shown (Fig 2).

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Figure 1: Conference logo.

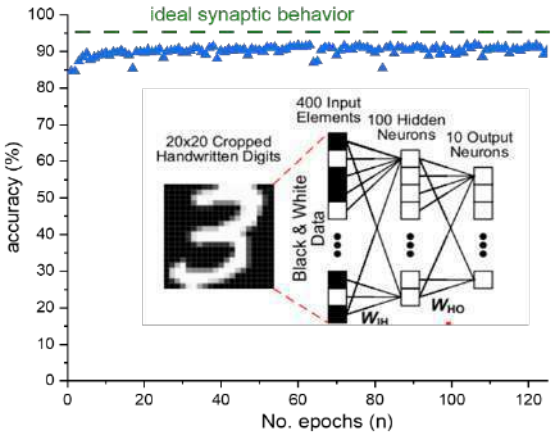

Figure 2: Stochastic Gradient Descent simulation of the neural network shown below the curve, with the synapses parameters extracted from the experimental data.

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