International workshop on 2D Heterostructures - Annual meeting 2025 of the GDR and IRN HOWDI

24-28 November

Abstract Booklet

MONDAY 24

Twisted Layers 1

Annual meeting 2025 of the GDR and IRN HOWDI
24-28 november 2025 Sète, France

Oral

CORRELATED PHASES IN MOIRE MATERIALS

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Stacking two or more layers of a two-dimensional material with a slight mismatch – either through a twist angle, or by using different materials with a different lattice constant – creates an interference pattern, which profoundly modifies the material's band structure. In these moire materials, fine tuning the superlattice can create a nearly flat band, which gives electron-electron interactions a prime role. Correlated phases such as superconductivity, strange metallicity, ferromagnetism, or the fractional quantum anomalous Hall effect have been observed in graphene based or transition metal dichalcogenide (TMD) based moire materials. In this tutorial, I will focus on correlated insulators observed in magic angle twisted bilayer graphene and in twisted TMDs. After presenting some of the correlated insulators occurring at commensurate filling, I will delve into the interplay of topology and interactions, which leads to fractional Chern insulators.

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OPTICAL CONTROL OVER TOPOLOGICAL CHERN NUMBER IN MOIRÉ MATERIALS

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Abstract

In recent years, moiré heterostructures of two-dimensional materials have emerged as a versatile and highly tunable platform to study strongly correlated electronic systems. In particular, devices based on twisted MoTe2 bilayers have gained significant interest due to their flat and topologically non-trivial valence bands. Recent studies showed that this system hosts the long-sought integer and fractional Chern insulating (ICI & FCI) states at moiré filling factors nu =-1 and nu=-2/3 with Chern numbers C = -1 and C = -2/3 (1-4). In this talk, we present a method to optically control the spin degree of freedom of itinerant holes in the moiré Chern bands of twisted MoTe2 bilayers. We show complete optical orientation by resonant excitation of the attractive polaron resonance for moiré filling factors ranging from nu = -0.4 to nu = -1.3, thus providing an ultra-fast, local, and non-invasive method to control the Chern number of FCI states. This opens up potential applications for quantum technologies, such as defining chiral edge states without the need for electrical contacts.
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*Speaker

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Oral

A REAL SPACE METHOD FOR EXCITONS IN HEXAGONAL BORON NITRIDE: APPLICATIONS TO DISORDER AND TWIST

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Hexagonal Boron Nitride (hBN) is well-known for its peculiar excitonic effects [1,2,3]. Here, we report on the extension of a real-space methodology for the computation of excitons in hBN [1,4] particularly suitable to the case of complex unit cells and its applications to static disorder and large-angle twisted hBN bilayers (~30°). More specifically, we perturbatively construct the Bethe-Salpeter Hamiltonian in a basis of spatially localized electron-hole pairs whose size grows linearly with the unit cell size. Combined with linear scaling algorithms [5,6], this allows for the efficient computation of properties of interest, such as the optical absorption spectrum, for structures containing thousands to tens of thousands of atoms.

As a first application, we illustrate its performances in the case of single layer hBN in the presence of Anderson disorder, showing its effects on the optical response and the exciton localization. We successively apply it to study twisted bilayer hBN in the neighborhood of the quasicrystalline limit (twist angle close to 30°) [2]. We first fix the parameters of the model relying on *ab initio* BSE calculations carried out on small approximants, and then apply it to study larger quasicrystal approximants, which are better representations of the quasicrystal limit (30°). The dependence of optical absorption on stacking and twist angles between ~20° and ~40° is further scrutinized, as well as the localization of electron-hole pairs in real space [2].

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TUESDAY 25

2D Magnets 1

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Oral

DOPING-CONTROL OF EXCITONS AND MAGNETISM IN FEW-LAYER CRSBR

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In two-dimensional (2D) magnets, phenomena distinct from bulk magnetism have been revealed, such as sensitivity to charge doping and electric field in few-layer CrI_3 [1]. Within the class of 2D magnets, air-stable CrSBr stands out as an antiferromagnetic semiconductor with a high Néel temperature, excitons coupled to the magnetic order [2], and exciton-magnon coupling [3]. In this talk, I will present our work on doping-control of excitons and magnetism in few-layer CrSBr [4,5]. We demonstrate that both exciton and magnetic transitions are sensitive to field-effect charging, exhibiting bound exciton-charge complexes and doping-induced metamagnetic transitions. We further visualize magnetic domain formation induced by magnetic field or charge-doping at the metamagnetic transition all-optically by raster-scan reflectance imaging. Our work identifies few-layer CrSBr as a rich platform for exploring collaborative effects of charge, optical excitations, and magnetism.

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Oral

ENGINEERING ANTI-FERROMAGNETIC DOMAINS IN 2D CRSBR

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CrSBr is an emerging van der Waals magnet that has been gaining significant attention, as it exfoliates easily down to the monolayer, and remains stable under ambient conditions. It also supports a relatively high Curie temperature of 140 K and exhibits magneto-optical coupling through its excitons [1].

A key challenge in working with anti-ferromagnetic (AF) materials is the control and measurement of their order parameter. In our work [2], we propose a novel method to manipulate the AF order in a CrSBr bilayer by leveraging lateral exchange interactions within a single crystalline flake.

Using scanning NV center magnetometry in a cryogenic environment [3], we were able observe for the first time the presence of AF domains in an atomically thin vdW magnet, and to characterize the structural and topological properties of their domain walls.

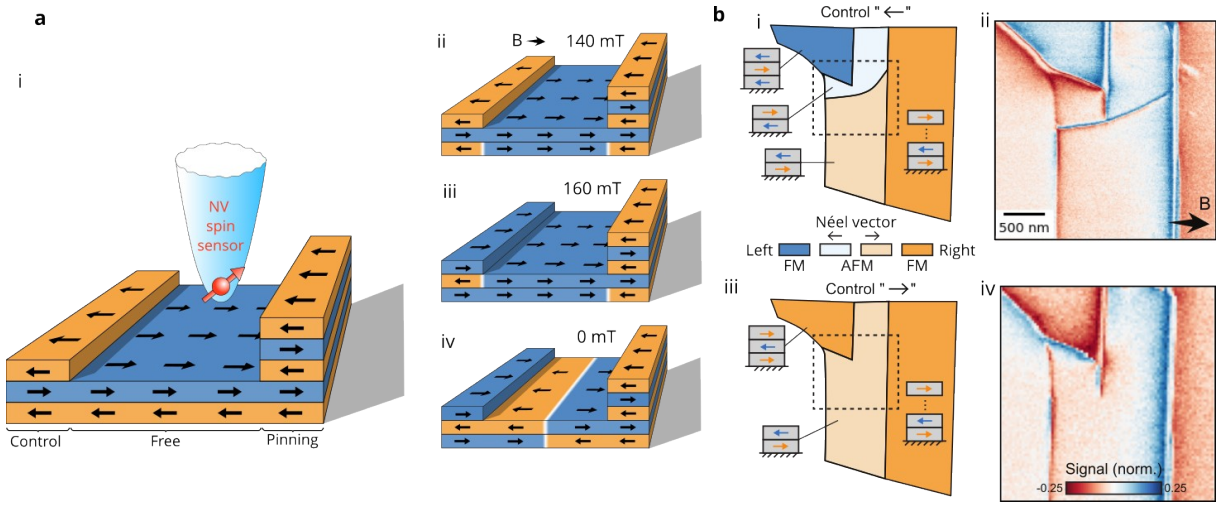

Figure **a** : Schematics of the lateral exchange protocol used to create anti-ferromagnetic domains. **b** : Magnetic imaging of an anti-ferromagnetic domain wall in a CrSBr bilayer.

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Oral

IMAGING VAN DER WAALS MAGNETS WITH SCANNING NV MAGNETOMETRY

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Two-dimensional (2D) van der Waals (vdW) magnets offer various opportunities both for fundamental science and for the design of innovative, atomically-thin spintronic devices, and magnetic imaging techniques are crucial for studying magnetic phases and magnetisation patterns in these materials. The thickness of the samples studied is often only in the order of nanometers, and therefore imaging techniques that are able to detect small magnetic stray fields at the nanoscale are required. In this work, we employ a a single-spin scanning probe technique to study the magnetism in two types of 2D magnets with high sensitivity and nanoscale spatial resolution.

First, we study the vdW magnet Fe_5GeTe_2 for which ferromagnetic order at room temperature has been recently demonstrated in thin samples grown by Molecular Beam Epitaxy (MBE) [1], making it a candidate for spintronic applications which require room temperature magnetism and large-scale fabrication. We use scanning nitrogen-vacancy (NV) magnetometry to quantitatively image the magnetic texture in 12 nm-thin MBE-grown Fe_5GeTe_2. We investigate the effect of patterning on the magnetic order and demonstrate the stabilisation of magnetic vortices in micron-sized structures at room temperature (Fig. 1) [2]. Our results show the role of confinement for the stabilisation of complex magnetic structures in 2D magnets and highlight the potential of the room temperature vdW magnet Fe_5GeTe_2 for applications in spintronics.

The second material we study is the intercalated vdW magnet $CoTa_3S_6$ which has an unconventional non-coplanar antiferromagnetic spin structure at cryogenic temperatures, and exhibits interesting magnetic phenomena induced by its spin topology such as a large anomalous Hall effect despite its negligible net magnetisation [3]. Using scanning NV magnetometry, we acquire the first magnetic images of thin exfoliated $CoTa_3S_6$, revealing the presence of nanometre-sized domains in the material (Fig. 2), and thereby providing insight into the magnetisation patterns of complex spin textures hidden to other characterisation techniques.

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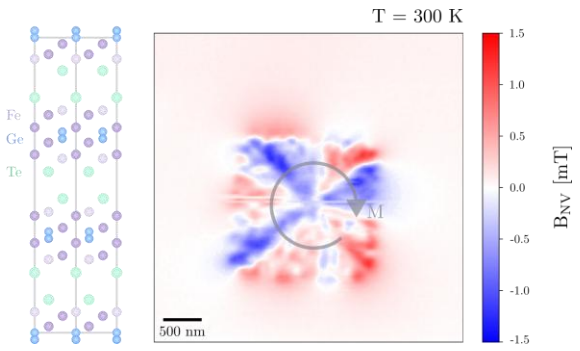

Figure 1: Crystal structure of Fe_5GeTe_2 (left) and NV magnetometry scan (right) showing the stray field of a magnetic vortex in a 12 nm-thin square Fe_5GeTe_2.

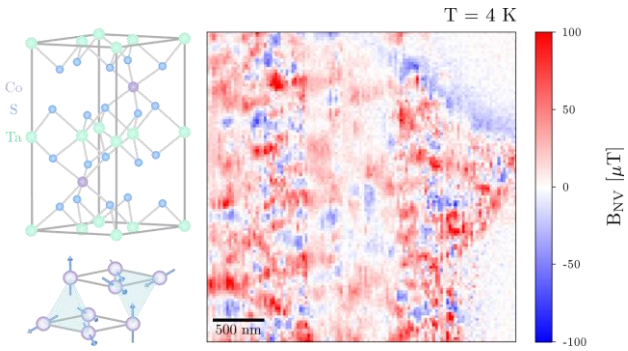

Figure 2: Crystal structure (left) and NV magnetometry scan (right) of thin $CoTa_3S_6$.

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Oral

MAGNETIC IMAGING UNDER HIGH PRESSURE WITH A SPIN-BASED QUANTUM SENSOR INTEGRATED IN A VAN DER WAALS HETEROSTRUCTURE

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Pressure is a powerful thermodynamic parameter for tuning the magnetic properties of van der Waals magnets owing to their weak interlayer bonding. However, local magnetometry measurements under high pressure still remain elusive for this important class of emerging materials. Here we introduce a method enabling in situ magnetic imaging of van der Waals magnets under high pressure with sub-micron spatial resolution. Our approach relies on a quantum sensing platform based on boron-vacancy (V_B) centers in hexagonal boron nitride (hBN), which can be placed in atomic contact of any type of two-dimensional (2D) material within a van der Waals heterostructure. We first show that the V_B center can be used as a magnetic field sensor up to pressures of a few GPa, a pressure range for which the properties of a wide variety of van der Waals magnets are efficiently altered. We then use V_B centers in a thin hBN layer to perform magnetic imaging of a van der Waals magnet under pressure. To illustrate the performances of the method, we image the pressure-dependent magnetization in micrometer-sized flakes of 1T -$CrTe_2$ (see Fig 1), whose evolution is explained by a shift of the Curie temperature. Besides providing a new path for studying pressure-induced phase transitions in van der Waals magnets, this work also opens up interesting perspectives for exploring the physics of 2D superconductors under pressure via local measurements of the Meissner effect.

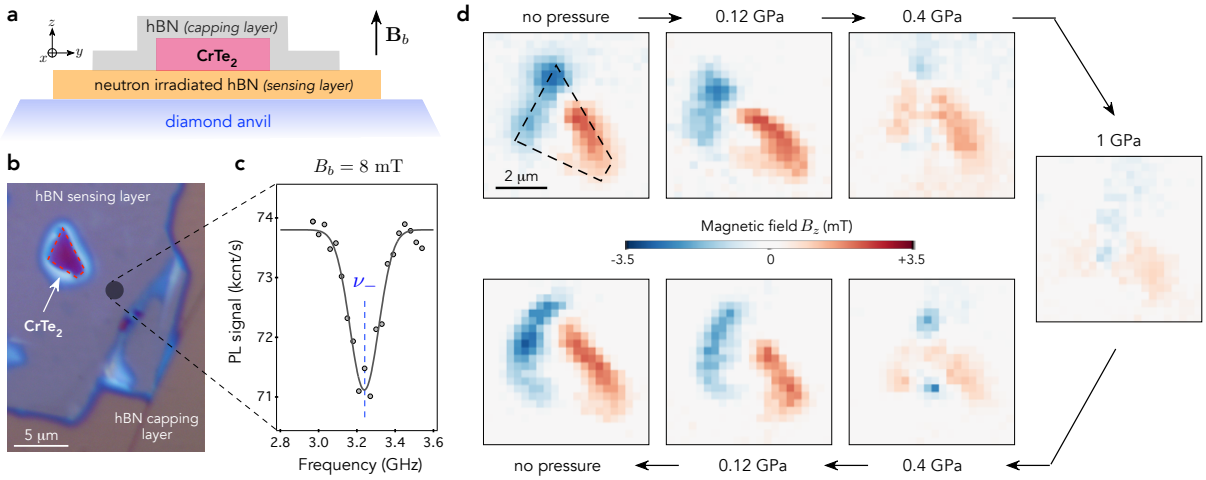

Figure 1: Magnetic imaging under pressure with V_B centers integrated in a van der Waals heterostructure. (a) Sketch and (b) optical image of the heterostructure deposited in the high-pressure chamber of a diamond anvil cell (DAC). (c) Spectrum of the low-frequency magnetic resonance of the V_B center recorded far from the $CrTe_2$ flake at zero external pressure with a bias field B_b = 8 mT. (d) Images of the magnetic field component B_z produced by the $CrTe_2$ flake for increasing (top) and decreasing (bottom) pressure. For all images, the pixel size is 300 × 300 nm^2 and the acquisition time per pixel is 60 s.

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TUESDAY 25

Optical Properties 1

CHARACTERISING INTERLAYER EXCITONS BY SPECTRAL SIGNATURE IN SCATTERING VISIBLE NEAR-FIELD MICROSCOPY

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Abstract

Interlayer excitons (IXs) in van der Waals heterostructures are quasiparticles formed by electrons and holes that are spatially separated across adjacent atomic layers. Due to their out-of-plane dipole moments, long lifetimes, and weak oscillator strength, IXs hold promise for applications in optoelectronics and quantum technologies. However, these same characteristics make them difficult to detect using conventional far-field optical spectroscopy. In this work, we use scattering-type scanning near-field optical microscopy (s-SNOM) to directly probe the dielectric response of IXs (Fig. 1) with nanometer-scale spatial resolution(1). We develop a model to extract key excitonic parameters, including resonance energies and damping rates. To validate our approach, we first study a pristine monolayer of MoS on hexagonal boron nitride (hBN) and a four-layer MoS sample that has been modified by ion irradiation. From the s-SNOM images, we extract the complex dielectric function. The excitonic parameters obtained agree well with those from photoluminescence (PL) measurements and previously published data. We then apply this method to MoSe/WSe heterobilayers, which are well-known systems for hosting interlayer excitons. At a photon energy of 1.35 eV, we observe a Lorentzian resonance in the s-SNOM signal that is characteristic of interlayer excitonic absorption. The measured linewidth indicates that broadening is dominated by non-radiative decay mechanisms, as opposed to the radiative limits typical of high-quality monolayers. Our results demonstrate that s-SNOM is a powerful tool for the nanoscale optical characterization of weakly absorbing excitonic species in two-dimensional monolayers and heterostructures. This technique enables spatially resolved studies of inter- and interlayer excitons and sets the stage for future investigations into many-body effects and device-relevant exciton dynamics in complex 2D systems.

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*Speaker

Oral

EXCITONIC TRANSPORT IN HIGHLY STRAINED WS2 MONOLAYER DOME

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Transition metal dichalcogenides (TMDs), such as $MoSe_2$, MoS_2, WSe_2, and WS_2 exhibit remarkable optical properties, including strong light absorption, and a very large excitonic binding energy making excitons robust at room temperature. In the pursuit of developing new optoelectronic devices based on TMDs, it is therefore essential to identify a physical property that allows the control of exciton flow [1-2]. However, as excitons are electrically neutral, their transport cannot be controlled by an electric field.
In our work, we focused on mechanical strain as a means to induce exciton transport. Recent studies have shown that applying mechanical strain to a TMD monolayer alters its band structure, thereby modifying the exciton energy and lifetime [3]. Since these two quantities are directly related to transport properties, it appears highly relevant to investigate exciton transport under strain.
We optically studied exciton transport in a WS_2 monolayer domes of a few microns diameter and hundreds of nanometers height [4]. The strain induced is relatively important (>1%) and induces a transition from direct to indirect gap. In particular, exciton transport was revealed using space-time-resolved PL spectroscopy, as well as space- and energy-resolved spectroscopy (hyperspectral). Due to the relatively complex spatial variation of both energy and lifetime (i.e. spatial variations in PL intensity are not a direct image of variations in exciton density), we model the excitonic transport to better highlight and understand the PL based experiements. We evidence a depletion of excitons at the edge of the dome and an increase in concentration at the center. Therefore, the results point out an efficient 2D transport towards the center of the domes.

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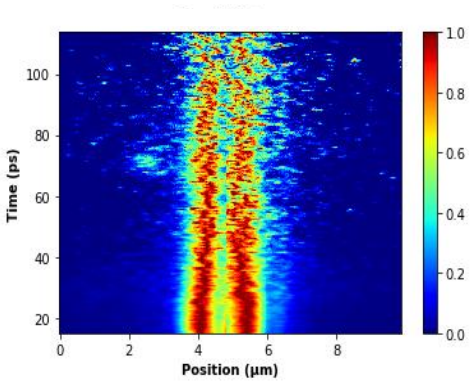

Figure 1 : Time-resolved photoluminescence PL intensity profile from the WS_2 dome

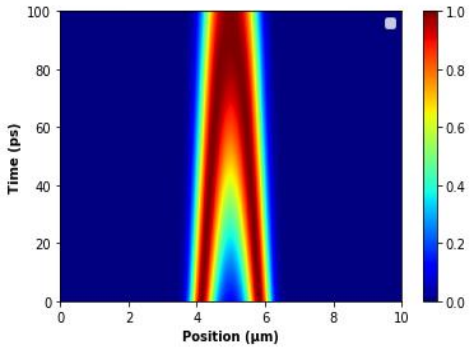

Figure 2 : Modeling resuts of Modeling the time-resolved photoluminescence PL intensity profile from the WS_2 dome

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EXCITONS AS A PROBE OF INTERFACIAL COUPLING IN A WSe_2/GRAPHENE VAN DER WAALS HETEROSTRUCTURE

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Interfacial coupling plays a crucial role in the properties of van der Waals (vdW) heterostructures. For instance, by altering the dielectric environment of a semiconducting Transition Metal Dichalcogenide (TMD) monolayer, considerable variations may occur in the exciton binding energy and in the free particle bandgap energy [1]. Hence, vdW engineering offers an efficient lever to control and fine-tune the physical properties of those stacks [2].

Besides, the sub-nanometer vdW gap between neighbouring layers may also lead to beneficial optical property changes. Indeed, we have recently demonstrated the use of monolayer graphene (Gr) to filter the complex emission spectra of some semiconducting TMDs at cryogenic temperatures (<20 K) [3]. The optical filtering effect results in single and narrow-line TMD-based emitters.

However, so far, the microscopic details of this effect have been mainly studied on $MoSe_2$, notably because this TMD exhibits a rather simple photoluminescence (PL) spectrum. Interestingly, contrary to the case of $MoSe_2$, in tungsten based TMDs such as WSe_2, the existence of a spin-dark state lying below the bright exciton induces more complex PL spectra, featuring multiple peaks [4].

Owing to its rich excitonic structure, WSe_2 constitutes a promising candidate to study in detail the optical filtering effect on various exciton types as well as the underlying microscopic mechanisms.

Here, we investigate in depth the interfacial coupling between WSe_2 and graphene as a function of spatial homogeneity, dielectric disorder and local strain. For this purpose, we have fabricated a WSe_2/Gr vdW heterostructure capped in h-BN in an argon filled glovebox. The sample was then optically characterized both at room temperature and low temperature (<10 K) through various optical spectroscopy means (PL, Raman spectroscopy and differential reflectance).

Optical spectroscopy techniques combined with hyperspectral mapping provide a valuable and powerful tool to characterize interfacial coupling in vdW heterostructures. Subtle changes in the excitonic features in the PL spectra have been studied via robust and quantitative parameters such as the quenching factor of the PL intensity, the exciton binding energy and the peak position of the neutral exciton. We have, thereby, identified diverse regions of interest exhibiting distinct degrees of interfacial coupling, dielectric screening and spatial homogeneity.

Unexpectedly, despite an efficient coupling between WSe_2/Gr, hyperspectral PL maps often reveal additional low-energy peaks alongside the neutral exciton, most particularly in the WSe_2/Gr-bilayer regions. These features tend to be evenly spaced, show a consistent fine structure splitting (~0.6 meV) and sharp linewidths (~ 100-200 µeV), thus suggesting the emergence of localized states, definitely worth further investigation.

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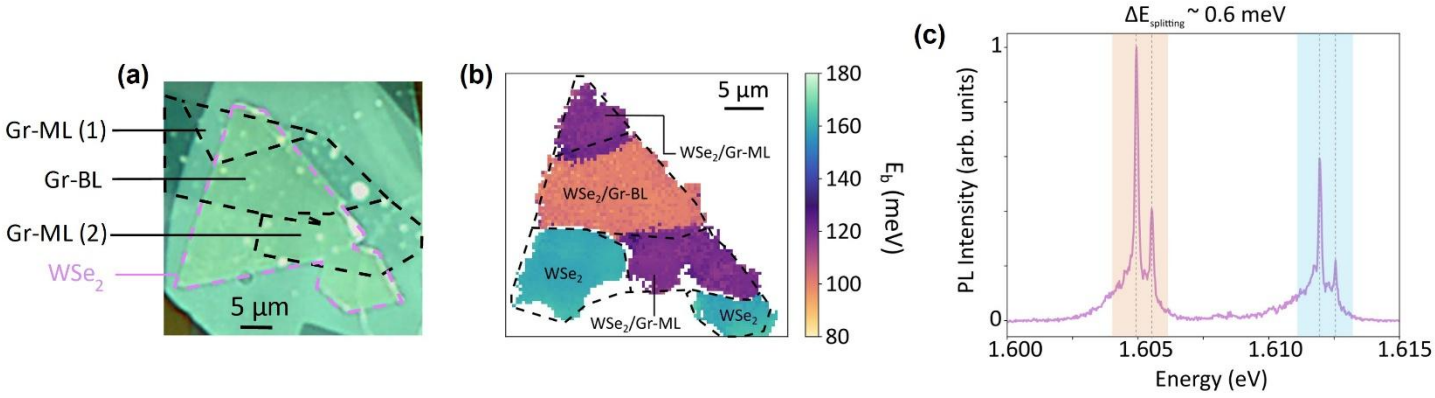

***Figure** : **(a)** Optical micrograph of a WSe_2/Gr van der Waals heterostructure. ML and BL stand for monolayer and bilayer respectively. **(b)** Map depicting the spatial evolution of the exciton binding energy of the neutral exciton (E_b). **(c)** PL spectrum evidencing two typical low energy peaks in a WSe_2/Gr-bilayer region and their fine structure splitting ~0.6 meV.*

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Oral

DYNAMICS OF MULTI-VALLEY EXCITONIC COMPLEXES IN HEAVILY DOPED WSE_2 MONOLAYER

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Monolayers of transition metal dichalcogenides (TMDs), such as MoS_2 and WSe_2, exhibit strong Coulomb interactions, leading to large exciton binding energies. These two-dimensional semiconductors can be integrated into van der Waals heterostructures which allow electrostatic tuning of the charge carrier density. Additionally, carriers can occupy distinct valleys in the Brillouin zone, split by spin-orbit coupling. This unique combination of properties makes TMD monolayers an ideal platform for exploring a wide variety of excitonic complexes [1]. This is particularly evident in WSe_2 monolayers, where the sign of the conduction band spin-orbit splitting gives rise to a rich spectrum of excitonic transitions. For example, Fig 1a shows the absorption (measured via reflectivity contrast) as a function of carrier density.

Until now, most studies have focused on carrier densities below a few 10^{12} cm^{-2}. In this work, we fabricated a charge-tunable device enabling access to electron densities exceeding 10^{13} cm^{-2}. In this high-density regime, carriers begin to populate both the first and second conduction bands at the K points, leading to the formation of multi-particle excitonic complexes: six-particle (H, "hexciton") and eight-particle (O, "oxciton") states [2] (Fig 1b). At the highest doping levels, a new transition (labeled M) emerges, which we interpret as a multi-valley complex involving electrons in the Q valleys.

We will present continuous-wave and time-resolved photoluminescence (PL) measurements in these high doping regimes, revealing strong dependencies on both doping level and excitation power. Our results underscore the potential of multi-valley excitonic complexes in the high-doping regime for use as efficient light emitters and for integration with optical cavities in future polaritonic applications.

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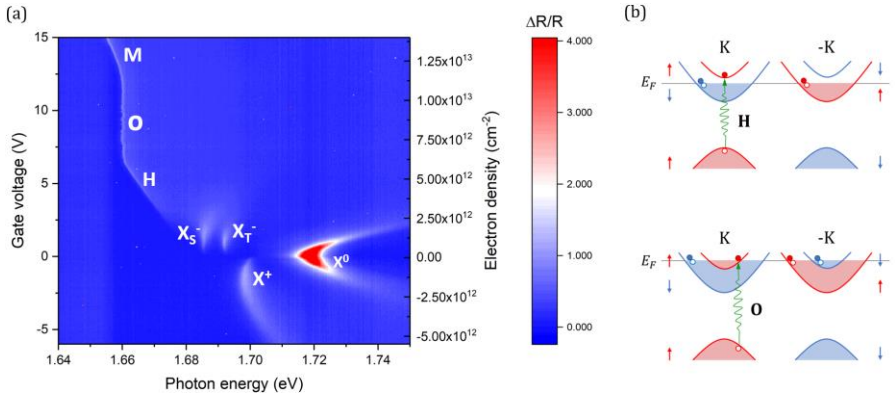

Figure 1: (a) Reflectivity contrast of a WSe2 monolayer as a function of doping density. X^0 is the bright neutral exciton, X^+ the bright positive trion, X_S^- and X_T^- are the singlet and triplet negative trions. At high electron doping densities, the hexciton (H), oxciton (O) and a multivalley complex M appears. (b) Sketch of the hexciton and oxciton.

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TUESDAY 25

Twisted Layers 2

Annual meeting 2025 of the GDR and IRN HOWDI
24-28 november 2025 Sète, France

Oral

OPTICAL SPECTROSCOPY OF CORRELATED STATES IN 2D MOIRÉ MATERIALS

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The field of two-dimensional (2D) materials offers unprecedented opportunities to engineer nanoscale magnetic, electronic, and optical devices. Creative stacking and twisting of atomically thin layers has become a powerful paradigm for realizing exotic phases of matter. Transition metal dichalcogenide (TMD) moiré heterostructures are particularly promising because they combine strong Coulomb interactions with robust excitons and tunable band topology. At small twist angles, they host topological flat bands that closely resemble the lowest Landau level but without an external magnetic field. In this talk, I will show how cryogenic optical spectroscopy uncovers ferromagnetism, correlated insulators, and fractional Chern states in twisted homobilayer TMDs. I will also highlight how tailored device architectures enable access to complementary observables such as magnetic susceptibility and electronic compressibility, revealing essential properties of correlated quantum phases.

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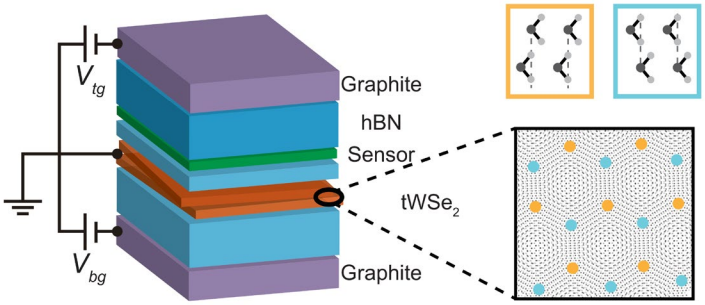

Figure 1: Twisted WSe2 device structure for optical sensing of correlated insulators.

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Oral

CORRELATED ELECTRONS AND LAYER PSEUDOSPIN PHYSICS IN A PURELY ELECTROSTATIC MOIRÉ POTENTIAL

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Moiré heterostructures based on transition metal dichalcogenide (TMD) hetero- and homobilayers have emerged as a versatile platform for exploring correlated electronic states. Introducing a twisted hexagonal boron nitride (h-BN) interface offers a novel and flexible method to externally induce a periodic superlattice for any van der Waals material. In this work, we demonstrate the potential of twisted h-BN in combination with TMDs to probe and manipulate correlated electrons [1, 2]. Specifically, we integrate two $MoSe_2$ monolayers with a twisted h-BN bilayer in a dual-gated, charge- and electric-field-tunable device. The periodic ferroelectric domains of twisted h-BN create a purely electrostatic potential for charge carriers in the $MoSe_2$ layers. Although the charge-neutral TMD exciton remains largely insensitive to the potential, it serves as a spin-valley- and layer-sensitive probe of the electronic state. Notably, the electrostatic potential generated by the twisted h-BN aligns potential minima across the two TMD layers, creating a weakly broken SU(2) symmetry in the layer pseudospin degree of freedom. This platform opens up opportunities to investigate a range of exotic phenomena, including spin-polaron formation through kinetic pairing, and the emergence of chiral layer-pseudospin liquids.

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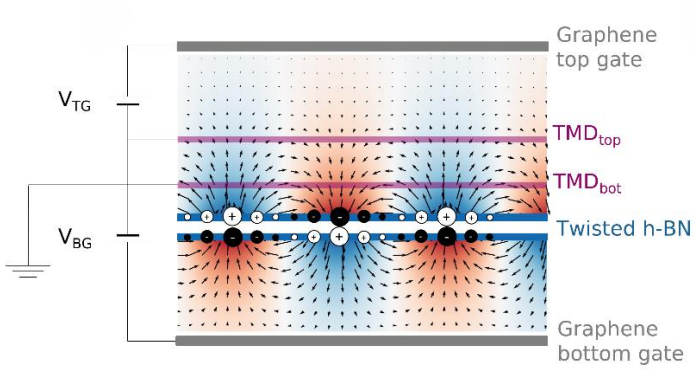

Figure 1: Illustration of the studied structure consisting of two $MoSe_2$ monolayers above a twisted h-BN interface within a charge- and electric field-tunable device.

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Oral

NANOSCOPIC STRAIN TO SECOND HARMONIC GENERATION SIGNAL IN 2D MOIRÉ HETEROSTRUCUTRES

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2D Moiré heterostructures – namely the resulting super-lattice arising from the superposition of two 2D material monolayers – have dragged a lot of attention for past few years for the ability to display stronlgy correlated states that can be tuned through a large number of parameters such as electronic doping, electric and magnetic fields and temeperature for examples[1,2]. Yet, the properties of these new materials strongly depends on the homogeneity of the moiré super-lattice which can display local strain due to the presence of bubbles, wrinkles or dust occurring during the nano-fabrication process. The devices being often encapsulated with hBN, the local moiré is no longer accessible and second-harmonic generation is preferred to access it[3,4]. If this latter technique is in-situ and non-destructive, it averages the local information over the diffraction limit and loses its local information. In this talk, I will show how the local and optical information can be linked using Lateral Force Microscopy and the geometric phase analysis[5] followed by an excitonic-resonant bichromatic polarization resolved second-harmonic generation.

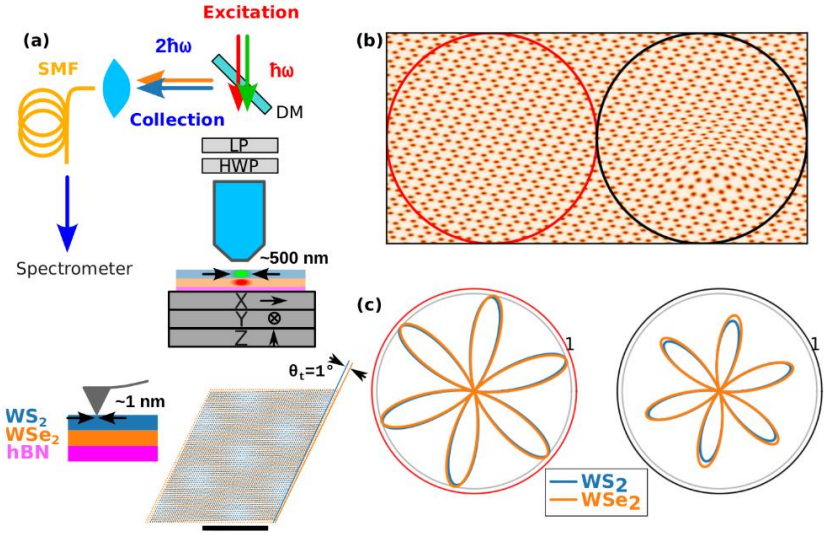

Figure 1.(a) Top : Experimental scheme of excitonic-resonant bichromatic polarization resolved second harmonic generation. Bottom : Lateral Force Microscopy on a WS2/WSe2 moiré heterostructure . (b) Simulated hexagonal lattice for a twist angle of $\theta_t = 1°$ with a local deformation. (c) Computed polarization resolved SHG signal for both monolayer on the coloured circle depicted in (b).

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Annual meeting 2025 of the GDR and IRN HOWDI
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Oral

STRUCTURAL & ELECTRONIC PROPERTIES OF TWISTED BILAYER MOS_2

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2D layered structures of transition metal dichalcogenides (TMDCs) such as molybdenum disulfide (MoS_2) are attracting increasing attention due to their rich and tunable electronic properties [1]. In analogy to the well-known twisted graphene-based systems, when MoS_2 layers are stacked with a relative twist, a moiré superlattice is formed, inducing new interlayer coupling which significantly modifies the corresponding electronic structure [2]. The twist angle between MoS_2 layers can strongly influence both the electronic band gap and the emergence of flat bands at small angles, where enhanced electron localization occurs, allowing the exploration of correlated electronic states and novel quantum effects [3]. In addition, atomic reconstruction occurring in small twist-angle moiré structures substantially alters the band structure, further enriching their electronic properties [4]. Furthermore, the twist angle and atomic reconstruction also have a profound impact on the vibrational (phononic) properties, which are important for understanding thermal transport and electron-phonon interactions in these systems [5]. Despite rapid progress, a comprehensive understanding of how the twist angle governs these electronic properties and vibrational characteristics remains an open question. In this work, we systematically investigate the influence of moiré effects in twisted bilayer MoS_2, demonstrating twist-angle-dependent valley manipulation and flat electronic band formation while revealing the emergence of moiré phonon modes in phonon spectra. This is achieved through a comprehensive comparison of atomistic modeling approaches, ranging from semi-empirical methods to machine learning potentials.

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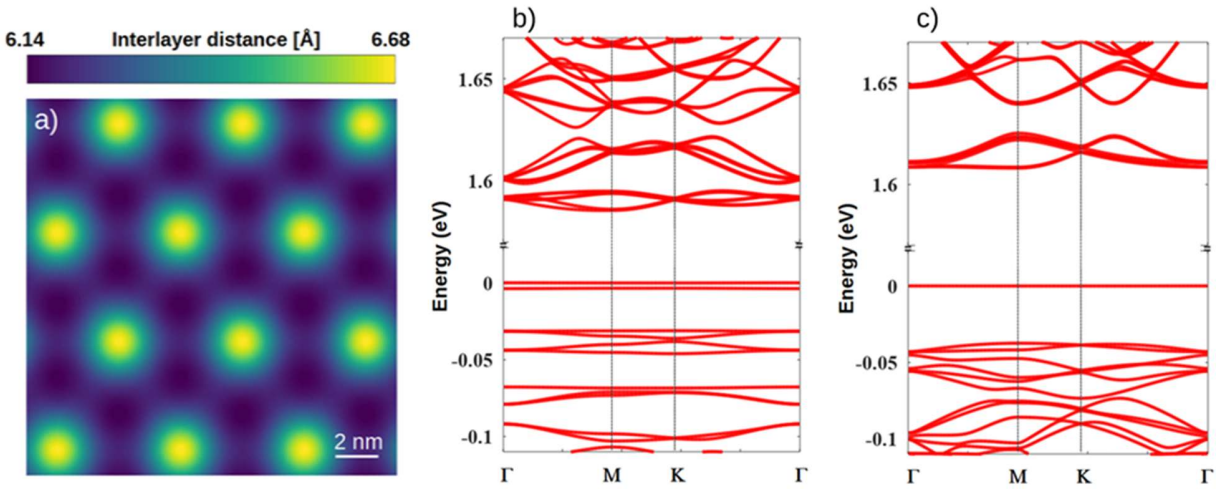

Figure 1: Moiré superlattices arising in twisted bilayer MoS_2 system. (a) Spatial map of interlayer distance(corrugation) in 3.15° twisted bilayer MoS_2 (b,c) Electronic band structure of 3.15° twisted bilayer MoS_2 with and without structural relaxation, respectively.

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TUESDAY 25

Single Photon Emission and Detection

Twisted Quantum Photovoltaics

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Abstract

Twisted van der Waals heterostructures-atomically thin crystals stacked with a relative twist-exhibit striking emergent properties driven by their moiré superlattices. From an optoelectronic perspective, their spectral response can be engineered across an exceptionally broad wavelength range, bridging visible to terahertz regimes. At the same time, their enlarged superlattice unit cells enhance quantum effects that open pathways toward next-generation quantum photovoltaic devices, where rectification arises from the wavefunction geometry of electrons. In this talk, I will present newly observed forms of quantum photovoltaic response in twisted van der Waals heterostructures. I will discuss terahertz photocurrent experiments in moiré superlattices that probe the interplay between quantum geometry and many-body interactions characteristic of flat-band systems1. I will then describe high-field measurements in these systems that establish a new platform for single-photon detection at long wavelengths2.
R. Krishna Kumar *et al*, *Nature Materials* **24,** 1034-1041 (2025) K. Nowakowski *et al, Science* **389**, 6760, 664-649 (2025)

*Speaker

Annual meeting 2025 of the GDR and IRN HOWDI
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Oral

TOWARDS ON-DEMAND SINGLE-PHOTON EMISSION FROM H-BN

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Single-photon emitters are instrumental in the transport of quantum information and in quantum sensing. However, the integration of single-photon emitters in optoelectronic devices remains a major challenge for the development of quantum photonics-based technologies. To be deployed on a large scale, these technologies require deterministic single-photon emitters (SPE) that can operate at room temperature and be electrically driven. Hexagonal boron nitride (hBN) hosts a variety of atomic defects which act as stable single-photon sources and thus represents a promising SPE platform.

In particular, the blue emitter displaying a Zero Phonon Line (ZPL) centered at 436 nm, first reported by Fournier *et al.* [1], can be created by low-energy electron-beam irradiation and remains stable at room temperature. The optical properties of this emitter have been the subject of several studies. Yet, its electrical and optoelectronic properties are still widely unexplored.

To investigate these properties, we first demonstrate the deterministic creation of blue emitters in exfoliated carbon-doped hBN [2] (C:hBN) flakes (Figure 1.a). The emitter generation is optimized according to the flake thickness by monitoring their photoluminescence (PL) and photon-correlation properties (Figure 1.b).

Then, we delve into the electrical behavior of defect-assisted tunneling in Graphene/C:hBN/Graphene junctions (Figure 1.c) with and without preliminary electron-beam irradiation. Current-voltage characteristics of the devices are carried out within the PL optical assembly, allowing light emission to be collected at different bias voltages. By analogy to previous work on different emitters [3], we expect to demonstrate controlled electroluminescence from the blue emitters.

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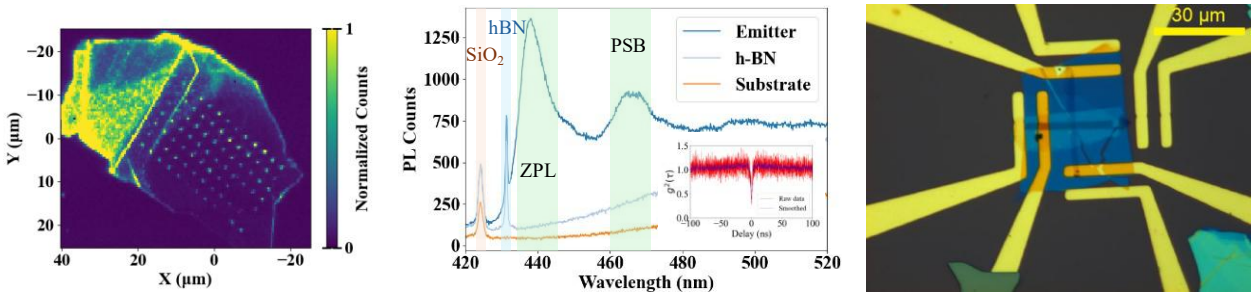

Figure 1: Deterministic blue emitter generation in carbon-doped hBN. a. Photoluminescence (PL) intensity map, filtered between 430 and 470 nm, of an electron-beam irradiated C:hBN flake according to an array pattern. b. PL spectra of the same flake in 3 different areas: the SiO_2/Si substrate, non-irradiated C:hBN and irradiated bright spot (Emitter). The zero-phonon line (ZPL) and phonon sideband (PSB) emissions are selected for photon-correlation measurement ($g^{(2)}(\tau)$), shown in the insert. c. Optical micrograph of a hBN/Graphene/C:hBN/Graphene stack deposited on Ti/Au contacts for electrical characterization.

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REPRODUCIBLE GENERATION OF GREEN-EMITTING COLOR CENTERS IN HBN USING OXYGEN ANNEALING

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Abstract

Oral Presentation

The ability to generate quantum emitters with reproducible properties in solid-state matrices is crucial for quantum technologies (1). Yet when it comes to the emerging material platforms based on 2D materials, most methods yield emitters with a large wavelength spread, including in hexagonal boron nitride (hBN), a 2D insulator that hosts the single-photon emitters (SPEs) with arguably the most advantageous properties (2). The difficulty of obtaining visible-range SPEs with reproducible wavelength hinders the scalability of their applications to quantum information.

Here, we show that a high density of close-to-identical single-photon emitters can be created in commercial hexagonal boron nitride using annealing under oxygen atmosphere. This simple procedure yields uniform in-plane distributions of color centers consistently emitting at 539.35 ± 0.45 nm. We present an extensive characterization of their photophysical properties. At room temperature, we show that the emitters are bright and stable, and exhibit a high purity. We also show that at low temperature, the emitters emit predominantly in a narrow zero-phonon line with minimal spectral diffusion. We provide a stastistical analysis that demonstrates the high reproducibility of these properties (3). Altogether, these characteristics make this family of quantum emitters highly appealing for applications to quantum information science.

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Oral

CREATION OF SINGLE-PHOTON EMITTERS IN 2D SEMICONDUCTORS BY CONTROLLED THERMAL ANNEALING

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Two-dimensional (2D) semiconductors such as monolayer WS_2 are promising materials for quantum light sources, as they can host optically active defect-bound excitons. Narrow photoluminescence (PL) emissions with single-photon characteristics have been observed from defect states in 2D TMDs [1]. Here, we investigate the controlled formation of sulfur vacancies in monolayer WS_2 via thermal annealing, as recently demonstrated in MoS_2 [2], to create localized excitonic states suitable for single-photon emission.

To thermally engineer defects in situ under cryogenic conditions, we transfered hBN-encapsulated monolayer WS_2 onto suspended SiC membranes, enabling localized Joule heating inside a cryostat. PL spectra were measured at cryogenic temperature (~4K) after annealing the same flake at increasing annealing temperatures.

A significant spectral change is observed after annealing above 1200 K, with the emergence of a sharp emission peak (X_L) centered at 1.945 eV - approximately 100 meV below the neutral exciton (X_A^0). The XL peak exhibits a narrow linewidth (~0.25 meV) and clear power saturation behavior, indicating localized emission from discrete defect states. To verify the quantum nature of this emission, we peformed second-order correlation $g^2(\tau)$ measurements under pulsed laser excitation. The results show a pronounced dip at zero delay with $g^2(0) < 0.5$, confirming that the X_L emission originates from a single-photon emitter.

Our results demonstrate that thermal annealing provides a reproducible and tunable method to activate single-photon emitter candidates in monolayer WS_2.

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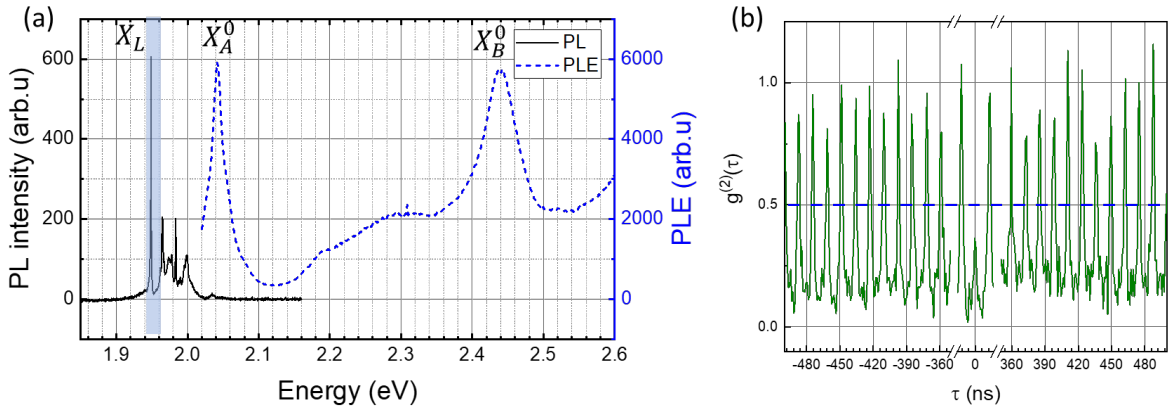

Figure 1. (a) Photo-luminescence (PL) spectrum of hBN encapsuated monolayer WS_2 after high temperature annealing at 1200K and Photoluminecence Excitation (PLE) spectrum measured for the newly appeared narrow peak (X_L), (b) Pulsed excitation measurement of $g^{(2)}(\tau)$ of the narrow peak (X_L)

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WEDNESDAY

26

Optical Properties 2

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Poster

ELECTROLUMINESCENCE AND ENERGY TRANSFER IN HBN-ENCAPSULATED GRAPHENE TRANSISTORS

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In this talk, I will present our recent discovery of graphene's electroluminescence in the middle infrared. Electroluminescence is the phenomenon by which a material emits light in response to the passage of an electrical current. In solids, it is the prerogative of semiconductors and related organic materials, and it results from the radiative recombination of electrons and holes.

We investigate high-mobility graphene field-effect transistors encapsulated in hexagonal boron nitride (hBN) at ambient conditions. Despite the semimetallic nature of graphene, which theoretically precludes electroluminescence, we observe this phenomenon due to (i) inefficient non-radiative carrier relaxation and (ii) a unique carrier injection mechanism specific to 2D semimetals: Zener-Klein tunneling.

Our results reveal two important consequences of graphene electroluminescence. First, it leads to mid-IR emission in the far field. Second, it significantly affects the energy transfer within the hBN-encapsulated heterostructure. Using far-field mid-IR spectroscopy, we demonstrate the far-field electroluminescence of graphene at 6.5 µm, made possible by the elastic scattering of hyperbolic phonon polaritons (HPhPs) of hBN at heterostructure discontinuities. We quantify the associated radiative energy transfer using mid-IR pyrometry of the substrate receiving the thermal energy.

Surprisingly, we find that radiative energy transfer is reduced in hBN with nanoscale inhomogeneities, underscoring the crucial role of the electromagnetic environment and opening interesting technological possibilities.

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Oral/Poster *(please, delete the unnecessary option)*

ULTRAFAST ELECTRON-HOLE PLASMA PHOTOLUMINESCENCE IN MONOLAYERS MOS2 AND WS2

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Semiconducting two-dimensional Transition Metal Dichalcogenide (TMD) monolayers are characterized by a direct bandgap yielding a high photoluminescence (PL) efficiency, and by large exciton binding energy (around 0.5 eV), resulting in thermally stable excitons at room temperature and above [1]. However, in the high excitation density regime, the strong electron-electron exchange and correlation terms lead to a huge band-gap renormalization and to the reduction of the exciton binding energy, leading to the ionization of free excitons (FE) to an electron-hole plasma (EHP). This is a limitation for the exciton-based light-emitting devices but at the same time it opens the possibility to ultra-bright and broadband light emission sources. EHPs in TMD monolayers have been theoretically predicted and investigated by means of power-dependent steady state PL experiments [2,3,4]. However, a study of the out-of-equilibrium properties and time evolution of the EHPs in TMD monolayers is still lacking. Time resolved photoluminescence (TR-PL) is a suitable technique to directly access the dynamics of the EHP generated after a pulsed photo-excitation at high excitation density (proportional to the excitation fluence).

Here, we report TR-PL experiments on mechanically exfoliated monolayers MoS2 and WS2, on SiO2 substrates, giving access to the time evolution of the PL spectrum after an above-band-gap pulsed photo-excitation (300 fs, hv=2.4 eV), with a time resolution of 50 ps and spectral resolution of 20 meV. Our data allow to capture the ultra-fast time evolution of the EHP after the pulsed photo-excitation, and to identify the threshold fluence for the transition from FE to EHP.

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Figure 1: Conference logo.

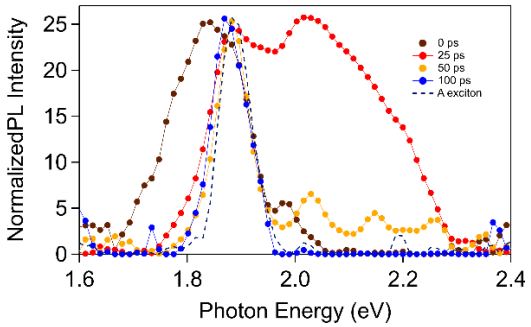

Figure 2: TR-PL spectra of monolayer MoS2 after a high fluence pulsed photo-excitation.

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Oral

SPIN COHERENCE PROPERTIES OF V_B^- CENTERS IN ULTRATHIN HBN LAYERS

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Spin defects with optically detectable magnetic resonances in hexagonal boron nitride (hBN) arecurrently attracting a deep scientific interest for the deployment of quantum sensing technologies on a two-dimensional (2D) material platform [1]. Among several optically-active spin defects recently discoveredin hBN, the negatively-charged boron vacancy (V_B^-) center stands out due to its well established atomic structure and ease of creation by various irradiation methods. This defect features a spin triplet groundstate whose electron spin resonance (ESR) frequencies can be interrogated by optical means and stronglydepends on external perturbations such as magnetic fields, strain, and temperature [1] [2]. Such propertiesmake the V_B^- center in hBN a promising candidate for the design of a flexible 2D quantum sensing unit, that could be placed in atomic contact of any type of 2D material within a van der Waals heterostructure. Despite such appealing prospects, the properties of V_B^- centers embedded in ultrathin hBN layers still remain poorly documented.

In this work, we study the optical and spin properties of V_B^- centers in atomically-thin hBN flakes obtained by mechanical exfoliation of neutron-irradiated hBN crystals isotopically purified with ^{15}N and ^{10}B [3]. We first show that the ESR frequencies of V_B^- centers remain optically detectable in the 2D limit [4] [5]. We then analyze how the spin relaxation times, T1 and T2, evolve with the hBN thickness underambient conditions. While T1 is significantly reduced in thin flakes, the spin echo coherence time T2 is preserved and can even be improved in ultrathin films despite the nanoscale proximity of the crystal surface that usually leads to a degradation of the spin coherence properties of solid-state spin defects. This work provides important insights into the properties of V_B^- centers embedded in ultrathin hBN flakes, which are valuable for future developments of foil-based quantum sensing technologies.

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WEDNESDAY

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0D and 1D van der Waals

Annual meeting 2025 of the GDR and IRN HOWDI
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Oral

FILLED SINGLE-WALL CARBON NANOTUBE FOR FUTURE ADVANCE IN PHOTOCATALYSIS

Y. Midiladji Bakary[1], J. Gillette[2], L. Bois[1], C. Marichy[1], F. Toche[1], R. Chiriac[1], F. Vialla[3], D. Bouyssi[2], N. Monteiro[2], A. Amgoune[2], C. Desroches[1], and S. Forel [1]

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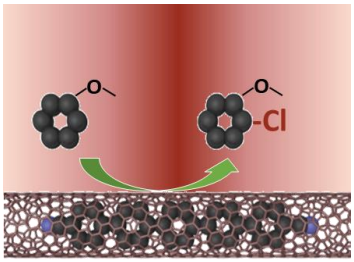
The development of photocatalysts offers a promising approach to driving chemical reactions under milder conditions by using light as an energy source. This strategy has significant potential for advancing green chemistry, providing sustainable alternatives to traditional catalysis. Current research in photocatalysis predominantly focuses on two main material types: transition metal-based catalysts and organic dye photocatalysts. Transition metals, such as platinum and ruthenium, are highly effective under visible or UV light; however, their high costs, limited availability, and the environmental impact of their extraction pose significant barriers to large-scale, sustainable use. Organic dyes, on the other hand, are cost-effective and can operate under low-energy light but suffer from photobleaching, which compromises their stability and long-term functionality.

In this work, we developed hybrid photocatalytic materials by encapsulating organic dyes within single-walled carbon nanotubes (SWCNTs). This approach aims to improve the efficiency, stability, and recyclability of the photocatalyst[1]. SWCNTs are known for their exceptional charge mobility[2], high chemical stability, and unique nanoscale tubular structures, which enable them to act as protective layers[3] while simultaneously enhancing photocatalytic properties.

Building on the work of Lamar et al. [4], who demonstrated that methylene green can catalyze visible-light chlorination of arenes, we encapsulated a related dye, methylene blue (MB), within SWCNTs as a proof of concept. The resulting SWCNT–MB hybrid materials catalyzed the chlorination reaction with a turnover number 35 times higher than that of free MB, underscoring their potential to advance green and sustainable catalytic processes.



Photocatalysis

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Oral

CHARACTERIZATION OF CARBON NANOTUBES DOPED BY ENDOHEDRAL FILLING

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Filling carbon nanotubes with electron-donor or electron-acceptor molecules has emerged as a promising strategy to tune their electronic properties in a controlled and stable manner [1]. This stability arises from the encapsulation of dopant species within the hollow core of the nanotube, protecting the molecule from environmental interactions. These hybrid systems can find potential applications in transparent conductive films, sensors, and nanoelectronic devices [1].

Despite previous reports demonstrating both p- and n-type doping of carbon nanotubes, a clear and consistent spectroscopic characterization of doping remains elusive. In particular, the changes observed in the characteristic Raman features of the nanotubes vary widely across the literature, with no consensus on how doping impacts those vibrational modes. This ambiguity arises not only from the variability of the effects across different carbon nanotube diameter regimes but also from the lack of a well-defined undoped reference, as carbon nanotubes are commonly found to be slightly p-doped due to oxygen adsorption.

Additional complexity arises from the diverse forms in which carbon nanotubes are studied—powders, dispersions, or films—each of which introduces differences in the Raman and absorption spectra. Effects such as bundling, strain, environmental interactions with water or oxygen compete and affect spectral features such as shifts of the vibrational G-band in a similar manner, thereby making the assessment of doping ambiguous [2,3].

To address these challenges, we have conducted a combination of spectroscopic techniques on filled nanotube samples, benchmarking their behavior compared to a neutral reference sample. These efforts aim to provide clearer insights into the spectroscopic signatures of doping and advance a more consistent framework for the characterization of doped carbon nanotubes. We then employ this characterization platform to investigate the efficiency of different filling methods, including liquid- and vapour-phase filling methods.

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Acknowledgments

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Oral

NANOCARBONS PHASE TRANSITIONS INDUCED BY ANISOTROPIC STRAIN UNDER HIGH PRESSURE

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High-pressure is as a powerful tool to explore the phase diagram of carbon materials and to synthesize novel structures. In the case of nanocarbons, their reduced dimensionalities and the necessary use of a supporting substrate imply that the environmental 3D high pressure produced in an anvil cell is transmitted anistropically to these systems. Here we will discuss exotic behaviours experimentally observed on a wide range of nanocarbon samples and high pressure environments. Such studies are enabled by the development of precise transfer methods inside the anvil cell and the use of corrected microscope objectives to allow optical spectroscopies with diffraction limited spatial resolution. Firstly, 1D carbon nanotubes present a reversible buckling threshold at high pressure which depends on their diameter (Figure 1) [1]. Secondly, supported 2D graphene shows strong biaxial compressive strain and doping effects mostly governed by the nature of the (usually less stiff) substrate and the pressure transimitting medium [2]. Interestingly, these changes are well transmitted to suspended regions of the graphene [3]. Finally, making use of this strong in-plane biaxial strain induced by the substrate, we can reduce the pressure threshold inducing the sp^2-to-sp^3 phase transition in few layer graphite (Figure 2) [4].

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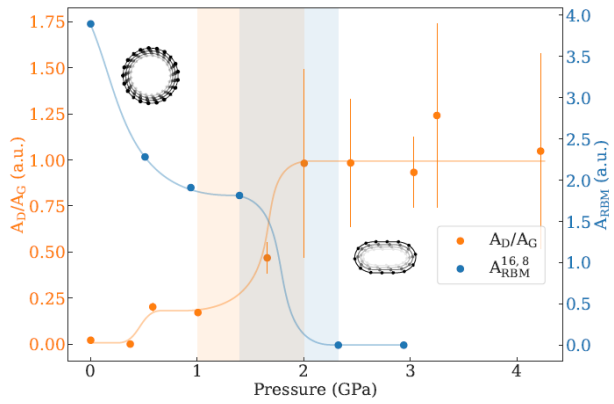

Figure 1: Raman spectroscopic features (D over G peaks ratio and RBM intensity) showing the buckling threshold of a single chirality nanotube under high pressure. From [1].

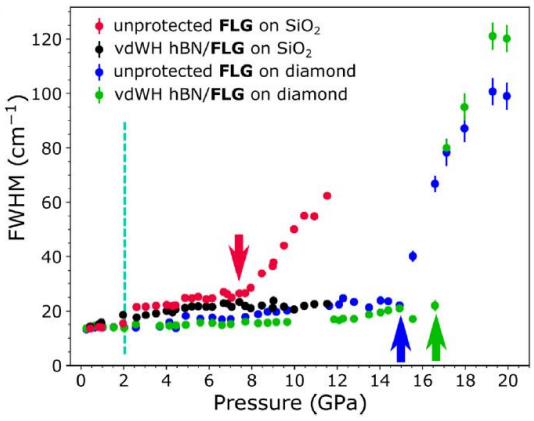

Figure 2: Evolution of the G peak full width at half middle of few layer graphite under high pressure with different substrates and interfaces (hBN encapsulation), highlighting a reduced sp^2-to-sp^3 phase transition threshold. From [4].

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HETEROSTUCTRE OF GRAPHENE QUANTUM DOT AND HEXAGONAL BORON NITRIDE FOR STABLE SINGLE QUANTUM EMITTER

Suman Sarkar[1], Daniel Medina-Lopez[2], Christophe Voisin[3], Yannick Chassagneux[3], Emmanuel Baudin[3], Stéphane Campidelli[2], Jean-Sébastien Lauret [1]

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Indistinguishable single photon sources are key components for quantum information technology. Although there are several single photon sources made of organic molecules available, most of them are in the form of guest-host matrix, which have some technical difficulties. At low temperature, some of them are capable of producing indistinguishable photon but due to low FCDW factor, the zero phonon line (ZPL) contains below 40% of all the emitted photons.

Bottom-up synthesized graphene quantum dots (GQDs)[1] have emerged as exceptional single-photon emitters[2], with quantum yields approaching near to 100%. The choice of substrate or environmental conditions for GQD deposition plays a pivotal role in stabilizing monomers on-surface. Achieving absolute control over these factors is critical for exploring indistinguishable photon emission.

In this talk, we will present the single-photon emission properties of GQDs, and the results on the role of hexagonal boron nitride (hBN) as a high-performance dielectric substrate. In our recent studies of $C_{114}tBu_{10}$ GQD on mechanically exfoliated hBN flake surfaces, we show that it is possible to find single molecule. More importantly the single molecules are stable in order of few minutes in air at room temperature. At low temperature we found very narrow ZPL whose linewidth is below the resolution of our spectrometer resolution and vibronic peaks are weak compared to the ZPL, which all together can be a promising factor for a source of indistinguishable photons.

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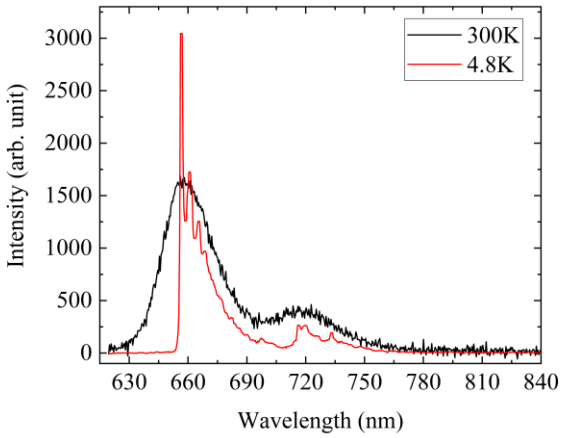

Figure 1: A typical room temperature vs low temperature spectra of C_{114} GQD on hBN surface.

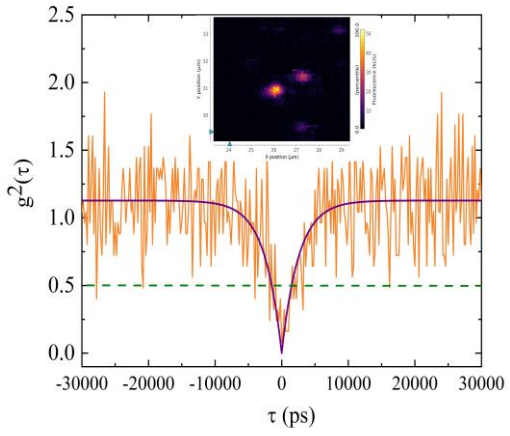

Figure 2: Antibunching value in autocorrelation measurement shows below 0.5 at zero delay on a diffraction limited spot of GQD (shown in the inset).

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WEDNESDAY

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Electronic Spectrocopies and Microscopies

Oral

Floquet-Bloch Valleytronics in TMDCs

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Driving quantum materials out of equilibrium enables the realization of exotic states of matter beyond conventional equilibrium tuning methods. When electrons are periodically driven by electromagnetic fields, Floquet-Bloch states emerge, allowing for the creation of nonequilibrium quantum phases without ground state analogs. In transition metal dichalcogenides (TMDCs), the broken inversion symmetry in monolayers gives rise to a nonzero orbital angular momentum and Berry curvature at the K and K' valleys, leading to chiroptical selection rules central to valleytronics. Here, we establish a connection between Floquet engineering and valleytronics.

First, using below-bandgap pumping, we demonstrate the formation of valley-polarized Floquet-Bloch states in 2H-WSe_2. We reveal quantum path interference between Floquet-Bloch and Volkov states, showing its dependence on valley pseudospin and light polarization. Extreme ultraviolet (XUV) photoemission circular dichroism in this nonequilibrium regime further illustrates the potential for orbital character control in Floquet-engineered states [1].

Second, we explore a distinct regime of resonant pumping, where non-equilibrium electronic populations coexist with light-field dressing. In this regime, we observe a pronounced enhancement of valley polarization in Floquet-Bloch states originating from transient photoexcited states. Circular dichroism in photoemission from the valence band and transient photoexcited states provides insight into a potential mechanism linked to the local orbital angular momentum of the involved electronic states, which underlies the enhanced valley polarization [2].

These findings bridge Floquet engineering and quantum geometric light-matter coupling in two-dimensional materials. They provide a pathway toward novel nonequilibrium phases of matter by dynamically breaking symmetries through coherent dressing of winding Bloch electrons with tailored light pulses.

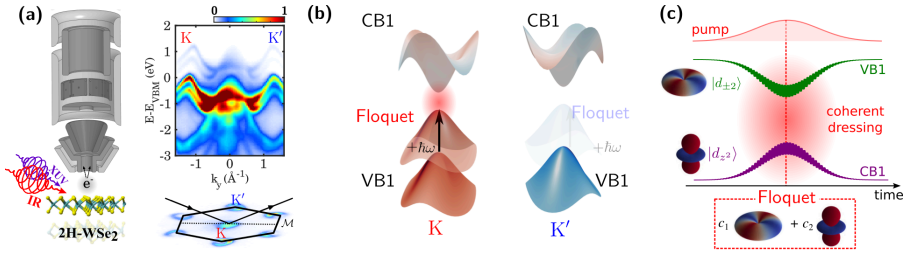

Figure 1: Experimental scheme and concept of Floquet valleytronics. (a) Schematic of the time- and polarization-resolved XUV ARPES setup and nonequilibrium band mapping. (b) Illustration of the Floquet-engineered electronic structure of 2H-WSe_2 near the K and K′ valleys. (c) Representation of the population dynamics in VB1 and CB1 induced by sub-gap coherent dressing and orbital hybridization upon the formation of Floquet sidebands.

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Oral

HIGHER ORDER TOPOLOGICAL DEFECTS IN THE MOIRÉ LATTICE OF A VAN DER WAALS MAGNETIC MATERIAL

E. Gambari[1], S. Meyer[2], S. Guesne[1], P. David[1], F. Debontridder[1], L. Limot[3], F. Scheurer[3], C. Brun[1], B. Dupé[2], T. Cren[1], M. Hervé[1]

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Van der Waals materials are emerging as extremely versatile building blocks for many fields of research, both at the fundamental and applied level. They offer tremendous possibilities for fine tuning spintronics, superconducting, nanoelectronics, optical devices. They appear extremely attractive for exploring new exotic physics due to their ability to be staked with an infinite number of combinations that leads to unexpected physical properties. The toolbox of van der Waals heterostructures is continuously growing with for instance the recent discovery of ferromagnetic order down to the monolayer limit in the family of chromium trihalide, CrCl3, CrBr3 and CrI3 (CrX3, X= I, Br, Cl) [1]. Several works have related some observations of moiré structure due to the mismatch between the CrX3 monolayers and their substrate which lead to a wealth of new exotic effects [2, 3]. Combining a chromium trihalide layer with a superconductor might lead for instance to topological superconductivity as recently reported in CrBr3/NbSe2 heterostructures [4]. In this hybrid structure, it was proposed that the mechanisms leading to a topological order in this hybrid structures was intimately related to the presence of a moiré pattern [2]. Another fascinating observation is about the influence of a moiré on the magnetic properties. In the CrX3 family, till now, the magnetization was shown to be essentially colinear, however, in CrI3 double bilayer some hint of non-colinear magnetism was found and was related to the moiré pattern which leads to a non- negligible spatial modulation of the magnetic interaction [3]. In this communication I will present our scanning tunneling microscopy investigation of a CrCl3 monolayer deposited on Au(111) which exhibit a second order moiré pattern. We report the presence of edge dislocations in this moiré pattern (see figure). Based on a comprehensive analytical model, I will show that these well know edge dislocations can be reexamined in the framework of topological concepts where they are described as topological defects analogous to vortices carrying a Berry phase characterized by a Chern winding number. They might therefore be use as a pinning center to host topological spin texture and / or Majorana bound states in CrX3/superconductor heterostructures.

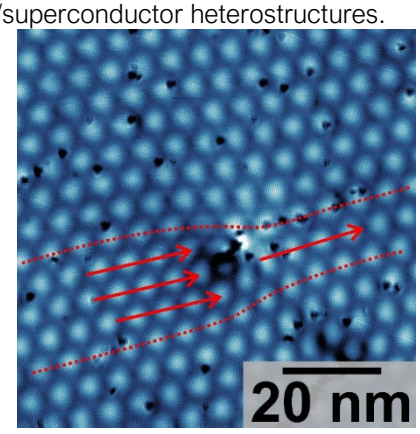

Figure: Edge dislocation in the moiré pattern formed between CrCl3 monolayer and Au(111). It exhibits a Burger vector 2 times larger that the moiré unit cell.

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Oral

HR-STEM-IDPC ATOMIC-SCALE CHARACTERIZATION OF 2D CRYSTALLINE MATERIALS

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Graphene and other two-dimensional materials (2DMs), composed of one or a few atomic layers, exhibit exceptional optoelectronic properties. Their integration into microelectronic devices—particularly on silicon and silicon-on-insulator (SOI) substrates—requires precise control over their microstructural characteristics. Achieving this control necessitates a thorough understanding of their structural, morphological, and chemical features across a broad range of length scales, from the micrometer down to the atomic level. Accurate multiscale characterization is therefore critical to optimizing both the performance and durability of these materials.The integrated differential phase contrast (iDPC) [1] a recently developed transmission electron microscopy technique enables electric field mapping within the sample through COM (center of mass) shifts detected along X and Y axes. By using four detectors it is possible to capture the smallest changes of the centroid position COMX and COMY and through an alignment difference obtaining a high-quality STEM-iDPC image offering insights into the structural and electric properties of the studied layers. Importantly, STEM-iDPC image intensity is directly proportional to the atomic number (Z) of the constituent elements, allowing for the identification of both heavy and light atoms within a sample.

This study focuses on two types of 2D crystalline materials: MoS_2 synthesized by molecular beam epitaxy (MBE) on a GaN/sapphire substrate, and graphene grown by chemical vapor deposition (CVD) on a 6H-SiC substrate (see Figure 1, left and right, respectively). STEM-iDPC analysis of cross-sectional samples revealed epitaxial growth in both systems, characterized by atomically flat, sharp interfaces and highly crystalline, defect-free layers. For the MoS_2/GaN system, detailed STEM-iDPC imaging allowed us to estimate a Ga–S interatomic distance of 2.21 Å—significantly shorter than expected for a van der Waals (vdW) interface—suggesting stronger interfacial interactions [2]. Atomic columns of Mo and S were clearly resolved, enabling direct visualization of the atomic stacking. For the graphene/6H-SiC system, the STEM-iDPC image (Figure 1, right) clearly distinguished the atomic positions of both Si and C atoms across the interface, with an interlayer spacing of 2.5 Å. Additionally, the graphene layer's undulations were observed and quantified, further showcasing the sensitivity of the technique.

These findings demonstrate the remarkable capability of the STEM-iDPC technique to resolve both light and heavy atoms at the atomic scale—capabilities that are difficult to achieve with conventional STEM imaging methods.

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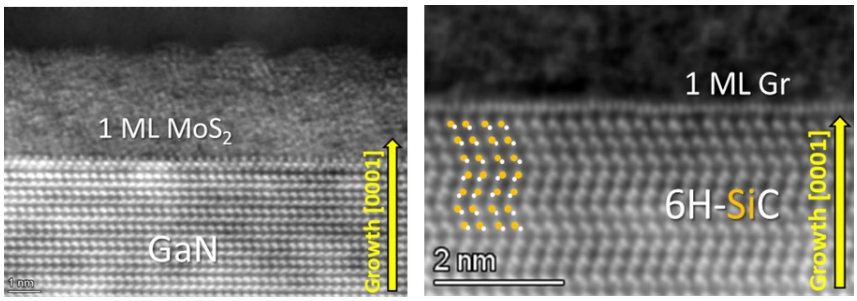

Figure 1: STEM-iDPC images of a MoS2 / GaN layer (left) and Graphene/ 6H-SiC layer (right) in a [11-20] cristalographic orientation illustrating the exact position of heavy Ga (Z=31), Mo (Z=42), Si (Z=14) and light C (Z=6) and S (Z=16) atoms.

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Oral

ROLE OF THE *DIRECT-TO-INDIRECT* BANDGAP CROSSOVER IN THE *'REVERSE'* ENERGY TRANSFER PROCESS

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Energy transfer (ET) is a dipole-dipole interaction, mediated by the virtual photon. Traditionally, ET happens from the higher (donor) to lower bandgap (acceptor) material. However, in some rare instances, a 'reverse' ET can happen from the lower-to-higher bandgap material, depending on the strong overlap between the acceptor photoluminescence (PL) and the donor absorption spectra. In this work [1], we report a reverse ET process from the lower bandgap MoS_2 to the higher bandgap WS_2, due to the near 'resonant' overlap between the MoS_2 B and WS_2 A excitonic levels. Changing the MoS_2 bandgap from direct-to-indirect by increasing the layer number results in a reduced ET rate, evidenced by the quenching of the WS_2 PL emission. We also find that, at 300 K, the ET timescale of ~45 fs is faster than the reported thermalization of the MoS_2 excitonic intervalley scattering ($K^+ \leftrightarrow K^-$) time.

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WEDNESDAY

26

Boron Nitride Synthesis

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Oral

RHOMBOHEDRAL BORON NITRIDE CRYSTALS GROWN BY THE IRON FLUX METHOD

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Boron nitride is a material with exceptional mechanical, thermal, optical, chemical and dielectric properties. Many of these characteristics stem from its extensive polymorphism, since BN exists in either sp^3 hybridization for cubic and wurtzitic phases or sp^2 configuration for the lamellar compounds. For 2D BN, numerous stacking variants have also been demonstrated experimentally (AA', AA, AB) or studied theoretically (AB2, AB3), which further enrich the electronic properties, which depend on the layer stacking arrangement and the symmetry of the crystal lattice [1]. The rhombohedral phase of boron nitride, rBN, which is non-centrosymmetrical, was mentioned as early as 1958, but is of new interest, because of its polar character, which leads to ferroelectricity and non-linear optics.

In this presentation, we will review rhombohedral BN, covering the various growth methods and physical characteristics. In particular, we will present the rBN samples that we have fabricated by the saturation of an iron solvent with nitrogen and boron at 1550°C, followed by slow cooling to precipitate BN [2]. The resulting metal ingots are covered with a white shell consisting of multiple triangular 3D crystals of submillimeter size (Fig.1). High-resolution X-ray powder diffraction reveals excellent crystalline quality, with the rBN phase dominating over the hBN polytype. This is confirmed by low-temperature micro-photoluminescence on a single crystallite, which has smaller peak widths than those observed in previous spectra (Fig.2). This enables fine analysis of high-energy phonon replicas and assessment of the indirect bandgap. These results are in good agreement with energy bands and phonon dispersion calculations. Finally, we will detail Raman and IR spectroscopies with specific structures that have not been observed in other BN polytypes yet.

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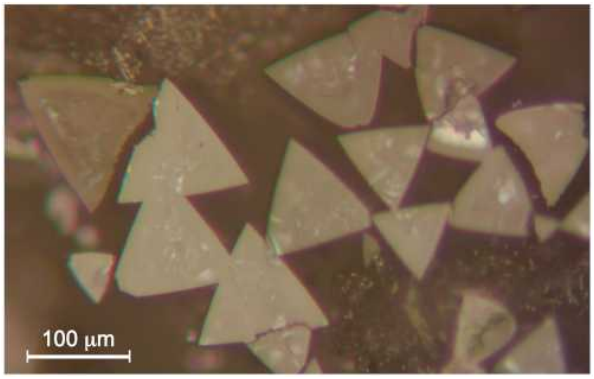

Figure 1: Triangular-shaped crystallites of rhombohedral boron nitride.

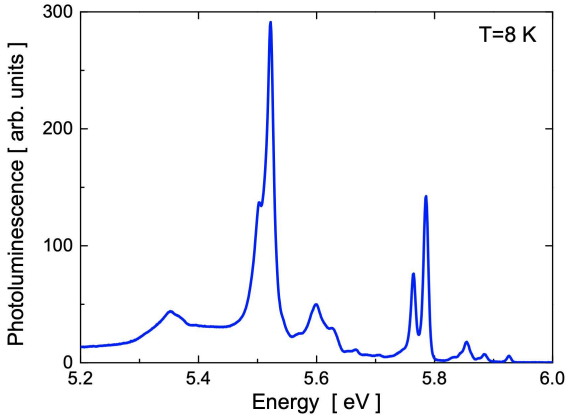

Figure 2: Low temperature photoluminescence of an rBN crystal.

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Oral

Thickness and stacking sequence control of BN layers epitaxially grown by Rapid Thermal CVD on Ni(111) substrate

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Among 2D materials, boron nitride has remarkable properties. It is an insulator with a large band gap (6 eV), atomically flat with no dangling bond, thermally resistant and chemically inert. It can be integrated in Van der Waals heterostructures with different roles : as a substrate or intermediate or protective layer, of great interest for the fabrication of nanodevices in optics, electronics and spintronics [1]. Most of the current proof of concept or devices with high-performances have been done with hBN flakes obtained by crystal exfoliation. This process provides hBN flakes of high quality in terms of crystallinity and low defect density, but with limited lateral size and it is hard to control their thickness. Mastering large area synthesis is essential for the development of 2D devices. To this end, large area synthesis is in development by techniques such as MBE, ALD, PVD or CVD [2]. However, so far controlling the film thickness with a high crystalline quality remains a challenge.

In this context, we develop a synthesis route for sp^2-hybridized boron nitride by CVD in a rapid thermal processing system with halogen lamps. The growth is done on Ni (111) substrate at low pressure with borazine as a precursor [3]. After growth, the films are transferred on TEM grid or SiO_2 substrate by a standard wet transfer (Figure 1) and characterized from the mm scale to the nm scale by optical microscopy, statistical Raman spectroscopy (Figure 2), AFM, MEB and in plane or cross sectional TEM. We have been able to synthesize and transfer homogeneous films of several mm^2 (Figure 1) and to vary the number of layers from 2 to 10 layers depending on the set of synthesis parameters, which are the substrate thickness, the borazine quantity, and the cooling rate. We discuss the impact of the different parameters on the BN films and how this study helps to understand the growth mechanism of BN on Ni(111) by CVD under low pressure.

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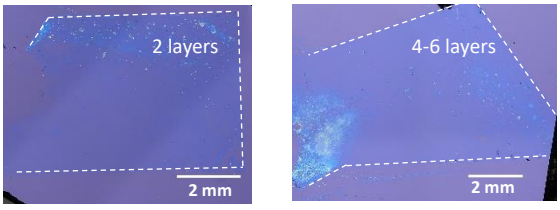

Figure 1: Optical microscopy images of BN films, 2 and 4-6 layers thick, transferred on 90 nm SiO_2/Si substrate

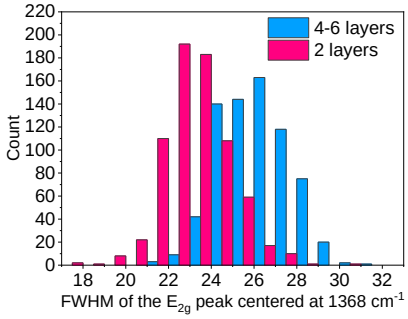

Figure 2: Histograms of the FWHM for the E_{2G} Raman mode recorded on 2 and 4-6 layers-thick BN films

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Oral

HEXAGONAL OR AMORPHOUS? STEERING BORON NITRIDE PHASE BY CVD OF BORAZINE

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Boron nitride (BN) has emerged as a highly promising material for current and next-generation electronic devices. Over the past decade, sp^2-hybridized BN has established itself as a key component in the development of graphene-based optoelectronic systems, thanks to its excellent insulating properties and its minimal lattice mismatch with graphene.[1,2] More recently, amorphous BN (aBN) has garnered increasing attention, particularly due to its ultra-low dielectric constant of 1.16−significantly lower than the value of 4.0 (at 1MHz) typically reported for hexagonal BN.[3] Notably, ultra-thin aBN films (e.g., 3nm-thick with k=2) have been successfully demonstrated as novel capping layers for copper interconnects, offering both low-k performance and compatibility with modern microelectronics architectures.[4]

To fully leverage BN's potential in electronics, optoelectronics, and spintronics, precise control over its structure − and therefore its properties − is essential.[5] Among the various thin-film deposition techniques, chemical vapor deposition (CVD) stands out as a versatile and widely adopted method, enabling the growth of high-quality BN films from a variety of precursors. In particular, borazine ($B_3N_3H_6$), a volatile compound with a 1:1 boron-to-nitrogen ratio, has proven to be highly effective for the CVD synthesis of sp^2-BN, offering stoichiometric control and efficient deposition. Nevertheless, the underlying deposition mechanisms and the influence of key parameters (e.g., temperature, precursor flux, carrier gas, and substrate) on the film's structural and functional properties remain insufficiently understood.

In this study, BN films were deposited by borazine-based CVD on native oxide Si wafers under a range of conditions spanning 400°C to 1350°C, with systematic variation of parameters such as precursor flux and carrier gas type. The resulting films were extensively characterized using a suite of complementary techniques including ellipsometry, XRD, SEM, EDS, TEM, XPS as well as Raman and infrared spectroscopy.

Our results reveal that both borazine flux and deposition temperature play crucial roles in determining film morphology, crystallinity, and chemical bonding. The data suggest a competition between two principal reaction pathways: (1) polycondensation of borazine into oligomeric species, and (2) thermal decomposition into reactive fragments such as BH_3 and NH_3. the dominance of one mechanism over the other is strongly influenced by the specific CVD conditions, thereby dictating the final film structure. Based on these findings, a proposed reaction mechanism is presented to explain the observed trends.

This work was supported by the project MINERVA - ANR-21-GRF1-0002, FLAG-ERA JTC 2021 - 2021

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Oral

ATOMIC-SCALE INSIGHT INTO THE OXIDATION BEHAVIOUR OF AMORPHOUS BORON NITRIDE FILMS USING ML-DRIVEN MOLECULAR DYNAMICS SIMULATIONS

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Amorphous boron nitride (aBN) has emerged as a critical material for advanced electronic and energy devices, where it functions as an ultrathin diffusion barrier and encapsulation layer thanks to its high thermal stability, low dielectric constant, and chemical inertness [1,2]. Its performance in harsh environments, particularly under oxidative stress, is of growing interest for applications ranging from interconnect protection in microelectronics to barrier coatings in energy systems [3]. However, a fundamental understanding of how aBN responds to oxygen exposure at the atomic level remains elusive.

Experimentally, techniques such as X-ray diffraction (XRD), NMR, or XPS offer limited structural resolution due to the absence of long-range order in amorphous materials, often yielding only average or statistical information about local bonding environments. Theoretically, empirical interatomic potentials lack the accuracy required to capture chemical reactivity and bond rearrangements, while density functional theory (DFT), although precise, is prohibitively expensive for simulating the large, disordered systems and long timescales involved in oxidation processes [4].

To bridge this gap, we develop a machine-learning interatomic potential using the Gaussian Approximation Potential (GAP) framework, trained on a DFT-derived B–N–O dataset. This model enables large-scale molecular dynamics simulations that retain near-DFT accuracy while allowing for the exploration of long-timescale oxidation processes. We apply this potential to generate realistic melt-quenched aBN structures and simulate their exposure to oxygen at different temperatures, capturing both surface oxidation and sub-surface diffusion phenomena. Our simulations reveal how structural features such coordination defects and short-range ordering influence the oxidation resistance of aBN [5]. This machine-learning-driven approach provides a predictive, physically grounded framework for understanding oxidation in disordered materials and opens the door to rational design of more robust aBN-based barrier layers for energy and nanoelectronic applications.

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THURSDAY 27

2D Magnets 2

Oral

EPITAXIAL VAN DER WAALS MATERIALS FOR MAGNETISM AND SPIN-CHARGE CONVERSION

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Layered materials possess electronic properties of exceptional interest for several domains of solid-state physics. Their crystal structure with van der Waals bonding between unit layers makes it feasible to stabilize single 2D layers and to form a wide range of heterostructures without the constraint of lattice matching. In this family of materials, transition metal dichalcogenides and topological insulators hold great promise for spintronics owing to their large spin-orbit coupling and the locking between the electron spin and momentum [1]. The recent discovery of van der Waals 2D magnets has also opened exciting opportunities to explore low dimensionality magnetism, proximity phenomena in heterostructures and all-van der Waals spin devices.

While most research on these materials is currently performed with microflakes mechanically exfoliated from bulk crystals, molecular beam epitaxy is emerging as a powerful method to grow large-area 2D materials with fine tuning of the composition, control of the thickness down to the 2D limit and ability to fabricate heterostructures with sharp and clean interfaces. I will discuss the specificities and challenges of van der Waals epitaxy and review recent progress in the fabrication of van der Waals materials by this technique, including topological insulators [2], transition metal dichalcogenides [3] and 2D magnets [4,5]. I will then illustrate the potential of these materials for spintronics with examples of heterostructures in which spin-charge interconversion is implemented, leading to large spin-orbit torques and current-driven magnetization switching [6-8].

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High-Tc Ferromagnetic Oxide Nanosheets for Spintronic Applications

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Abstract

Spintronics intends to further develop electronic systems with the aim of reducing energy consumption while maintaining growing performances. In this framework, 2D oxide materials are a promising platform offering model properties ranging from high-k 2D dielectrics (1) to 2D ferroelectrics (2) or 2D ferromagnets (3) while being intrinsically air stable, an overall key asset for 2D spintronics.

This presentation focuses on the development of 2D-TFCO (Ti0.8–x/4Fex/2Co0.2–x/2O2) doped titanate oxide nanosheets, an original 2D oxide stable in ambient atmosphere with ferromagnetic properties at room temperature (3). TFCO oxide nanosheets are produced *via* the exfoliation of the bulk layered parent oxide KTFCO (K0.4Ti0.8–x/4Fex/2Co0.2–x/2O2), synthesized by solid-state chemistry methods. The optimization of synthesis parameters has led to the growth of millimetric KTFCO single crystals (see Fig.1a) suitable for bulk properties analysis prior to the exfoliation of large area TFCO nanosheets.

Latest results on KTFCO crystals characterizations will be presented, especially their magnetic properties with Curie point above room temperature. Structural properties of the layered phase will also be presented. Exfoliation of KTFCO crystals into TFCO-nanosheets (Fig.1b) will be demonstrated as a first step towards the integration of this 2D ferromagnetic insulator as a functional material in spintronics heterostructures (Fig.1c). Finally, a specific focus will be dedicated to the investigation of the electronic, magnetic, transport and

*Speaker

magneto-transport properties of 2D-TFCO single and multilayers.

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MAGNETOELASTIC COUPLING IN CHROMIUM OXYCLORHIDE DOWN TO THE 2D LIMIT

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Abstract

Chromium oxychloride (CrOCl) is a van der Waals magnet featuring a rich phase diagram (1,2) related to its low-symmetry structure, structural phase transitions, and a subtle competition of interactions potentially leading to magnetic frustration. In a recently published work (3), we showed how, exploiting the strong magneo-elastic coupling in the material, we can use Raman scattering spectroscopy, performed at variable temperature and magnetic field (up to very high fields), to decipher the magnetic phase diagram of bulk CrOCl. Here we extend this work to the investigation of thin flakes of CrOCl down to the single layer. While previous works on thin layers have used transport techniques and did not show a clear evolution of the properties with the thickness (4), we were able to highlight strong effects of the coupling of the lattice with the external field, leading to zone-folded phonons (produced by the magnetic supercell) or blue/red-shifts of the phonon energies at the metamagnetic transitions (see Figure 1) to build a phase diagram of the material at varying thickness. Moreover, we were able to demonstrate the existence of a strong magnetostriction effect at high magnetic field (up to 30T) , present for all thicknesses down to the monolayer.
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*Speaker

Pressure-dependent magnetism in 2D van der Waals materials : theoretical calculations

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Abstract

Two-dimensional (2D) van der Waals (vdW) materials have emerged as a rich platform for exploring novel quantum phenomena and next-generation device concepts. Among their many intriguing features, the recent discovery of magnetism in atomically thin layers (1) has opened new directions in spintronics and materials design.
Recent studies on CrBr (2) have shown that the strength and even the sign of the interlayer magnetic exchange can vary significantly depending on how the layers are stacked. A similar tendency to form different magnetic phases under pressure has also been reported in VI (3), highlighting a broader phenomenon across layered vdW magnets. These arguments suggest that both the phases with ferromagnetic (FM) and antiferromagnetic (AFM) interlayer interactions are present simultaneously in real samples, and their relative proportion depends on the pressure. Even recentally we found Pressure can supress complex non-collinear helimagnetic phase (HM) in NiBr2.

In this work, we investigate how applied pressure influences the magnetic properties of bilayer Chromium Bromide (CrBr), Vanadium triiodide (VI) and Nickel Bromide (NiBr2) prominent candidates for 2D magnetic vdW materials. We present how pressure changes the magnetic coupling between layers, which is responsible for formation of different stacking configuration. To understand how these mixed-phase environments influence the magnetic critical temperature (T_C/T_N), we conducted finite-temperature Monte Carlo simulations using a stochastic Landau-Lifshitz-Gilbert (LLG) framework (4). By modelling systems with varying proportions of AA and AB phase atoms-randomly distributed but differing in interlayer exchange-we quantify how the interplay between competing magnetic interactions shapes the thermal stability of magnetism under pressure.

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*Speaker

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THURSDAY 27

Growth and Synthesis

2D Materials from Crystal Growth to Exfoliation and Chemical Modification

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Abstract

2D materials offer vast variability, with nearly unlimited combinations of composition, properties, and structures. This versatility can be further extended through layer stacking and twisting, enabling unique electronic and mechanical behaviours. The diversity in chemical composition necessitates various approaches for their crystal growth and chemical modifications.
This discussion will cover the synthesis and crystal growth methods for different classes of 2D materials, including chalcogenides, halides, chalcogen-halides, and beyond. The impact of experimental conditions on their structural and functional properties will also be explored.

Exfoliation techniques, particularly those involving intercalation, provide a pathway for obtaining large-area monolayer flakes and bulk intercalated compounds with tailored properties. The effects of these methods on material characteristics will be examined. Additionally, chemical exfoliation methods for materials with layered structures held together by covalent bonds will be presented.
Finally, the applications of 2D materials across multiple fields will be discussed, including electronics, energy storage, catalysis, and beyond. This overview aims to highlight the transformative potential of 2D materials from fundamental synthesis to practical technological implementations.

*Speaker

COVALENT AND SUPRAMOLECULAR APPROACHES TO CONTROLLED 2D HYBRID HETEROSTRUCTURES GROWING.

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Abstract

Two-dimensional materials have captivated researchers thanks to their unique properties as anisotropic quantum confinement, tunable band gap, and heterogeneous catalyst, among others. The combination of these materials, combining various 2D layers, offers a compelling approach to obtain hybrid 2D heterostructures, permitting the synthesis of entirely new material systems, with great potential for next-generation technologies (1).
A typical approach to the production of 2D heterostructures is commonly based on the vertical stacking of 2D materials (2, 3), obtained by *in-situ* chemical vapor deposition (CVD), scotch tape exfoliation, and transfer of the structures. These approaches permit control over the stacking order of the 2D structure, limiting however the scalability of the production. More surprisingly, despite the chemical control developed during the last decades over 2D materials, fewer are examples of wet chemical approaches to 2D hybrid formation, exhibiting great synergistic effects and promising applications (4).

This talk will discuss the chemical covalent and supramolecular approaches recently explored by our group, aimed at synthesizing graphene-molybdenum disulfide (MoS2)/perovskite (PVK)/layer double hydroxide (LDH) 2D heterostructures (Scheme 1). The ordered stacking characterization and bulk properties of the hybrids will be presented showing synergistic effects in terms of time stability, electrical conductivity, and catalytic properties (5). Moreover, the colloidal synthesis of 2D hexagonal-shaped antimonene and bismuthene materials will be introduced, together with the production of their hybrids heterostructures with graphene and fullerenes (6).

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*Speaker

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(5) Articles in preparation
(6) Article in press

Annual meeting 2025 of the GDR and IRN HOWDI
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ORAL

SYNTHESIS AND CHARACTERIZATION OF INCLX (X=SE , S) LAYERED METAL CHALCOHALIDES AND THEIR HETEROSTRUCTURES.

Andres De Luna Bugallo[1],Mario Flores Salazar[1], David Sanchez[2], Uriel Castro Ibanez[1], Alan Cruz Gonzalez [1], Mauricio Terrones[2]

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Ternary 2D compounds provide additional degrees of freedom to tailor physical properties through stoichiometric variation, often enabling functionalities beyond those of their binary counterparts (e.g., transition metal dichalcogenides, TMDs). In this work, we report the successful synthesis of two ternary layered materials, InCIS and InCISe, via atmospheric pressure chemical vapor deposition (APCVD). Both systems were grown at relatively low temperatures (300–400 °C). The resulting crystals exhibit well-defined layered morphologies, as confirmed by optical microscopy and scanning electron microscopy (Figure 1). Energy-dispersive X-ray spectroscopy (EDS) reveals a stoichiometry close to In:1, Cl:1, and S or Se:1, consistent with a 1:1:1 ternary composition. Selected area electron diffraction (SAED) patterns obtained by transmission electron microscopy (TEM) indicate a hexagonal crystal structure (Figure 2).

To assess the vibrational and optical characteristics, Raman spectroscopy and photoluminescence (PL) measurements were performed. Raman spectra display distinct vibrational modes indicative of complex ternary bonding environments, and the PL response reveals strong emissions in the visible range, suggesting promising applications in optoelectronic and photonic devices. In particular, low-temperature PL measurements performed on InClSe flakes, show a notable blueshift of the main emission peak and a narrowing of the emission linewidth to ~27 meV at 90K(Figure 3).

Finally, we demonstrate the versatility of these materials by not only inducing the growth of vertical heterostructures composed of InClSe–InClS, but also by integrating them with conventional transition metal dichalcogenides (TMDs) such as MoS_2, $MoSe_2$, WS_2, and WSe_2 to form hybrid ternary–binary 2D heterostructures.

The combination of low synthesis temperature, well-defined layered structure, and strong photoluminescence emission makes these ternary compounds promising candidates for integration into back-end-of-line (BEOL) processes within CMOS-compatible technologies, while simultaneously expanding the library of 2D materials to include halogen-containing ternary systems.

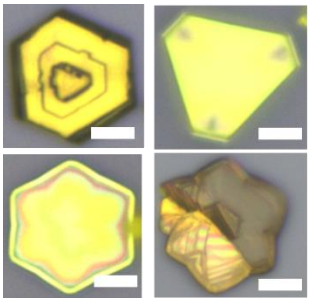

Fig.1 Optical images of InCIS and InCISe crystals (bar scale is 5um)

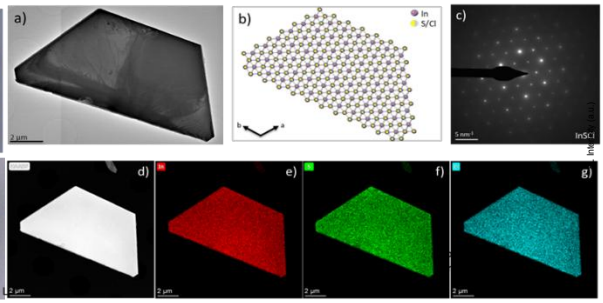

Fig.2 Low magnification TEM, atomic structure depiction, SAEDpattern and EDS of InClS

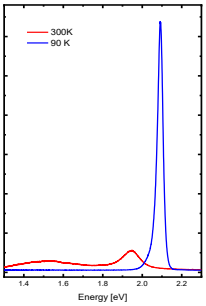

Fig 3. PL emission of InClSe at RT and 90K

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Oral

IN SITU GROWTH OF SUSPENDED ZIRCONENE ISLETS INSIDE GRAPHENE PORES

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Despite the growing interest and theoretical predictions[1] of suspended two-dimensional (2D) metals (or metallenes), direct observations of these one-atom-thick structures remain limited.[2] This innovative study presents a novel approach for the *in situ* synthesis of suspended 2D zirconium (zirconene) islets within graphene pores using electron beam irradiation inside a transmission electron microscope (TEM).[3] Unlike previous methods that rely on complex epitaxial growth on metallic substrates, our approach enables the fabrication of freestanding zirconene structures with atomic-scale precision.

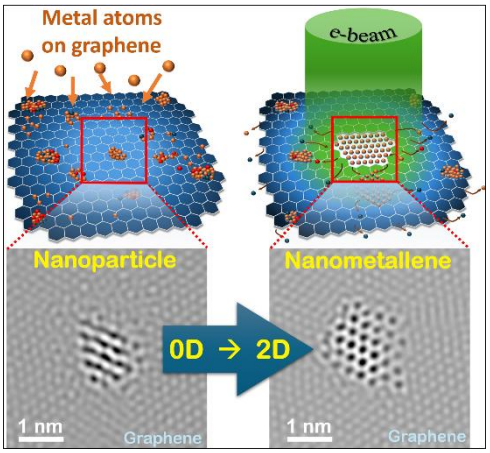

Figure 1: *In situ* growth of zirconene islets using TEM.

Experiments conducted with a TEM revealed that electron beam irradiation of zirconium acetylacetonate decomposed the precursor directly on graphene, leading to the formation of zirconium nanoparticles, which, under continuous irradiation, transform into zirconene islets embedded within the graphene lattice (see Figure 1). The originality of our results lies in the systematic observation of the formation and stability of zirconene islets under electron irradiation. Consequently, this work introduces unprecedented opportunities for studying the dynamic interactions between zirconium atoms and graphene, highlighting the key role of defect engineering in the confinement and stabilization of zirconene layers.

This work offers key insights into electron-driven growth and degradation of zirconene islets. It marks a step forward in using electron beams to fabricate atomically thin zirconene coatings for materials exposed to extreme evironments. Furthermore, this study paves the way for a broader exploration of metallenes in the fields of nanoelectronics, catalysis, and energy storage.

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FRIDAY 28

Transport

Quantum transport of heat in graphene

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Under high magnetic field and at low temperatures, electronic interactions in a graphene give rise to exotic, strongly correlated many-body quantum Hall states. These states have been proposed for the implementation of new quantum circuits, for instance realizing topologically protected quantum computing. Although exciting, they remain poorly understood, because the conventional experimental approach for their investigation, dc electron transport, only yields limited information. In particular, electron transport only probes the physics of the current-carrying edge channels of the quantum Hall effect propagating along the edges of the electron gas, leaving the physics of the bulk unexplored. To gain a better understanding of these exotic states and their origin, we propose a new, unconventional approach, based on heat transport measurements, which directly probes the charge-neutral, heat-carrying collective modes characterizing these interactions-induced states.

In this talk, I will introduce the principle of our heat transport measurements, and describe recent results on its application to quantum Hall physics in graphene.

Oral

Graphene/MoS_2 field-effect transistors with spin-dependent photovoltage

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Graphene exhibits a small intrinsic spin–orbit coupling (ISOC), typically around 45 μeV, as previously measured using techniques such as resistively detected electron spin resonance (RDESR) [1], and photovoltage-detected ESR (PV-ESR) [2]. This photovoltaic measurement technique enables the investigation of intrinsic spin–orbit coupling in graphene, as well as its topological properties, over a broad frequency range from GHz to THz. To enhance this weak ISOC, graphene can be combined with transition metal dichalcogenides like MoS_2, a material known for its strong spin–orbit interaction in order to enhance graphene's SOC via the proximity effect.

In this work [3], we use PV-ESR in the 55–115 GHz range, using a plasma wave detector based on a monolayer graphene/MoS_2 field-effect transistor, in order to investigate both the graphene/MoS_2 heterostructure and the origin of the observed ESR signals.

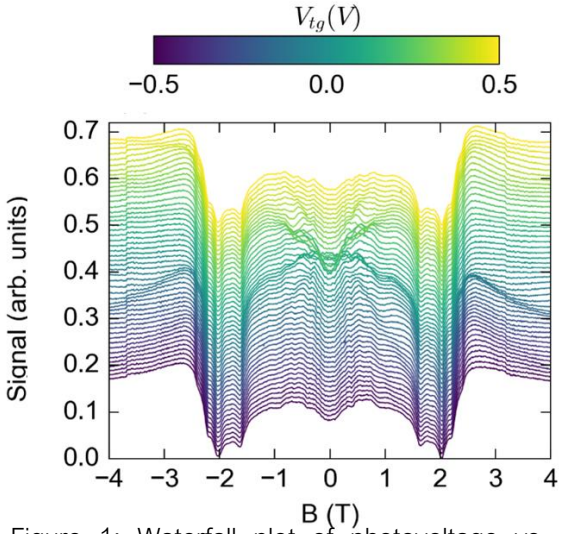

Figure 1: Waterfall plot of photovoltage vs. magnetic field for various top gate voltages as at 1.7 K and under an excitation at 56 GHz. (adapted from [3])

We observe four electronic spin resonances which are completely independent of gate voltage. Among the four resonances observed, one corresponds to intrinsic spin–orbit coupling (ISOC), two are attributed to sublattice potential asymmetry, and the fourth arises from a spin-flip transition between Zeeman-split bands, with an extracted Landé g-factor of 2.09.

Compared to previous results, our results show that the presence of the MoS_2 layer does not significantly enhance spin–orbit coupling in graphene. Tight-binding simulations suggest that the strength and nature of the proximity-induced SOC in graphene/MoS_2 heterostructures are highly sensitive to the moiré angle [4], a parameter not controlled in our samples, which may explain the absence of enhancement.

In parallel, we observe that this four ESR resonances consistently appear as drops in the photovoltage, regardless of the signal's polarity or rectification mechanism, whether arising from plasma-wave or Seebeck effects. We interpret this behavior as a decrease in the system's spin polarization during resonant excitation, possibly due to spin-dependent scattering or a return to a randomly polarized spin state.

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Annual meeting 2025 of the GDR and IRN HOWDI
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Oral

CRYSTAL FIELD in BILAYER GRAPHENE/hBN HETEROSTRUCTURES

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The crystal field describes how the spatial variation of the crystal potential—such as near the surfaces of 3D systems or at the interfaces between different materials in heterostructures—affects the electronic structure. Its effects are primarily significant at these surfaces of 3D systems. In Van der Waals heterostructures with the few-atomic-layer thickness [1], crystal fields can, however, significantly alter the electronic properties of the entire system. Therefore, investigating the crystal field is crucial for understanding the impact of the combination of 2D layered materials and, consequently, for understanding the properties of Van der Waals heterostructures [2-4]. In this talk, we will present a recent study [5] on the crystal field in Bernal bilayer graphene/hexagonal Boron Nitride (h-BN) heterostructures, conducted by atomistic simulations and experimental transport measurements. Simulation results show the strong dependence of crystal field on the angular alignment angle between graphene and hBN layers. In addition, their commensurate state and symmetry properties also play important roles, which nicely re-confirms the 120° periodicity in the transport properties previously reported [6]. Transport measurements using the newly developed device architecture (see Fig.1)—which integrates dynamically rotatable van der Waals heterostructures and the control over both top and bottom gates—have confirmed these theoretically predicted properties of the crystal field.

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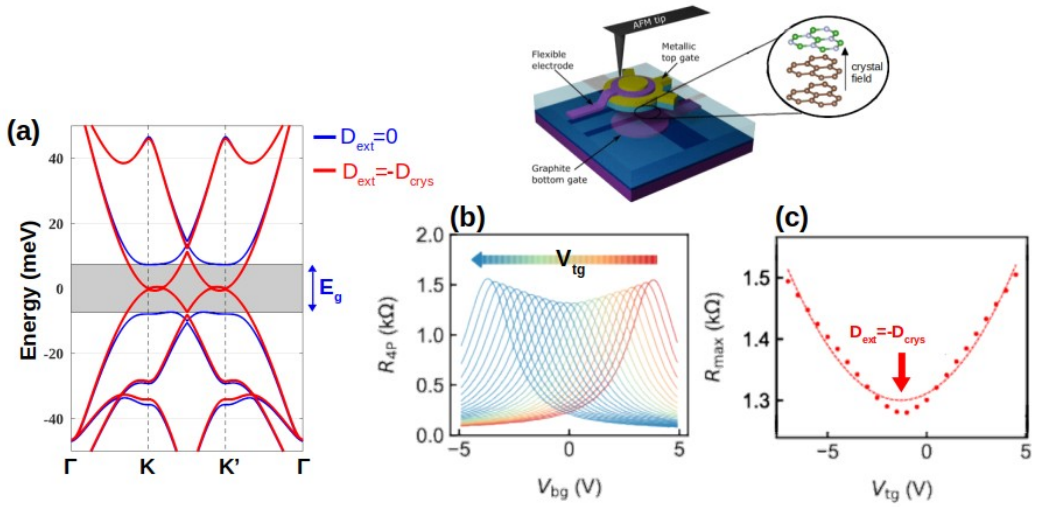

Fig.1: Bilayer graphene/hBN heterostructures. (a) Bandgap induced by a crystal field and closed by an external displacement field, computed in the 60° alignment case. The top-right panel illustrates the new device architectureexperimentally developed [5]. (b) Resistance as a function of the bottom gate for different top gates and (c) Resistance at the charge neutrality point for different top gate voltages.

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Oral

MULTIFERROIC EPITAXIAL EUROPIUM OXIDE UNDER TOPOTACTIC REACTION

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2D van der Waals heterostructures are a promising technology to induce new properties in materials through electrostatic interactions and hybridisation. Since the advent of spintronic and spin-dependent transport properties, the route towards magnetic proximity effects (MPE) has revealed its large potential. Nevertheless, the quest regarding a coupling between magnetic and electric orders is under great attention. The EuO/graphene heterostructure is grown by topotactic reaction with a polycrystalline structure. It has recently shown encouraging properties such as magnetic ordering (superparamagnetism) and a ferroelectric behaviour up to room-temperature (RT). Furthermore, a magnetic field dependence of the electric polarisation has been observed.

Through these observervations, two ways open up. The first one is to probe the magnetisation tunability by applying an electric field through transport measurements in a Hall bar-shaped heterostructure. That could be another proof of the magnetoelectric multiferroic coupling. The second one is to grow EuO on different layers in order to promote a monocrystalline growth that can lead to better magnetic properties.

Magneto-electric coupling characterisation by transport measurements

Transport measurements show an Anomalous Hall Effect (AHE) contribution in both the transversal and the longitudinal resistance, arising from the magnetisation induced in graphene by MPE. The electric field dependence of the AHE has an even contribution (Fig. 1), which is proportional to a magnetoelectric coupling term. This is another proof of magnetoelectric coupling in EuO, but a first highlight of the magnetisation dependence under an electric field in topotactic EuO layers.

Epitaxial europium oxide growth

Europium oxide (Eu_2O_3) is grown on epitaxial V(5 nm)/Cr(20 nm) by Molecular Beam Epitaxy at RT. First magnetic measurements were performed in SQUID VSM (Fig. 2) after deposition and showed a coercitive field of 20mT up to RT and a saturation magnetisation of 3 µB/at (with 1nm magnetic EuO). These results show that V can reduce Eu_2O_3 into EuO, leading to RT ferromagnetic behaviour, above the Curie temperature of EuO (69K). The reduction through topotactic reaction is enhanced during annealing and lets us suggest better properties to be reached.

Preliminary results of MPE in a graphene on a ferrimagnet insulator stack will also be discussed.

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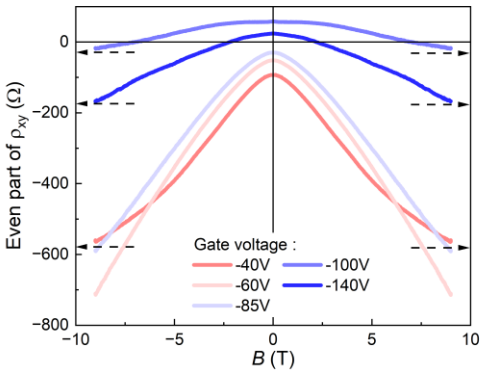

Figure 1: Even contribution of the magnetic field to the transversal resistance at different gate voltages at 2K.

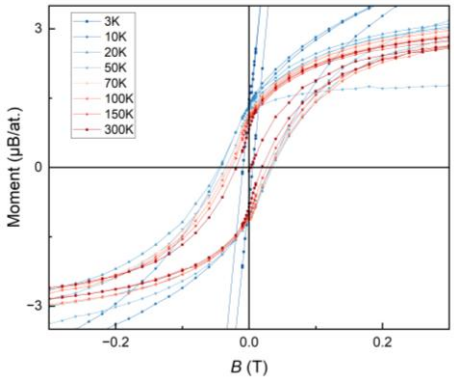

Figure 2: Magnetization as function of the magnetic field in EuO/V/Cr/MgO at different temperatures, supposing 1nm magnetic EuO.

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FRIDAY 28

Optical Properties 3

Annual meeting 2025 of the GDR and IRN HOWDI
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Oral

OPTICAL ABSORPTION IN LAYERED SEMICONDUCTOR TO SEMIMETAL PLATINUM DISELENIDE

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The transition metal dichalcogenide $PtSe_2$ exhibits the surprising property of transitioning from a semimetal to a semiconductor as it is thinned down to a few monolayers [1]. This strongly thickness-dependent 2D material hence allows the tuning of its electronic properties to address specific applications—such as near-infrared photodetection for fiber optics telecommunications. Yet, the light absorption mechanism in such materials is still not well understood.

In this talk, I will rely on broadband optical absorption spectroscopy (0.8–3.0 eV) of high-quality $PtSe_2$ few-layer crystals obtained by the Au exfoliation technique [2]. While previous studies conjectured that their absorption threshold originates from interband indirect transitions, we will rule out such a mechanism by studying the dependence of optical absorption on temperature and material quality. The quantitative comparison with *ab initio* density functional theory (DFT) simulations will allow us to conclude that the optical absorption arises solely from direct transitions, and to identify the transitions at play [3]. Based on this understanding, I will revisit the $PtSe_2$ semiconductor-to-semimetal transition with respect to the number of layers.

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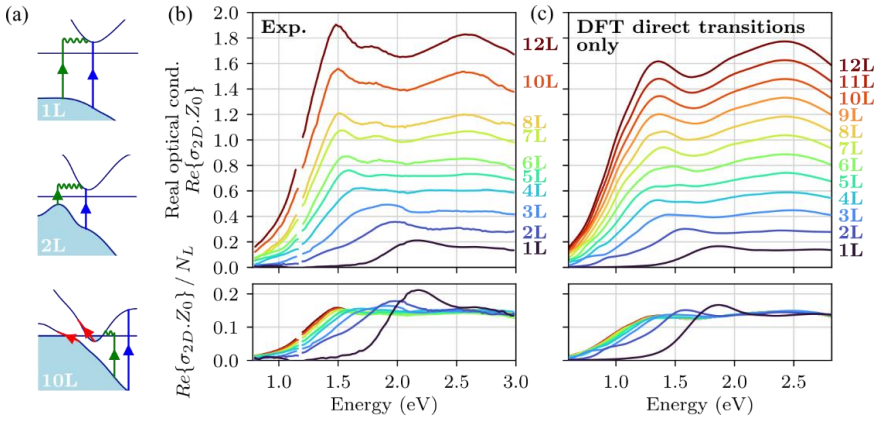

Figure 1: (a) Schematic of photon absorption mechanisms considered—depicting intraband (red), indirect interband (green), and direct interband (blue) transitions. (b) Experimental and (c) theoretical real 2D optical conductivities $Re\{\sigma_{2D}.Z_0\}$ (top plots), and their values normalized by the layer count N_L (bottom plots). Z_0 = 377Ω is the impedance of free space. Adapted from [3].

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Oral

EXCITON FORMATION IN TWO DIMENSIONAL SEMICONDUCTORS

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Robust excitons, which are tightly bound electron-hole pairs, dominate the optical properties of atomically thin semiconductors based on transition-metal dichalcogenides (TMDs). Exciton relaxation and formation dynamics in TMDs have been extensively studied by time-resolved optical spectroscopies.[1] Nonetheless, the crucial question, ***What is the microscopic exciton formation mechanism in two-dimensional semiconductor systems?*** persists**.** This study addresses this fundamental problem through polarization-dependent micro-photoluminescence (PL) studies performed at cryogenic temperatures (4K) on fully hexagonal boron nitride (hBN) encapsulated and charge-tunable (CT) TMD monolayers (MLs) close to the neutrality point. Our experiments results, performed on both WSe_2 and MoS_2 MLs, clarify the role played by the two potential formation mechanisms: a) geminate and b) bimolecular (Fig. 1). The geminate exciton formation process corresponds to the monomolecular annihilation of the photogenerated correlated electron-hole pair. In contrast, the non-geminate formation results from the random bimolecular binding of two free charges, losing the correlation between the excitation photon and the electron-hole pair of the exciton.[2] These two key processes control the exciton formation time.
We demonstrate that for a laser excitation energy below the band gap, the geminate mechanism prevails as expected, whereas above the band gap, both geminate and bimolecular phenomena coexist. These findings provide valuable insights on the exciton formation mechanism in 2D semiconductors, which is crucial for the optoelectronic applications, and may be applicable to a broader range of semiconductor nanostructures, emphasizing the intricate interplay between excitation energy, light polarization, and Coulomb interaction. Additional striking phenomena will be further discussed.

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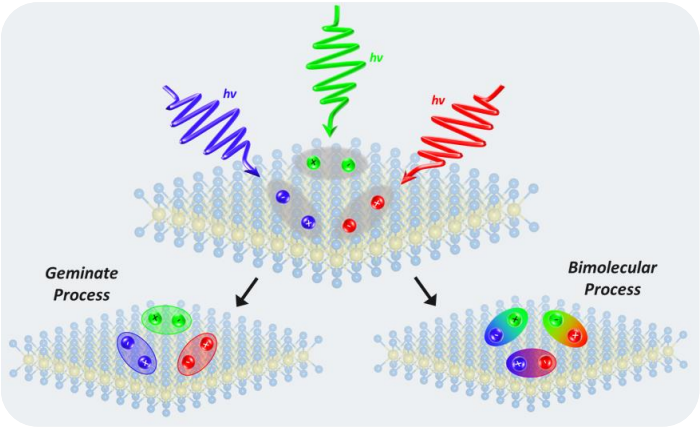

Figure 1: The two primary exciton formation processes in TMD monolayers: a) Geminate and b) Bimolecular.

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ULTRAFAST RELAXATION DYNAMICS OF MOSE2 PROBED WITH BROADBAND TUNABLE WAVELENGTHS

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Abstract

Van der Waals 2D materials have become a unique field of research over the last two decades, since the first successful exfoliation of graphene. Due to quantum confinement and weakly screened charge carriers, most of those materials present exotic behaviors, for exemple room-temperature excitonic properties in transition metal dichalcogenides (TMDs) (1). In this specific family, we decided to study MoSe2 because of his absorption resonance at around 800nm. As of now, ultrafast optical pump-probe studies on MoSe2 have mainly been focused on excitonic behaviors, attributing the two different dynamics in mono and few-layers to fast (ps) exciton-exciton annihilation and slow (100's ps) exciton relaxation in the material (2,3), overlooking other potential contributions : thermal, acoustic ...
Here we propose to precisely study the optical response of atomically-thin MoSe2 exfoliated sheets with advanced pump-probe optical measurements, using beams focused to their diffraction limit and wavelengths of both pump and probe independently tuned in the UV-visible-NIR (400-1100nm) range (figure 1). This approach is an expertise of our team here at ILM applied to plasmonic nanoparticles. By experimentally extracting the quantitative absorption spectrum and pump-probe signals at finely tuned pump and probe wavelengths, we are able to separate and study the different physical contributions forming the nanoparticule's relaxation : electronic, thermal, acoustic and the environment response (4,5).

We recently obtained some preliminary results with this approach, retrieving the two characteristic times previously mentioned yet highlighting a different probe wavelength dependence (figure 2).While a firstcoming fast decay remains positive in the probed range, the slow decay clearly shows a sign change around 810 nm, i.e. close to the excitonic resonance. We infer two different physical origins for these timescales that we are quantitively investigating via electronic and thermal modelization.

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Oral

Spin Relaxation of Rydberg Excitons in a Two-Dimensional Semiconductor

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Optical properties of atomically thin transition metal dichalcogenides are dominated by robust excitons characterized by a very large oscillator strength [1]. Encapsulation of monolayers such as WSe2 in hexagonal boron nitride (hBN) yields narrow optical transitions approaching the homogeneous exciton linewidth [2]. In this work, we have measured the optical and spin/valley properties of excitons in a very high quality encapsulated WSe2 monolayer allowing the observation of excited excitonic states up to n=5 using photoluminescence and reflectivity spectroscopy. This offers a unique possibility to investigate the spin relaxation of excited excitonic states. Until now, these studies in two-dimensional semiconductors (quantum wells or 2D materials) had only been carried out for the 1s exciton ground state [3,4]. Following circularly-polarized laser excitation, we have recorded the circularly-polarized luminescence polarization Pc of the different exciton states. Remarkably, we measure in cw optical orientation experiments very large polarization: Pc~30 %, 80% and up to 90% for 1s, 2s and 3s excitons respectively. Time-resolved photoluminescence experiments performed with a synchro-scan Streak camera with a typical time-resolution of ~1 ps demonstrate that the increase of the exciton polarization with n is not due to a decrease of the lifetime but the polarization dynamics evidence clearly an increase of the exciton spin relaxation time which varies from ~1.5 ps for 1s up to ~50 ps for 3s excitons. To our knowledge this is the first time that the Rydberg exciton spin relaxation time has been measured directly and the results will be discussed in the framework of the exciton spin relaxation mechanism driven by the long-range exchange interaction between the electron and the hole.

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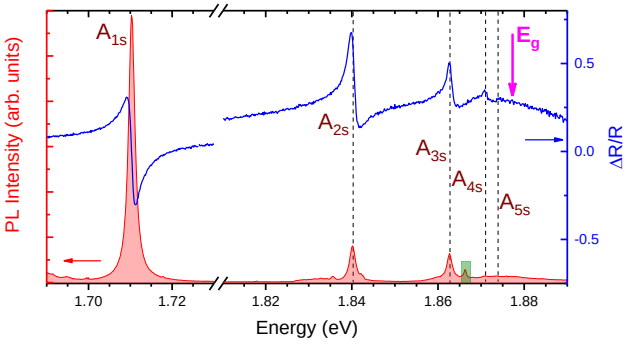

Figure 1: Photoluminescence (red) and reflectivity contrast (blue) measurements on monolayer WSe2 at 4 K, with signature of excited exciton states up to n=5, pink arrow marks the bandgap (E_g) for this material.

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POSTERS

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Oral

CONTROLLED FORMATION OF QUASI-FREE-STANDING GRAPHENE ON SIC VIA POST-GROWTH AND COOLING-PHASE HYDROGENATION

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Graphene growth on the Si-face of silicon carbide (SiC) is of great interest due to its potential for scalable, high-quality, and substrate-integrated 2D materials. However, the carrier density in such films (~10^{13} cm^{-2}) [1] is significantly higher than that of freestanding graphene (~10^{11} cm^{-2}). This high doping level is primarily attributed to the presence of the buffer layer and the unsaturated dangling bonds of silicon atoms at the SiC surface. Such carrier concentrations are detrimental for precision applications like the quantum Hall resistance standard (QHRS), which requires low intrinsic doping to achieve well-defined quantization at low magnetic fields.

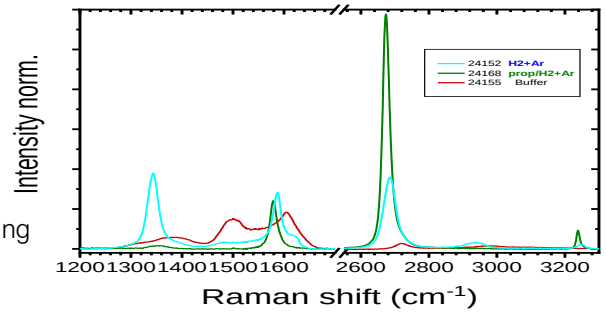
However, it's known that hydrogen intercalation [2] can turn the buffer layer into a monolayer graphene by breaking the silicon–carbon sp^3 bonds and passivating all the dangling bonds of silicon on the surface. This process leads to the formation of what is now known as quasi-free-standing graphene (QFSG).

In this work, we grow graphene on SiC by chemical vapor deposition in a hydrogen atmosphere [3] (H-CVD), a method presenting interesting features such as the self-limitation of the growth to a single layer [4]. Here, we are presenting two different approaches for the formation of quasi-free-standing monolayer and bilayer graphene (QFSMG and QFSBG)) using H-CVD.

(i) The **post-growth annealing** is a two-step process in which the desired graphene structure is first synthesized—either a buffer layer for QFSMG or a graphene/buffer stack for QFSBG—followed by hydrogen annealing at temperatures specifically adapted to each structure. In this study, particular attention is given to the role of annealing temperature, which is the key parameter explored in this approach.

(ii) The **hydrogenation during cooling** is an uncommon yet effective method where the buffer layer is first grown under optimized conditions, and hydrogenation is initiated during the cooling phase. In this method, we specifically investigate how the composition of the cooling gas mixture influences the efficiency of the hydrogenation process.

To characterize the structural and electronic properties of the resulting graphene layers, we will employ a set of complementary techniques. Morphological, spectroscopic, and electrical measurements such as AFM, XPS, Raman spectroscopy, and Hall effect will provide a comprehensive understanding of the modifications induced by hydrogenation. These methods will help assess uniformity, chemical composition, defect density, and carrier transport. As an illustration of the quality achievable with our new hydrogenation approach applied during the cooling phase, the figure presents the Raman spectrum, where the green curve corresponding to the sample cooled under propane/H_2/Ar displays a sharp, symmetric 2D peak and a nearly absent D band, indicating high-quality monolayer graphene comparable to pristine material. Finally, this work also explores the potential for scaling up the process toward the synthesis of quasi-free-standing graphene (QFG) on 2-inch wafer-sized SiC substrates.



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Generating long-distance magnetic couplings with flat bands

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Abstract

It is well known and intuitively understandable that magnetic couplings in materials decrease extremely rapidly as the distance between localized spins increases. In this study, we reveal an unusual and unexpected phenomenon that completely challenges this concept. Indeed, it is possible in flat-band (FB) materials to significantly amplify the magnetic couplings between widely separated spins. We show that the underlying mechanism that enables a boost of the magnetic couplings is connected to a geometric characteristic of FB eigenstates known as the quantum metric (QM). The QM provides a measure of the square of the typical spread of FB eigenstates. In particular, we believe that our findings could be of great interest for long-distance quantum communication that requires lossless transfer of a quantum state between distant quantum registers.

*Speaker

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Poster

ELECTRONIC TRANSPORT IN HBN-ENCAPSULATED GRAPHENE FIELD EFFECT TRANSISTORS UNDER LARGE BIAS

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Since the early 2010s, hBN encapsulation has enabled to reach the intrinsic properties of graphene electronics. Within the field effect transistor (FET) geometry, the graphene electron gas becomes mostly decoupled from the atomic lattice, which allows reaching exotic transport and optoelectronic regimes under large bias where far out-of-equilibrium electronic distributions develop.

In this poster, we review key phenomena observed at room temperature in high mobility graphene FETs under large electric bias, starting with transport and the emergence of interband Zener-Klein tunnelling and mesoscopic Schwinger effect. We develop a phenomenological model for the mechanism that leads to a realization of the 1D version of the Schwinger analogue mechanism in graphene.

These peculiar transport regimes are associated to new photoemission and energy transfer regimes revealed by the observation of electroluminescence cooling, as well as mid-infrared near-field and far-field electroluminescence.

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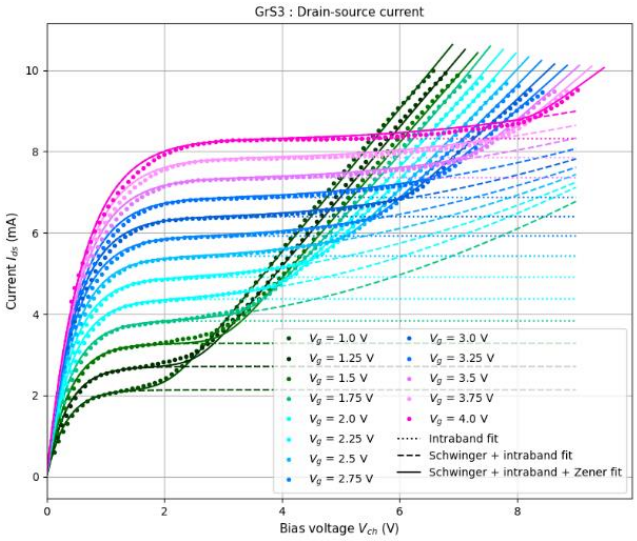

Figure 1: Electric current through the graphene FET as a function of the electric bias, for different values of the gate voltage.

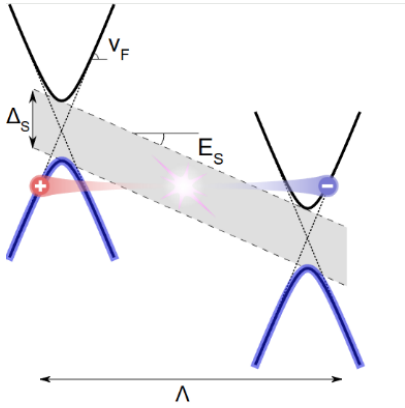

Figure 2: Schematic representation of the electron-hole pair creation process via the Schwinger mechanism. A gap Δ_s opens in the Dirac cones under the action of the electric field $E > E_s$ over a characteristic length Λ

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Poster

Probing electron-phonon coupling in encapsulated graphene

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Electron transport measurements and models have shown that the intrinsic room temperature mobility in graphene is mostly limited by the scattering of electrons by phonons [1]. Scattering is dominated by intrinsic acoustic phonons below 200 K, and by optical phonons at higher temperatures [2,3]. Even though a consensus seems to be reached about this mechanism, there is still remaining discrepancies between the expected theoretical and experimentally observed electron-phonon coupling strengths.

In this work, we fabricated Hall bars of monolayer and bilayer graphene encapsulated in hBN and studied in detail their transport properties between *10* K and *350* K. The charge carrier density, mobility, disorder and Fermi velocity are carefully estimated combining gate dependent and low magnetic field measurements. The temperature and gate dependent resitivity is clearly dominated by phonon scattering for both types of carrier for $|n| > 10^{12}$ cm^{-2}. It is well described by a phenomenological model: $\rho(T) = \rho_0(T) + \alpha T + \frac{A}{\exp(a/T)-1}$

where ρ_0 is the residual resistivity, α is an acoustic phonon scattering parameter, and the final term describes the contribution from optical phonons (*a* is the Bose-Einstein phonon activation term and *A* is the resitivity associated to optical phonon scattering).

At low temperatures (T < 150 K), resistivity increases linearly with temperature with a doping-independent scattering parameter α ≃ 0.05 Ω/K, consistent with acoustic phonon scattering (Fig. 1a). Above ~150 K, a doping independent phonon activation energy of ~ *86* meV (*a* ~*1000* K), indicates the onset of optical phonon scattering (see Fig. 1b). These results are supported by a theoretical model, and minor discrepancies are analyzed in details. These findings provide valuable insights into the fundamental scattering mechanisms in encapsulated graphene systems and their implications for device performance.

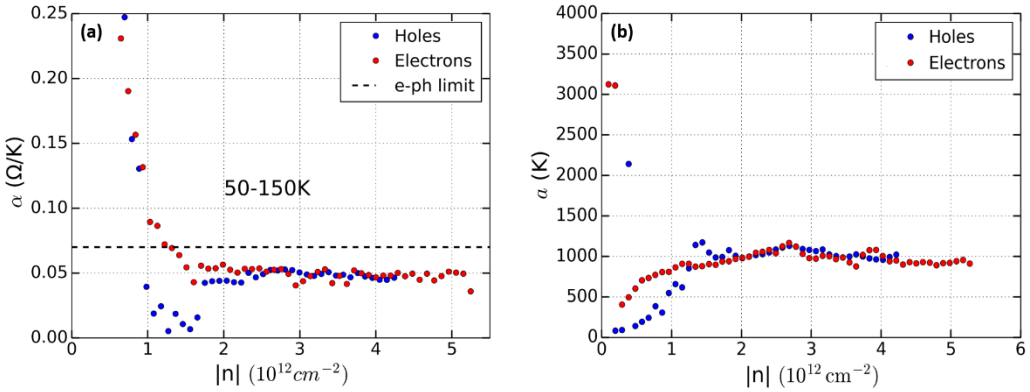

Figure 1: **(a)** Acoustic phonon scattering coefficient α as a function of carrier density. **(b)** Optical phonon activation parameter a versus carrier density, extracted from temperature-dependent resistivity fits.

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Carbon dimer in hexagonal and rhombohedral boron nitride

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Abstract

Identifying defects is an important goal in condensed matter physics. Once the natures of extrinsic and intrinsic defects are determined, processes to improve the quality and the purity of crystals can be optimized. Conversely, the controlled incorporation of dopants are basic tools for fabricating electronic and optoelectronic devices.
Hexagonal boron nitride (hBN) is a lamellar material, characterized by strong in-plane covalent bindings and weak Van der Waals interactions along the c-axis, leading to the formation of hBN under different stackings, called polytypes, such as rhombohedral boron nitride

*Speaker

(rBN). Moreover it has a wide indirect bandgap that allows the existence of several extended and point defects, in particular the deep-level UV emission at 4.1 eV. At low temperature, for natural isotopic abundance in AA'-stacked hBN, the typical photoluminescence (PL) spectrum of the 4.1 eV defect consists in a narrow line around 4.097 eV, called the zero-phonon line (ZPL), corresponding to the emission of a photon without the support of a phonon and then at lower energy, several phonon replicas located at _˜200meV from the ZPL. Today, there is a huge accumulation of experimental and theoretical studies dealing with this UV color center, nevertheless its atomistic origin is still debated. The four most probable structures proposed by theoretical calculations are the carbon dimer, the carbon tetramer, the carbon 6-ring and the Stone-Wales defect (SW), deformation of four hexagons into two pentagons and two heptagons (1,3).

Here we demonstrate that the 4.1 eV emission in hBN comes from carbon dimer by using isotope substitution and polytype control, with a systematic comparison with DFT calculations. Firstly, we studied the effect of isotopic purification of the host hBN matrix (boron and nitrogen atoms) on the PL signal of the 4.1eV defect. This experiment allows us to eliminate the SW defect as a potential candidate and to point out that the phonon replica at _˜200 meV originates from a local vibrational mode (LVM) of the defect. Then, by doping samples with carbon and purifying the incorporated carbon (NatC vs 13C), we have shown that the 4.1eV emission is indeed related to carbon by observing a 6 meV-isotopic shift of the LVM, consistent with the carbon dimer. Finally, we investigate the 4.1 eV signal for another polytype, in rBN crystals, in order to see the effect of stacking on this point defect.

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Poster

ELECTRONIC AND OPTICAL PROPERTIES OF BN TWISTED BILAYERS FROM MODERATE ANGLES TO THE QUASICRYSTAL LIMIT

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When a 2D lattice is rotated on top of another with a small angle (close to 0 or 60°), a super-periodic moiré pattern naturally arises as a regular array of in phase and out-of-phase local arrangements. It leads to low-dispersing states, or flat bands, that often bring novel phenomena, the most spectacular of which is the emergence of tunable superconducting phases in twisted bilayer graphene [1]. Differently, at high angle of misorientation (close to 30°) the emergence of mirrored Dirac cones inside the Brillouin zone of the two graphene layers (quasicrystalline behaviour) enhances double-resonance Raman scattering via Umklapp mechanisms [2].

In this context, twisted bilayers of boron nitride (t-BLBN) differ from graphene because (i) hBN has a wide gap, so flat bands are expected to influence optical properties rather than transport ones and (ii) it hosts two chemical species, so many more stacking configurations (angle *and* position of the rotation axis in atomic layers) are existing [3]. In this poster, we focus on the impact of the angle of twist and the stacking sequence on the electronic structure of t-BLBN by exploring them from the range of moderate angles [3] up to the large angle limit (close to 30°) [4]. Following the validation of our dedicated tight-binding (TB) model, we discuss the emergence of novel and intriguing electronic band structure features that may be specific to the stacking sequence and the range of angle, as well as their consequences on optical properties.

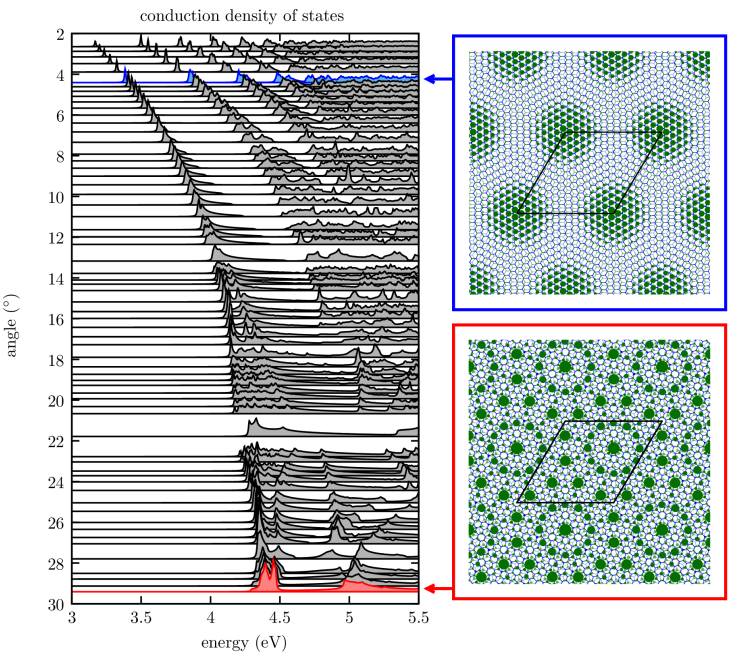

Figure 1: Left: Evolution of the conduction band density of states with the twist angle, calculated with our TB model. (The pivot is located at the center of the hexagon, starting point is non-twisted AA stacking). Right: the local electronic density of states of a twisted bilayer with low angle (4.40°, blue, above) shows evidence of localization. The one with high angle (29.84°, red, below) exhibits a quasicrystalline pattern. In both cases the local DOS is summed from the conduction bottom to 4.4 eV. Size of the circle is proportional to the local DOS on the atomic orbital.

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CONTROLLED GENERATION OF INDIVIDUAL QUANTUM EMITTERS IN HBN USING ELECTRON BEAM IRRADIATION AND IN-SITU CATHODOLUMINESCENCE MONITORING

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Abstract

Oral

The control of the position and wavelength of high-quality quantum emitters is crucial for the implementation of a top-down approach in solid-state quantum technologies. In this context, 2D materials offer new opportunities in this field, with specific integration techniques at the ultimate scale of single atomic layers.

We have recently demonstrated the local generation of quantum emitters ("B-centers") with reproducible wavelength and high quality photophysics in the visible range (1). The B-centers are generated by local irradiation in a scanning electron microscope. The limitation of this technique is the lack of control over the number of emitters created during irradiation. To overcome this limitation, we exploit the fact that B-centers can exhibit cathodoluminescence (CL) under irradiation conditions compatible with their generation (2), although these results were obtained on large ensembles. Based on this observation, we have implemented a new in-situ monitoring setup, sensitive to the CL of individual emitters. It allows us to observe the generation of B-centers in real time at the individual scale. A direct consequence is that the CL signal heralds the successful creation of individual emitters, so that the irradiation can be stopped without producing excess emitters, allowing deterministic generation of individual emitters. The controlled generation of quantum emitters in a 2D material opens up exciting prospects in quantum photonics with applications in optical quantum technologies.

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Miscibility gap and CVD growth of monolayer WSeTe

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Abstract

The dichalcogenide family of bi-dimensional (2D) materials host many iconic compounds such as MoS2 or WSe2 , which are well-know for their indirect to direct band gap transition when their thickness is reduced to a single monolayer. The telluride compounds of the family have received less attention that the sulfides and the selenides but they host interesting physics, such as 2D topological insulators for WTe2 (1). We focus here on growth and the properties of the ternary alloy WSe2xTe2(1-x) which sits between the near semi-metal (the2D topological gap is _˜50meV) WTe2 with orthorhombic symmetry and WSe2 with hexagonal symmetry and direct band gap (1,62eV) (2).
Compared to the corresponding W-based dichalcogenides (WSe2 or WS2), the CVD growth conditions of WTe2 are more challenging and require a Te partial pressure over two decades than the respective Se or S vapor phases. Using Raman, TEM and EDX we explore the different features of single monolayer WSe2xTe2(1-x) monolayer obtained by direct CVD growth. Remarkably, the ternary WSe2xTe2(1-x) alloys shows hints of a large miscibility gap between x=0,2 and x=0,8 associated with a change of crystal structure from hexagonal to orthorhombic.

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Poster

Deterministic positioning and energy tunning of QEs in TMDs

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Control of single photon emitters in terms of energy, decay channels, and spatial position is crucial for integrated quantum nanophotonic targeting applications toward quantum communication and quantum computing. 2D semiconducting crystals (e.g. TMD) enable to deterministically create such quantum emitters using various approaches based on strain [1,2,3], defect [3], or electrostatic [4] engineering of the exciton trapping potential. Here, we have deterministically created localized excitonic states by depositing monolayer MoSe2 on nano-pillars to generate local strain. Such strain is extracted through a detailed analysis of a high-resolution AFM micrograph as in the beam limit, the second derivative of the height is proportional to the strain tensor. By correlating the strain cartography with hyperspectral photoluminescence maps measured at 3K using a confocal scanning microscope, we can demonstrate how narrow emission lines (<1meV) are linked to quantum emitters formed in strained regions in MoSe2. With super-localization techniques [5,6], we are able to determine the position of these emitters with a resolution of 100 nm and conclude that they originate predominantly from the apex of each nano-pillar.
In addition, we will present preliminary results on individual Stark tuning of such self-assembled quantum emitters.

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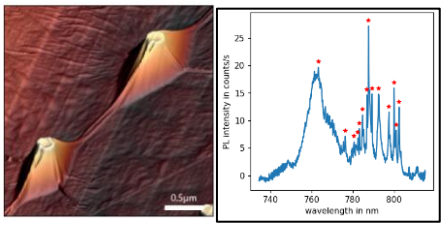

Figure 1: right panel: AFM micrograph of MoSe2 ML transferred on top of GaN pillars. left panel: PL spectrum acquired at 3K showing narrow line features.

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Poster

Mastering the growth of centimetric sp^2-hybridized boron nitride films for optoelectronic devices

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In the recent years, sp^2-hybridized boron nitride (sp^2-BN) has been identified as a key component for the development of high-performance 2D material platforms towards applied devices. Its unique properties - including a large band gap (> 6 eV), chemical inertness, atomically flat surface free of dangling bonds and small lattice mismatch with graphene (less than 1.7%) [1] - give it a pivotal role in van der Waals heterostructures elaboration. Indeed, sp^2-BN has been identified as the ideal insulating substrate and encapsulating layer to achieve the highest mobility or best optical properties in graphene or other 2Ds channels, with strong implications for efficient electronic, optoelectronic and spintronic devices [2]. However, realising the potential of BN-based electronic platforms requires continuous, atomically flat BN films on a large-scale with a controlled thickness ranging from a monolayer to 50 nm, depending on the targeted application. To date, proof-of-principle demonstrations showing ultimate performance have been obtained using exfoliated flakes from high-quality bulk crystals. This fabrication method seems unsuitable for practical applications due to the low yield and quality limitations of the nanosheets produced, such as the small lateral size, lack of homogeneity and thickness control [3]. In parallel, large-scale synthesis is being developed, in particular by MBE, ALD and CVD [4]. However, real control of film thickness with high crystalline quality has not yet been achieved.

In this context, the aim of the research we have undertaken is to develop the synthesis by chemical vapor deposition of multilayer sp^2-hybridized BN films with structural specifications that meet these requirements. In collaboration with Annealsys, we have developed an epitaxial growth process on Ni (111) substrates on the centimeter scale, using borazine molecule as a source of boron and nitrogen atoms [5]. We have characterised the structure and the quality of BN films from the centimetre to the atomic scale using a wide range of techniques (OM, SEM, TEM, AFM, Raman spectroscopy) and in a quantitative manner. We show that by adjusting the synthesis parameters, we can obtain BN films with controlled thicknesses between 2 and 10 layers, homogeneous over several mm^2 with the same crystalline orientation and a hexagonal or rhombohedral stacking sequence. These are essential control points for the future integration of BN films into large-scale devices with other 2D materials.

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Poster

SYNTHESIS AND OPTICAL PROPERTIES OF A WATER-SOLUBLE GRAPHENE QUANTUM DOTS FOR BIOLOGICAL APPLICATIONS

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Graphene exhibits remarkable mechanical and electronic properties. However, the semimetallic character of graphene constitute a severe limitation to its use for optical or optoelectronic applications. When the dimensions of a 2D graphene sheet are reduced to the nanometric scale, new properties coming from the confinement or electrons will emerge. Thus, we shine our interest in graphene quantum dots (GQDs). GQDs synthesis has been mostly described *via* top-down methods (*i.e.* lithography, harsh oxidative cutting conditions or hydrothermal treatments).[1] Though cheap and efficient, these methods do not allow for precise control of the size, shape and edges of the GQDs. In order to truly control, with the required level of precision, the morphology and the composition of the materials and of its edges, the bottom-up approach is the relevant way to proceed.[2]
In a previous study, our team synthesized a family of graphene nanoparticles soluble in classical organic solvents. Thanks to their particular functionalization, these nanoparticles are individualized in solution and in the solid state. They emit photons in the red and near-infrared regions and exhibit exceptional photoluminescence quantum yields ranging from 90 to 95%, a level never before achieved for particles of such size.[3] At the solid state, the GQDs also act as single photon emitters.[4] To extend the potential of these materials, my thesis aims at improving the solubility of these nanoparticles in water by grafting hydrophilic polymers such as polyethylene glycol (PEG). To this end, we decided to functionalize the nanographene with triple bonds and to perform Click Chemistry (CuAAC). I began my thesis work by functionalizing C_{60} and C_{96} nanoparticles with polyethylene glycol (Figure 1), and thoroughly characterized the final products. This modification is crucial to make them soluble in water and test these materials for biological and medical applications.

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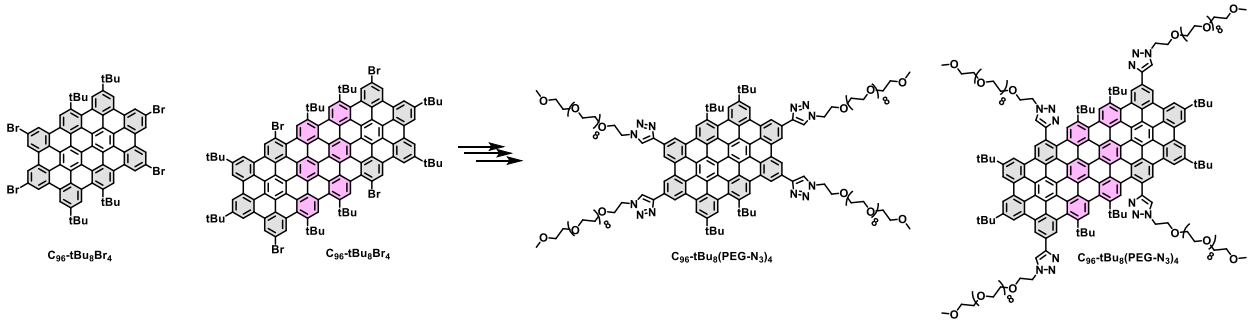

Figure 1: Schematic representation of PEG-functionalized graphene quantum dots.

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Tunable Superconductivity via Disorder in Systems with Quantum Geometry

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Abstract

Topological insulators host edge states that obey bulk-boundary correspondence, giving rise to quantum Hall physics. In this work, we demonstrate that the emergence of impurity-induced subgap states around impurity potentials is governed more by the *quantum geometry* of the occupied bands than by their topological invariants. Under strong electron repulsion, correlated states resembling Mott rings and associated Mott zeros appear, mirroring features in the non-interacting case. Conversely, in the presence of effective attractive interactions, we show that Cooper pairing can emerge within these ring-like impurity bands. Importantly, the impurity density acts as a tunable parameter, enabling a transition from a topological insulator phase to a superconducting phase. This highlights a new route for engineering tunable quantum phases via disorder and interaction in systems characterized by nontrivial quantum geometry. (1) Impurity-induced Mott ring states and Mott zeros ring states in the Hubbard operator formalism. Emile Pangburn, Anurag Banerjee, Catherine Pépin, Cristina Bena. arXiv:2503.05870 (2025)

*Speaker

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Poster

Harnessing Single-Photon Emission from color centers in hBN.

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Hexagonal Boron Nitride (hBN) is a 2D material that hosts color centers emitting single photons in the visible range. hBN has the property of displaying remarkable brightness and great photophysical properties at ambient temperature, making it a good candidate for single photon emission without requiring cryogenic cooling [1]. However, most of well-known solid state single photon emitters, such as NV centers, are hosted in a high refractive index crystalline lattice, making extraction and collection of photons challenging.

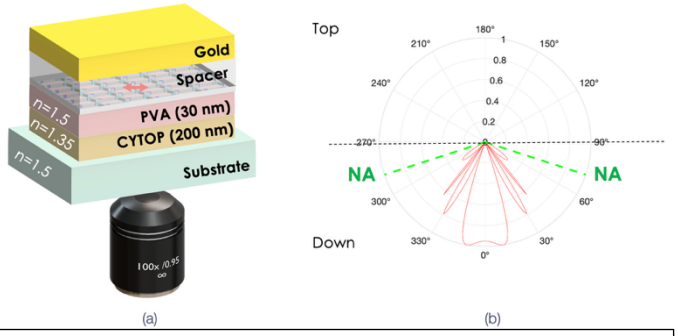

Figure 1: Example of a nanostructure designed to optimize the collection of the photon flux [2]. (a) Schematic of the structure, with an in-plane dipole emitter (red arrow) embedded in a dielectric structure covered by a metallic mirror. A high-NA microscope objective collects light from the bottom of the structure. (b) Radiation pattern of the emitter embedded in the nanostructure, with close to 100% collection within the aperture of the objective.

Here, we first built a confocal microscope to locate and characterize color centers hosted in hBN via fluorescence mapping. The setup allows us to measure photophysical properties such as brightness, spectrum or single photon purity by performing intensity correlation measurements. A single emitter can be hosted in crystals close to atomic thickness, making extraction from the host material much less impacted by dielectric screening. Then, we make use of the 2D nature of hBN to achieve coupling between color centers and nanostructures, in order to enhance the collection of single photons by high numerical aperture objectives. We are exploring designs of nanostructures through numerical simulations in order to shape the angular distribution of emission and to optimize the collection of the total flux emitted by a single color center, as displayed in Figure 1 [2]. Defects in exfoliated hBN flakes will be created by exploiting the field enhancement at the tip of a s-SNOM microscope. This will enable to form arrays of deterministically activated color centers at a subwavelength scale. The samples will be later transferred into the designed nanostructures. The planar nature of the structure releases the constraint of precise and deterministic positioning of the emitter in a small mode volume, as seeked in some nanophotonic architectures based on antenna-emitter coupling.

The longer-term goal is to demonstrate controlled positioning of emitters around nanostructures with advanced functionalities, including electrical biasing of the device to modify spectral properties of the emitters [3]. An upgraded version of the setup will be assembled, that will allow manipulation, transfer of 2D samples and characterization of emission to investigate the role of the nanophotonic structures in the modification of the spectral and angular features of single photon emission.

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Poster

HIGH-MOBILITY GRAPHENE TRANSISTORS SHED NEW LIGHT ON AN OLD QUANTUM FIELD THEORY CONTROVERSY

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A seminal result in high-energy quantum electrodynamics is the instability of the vacuum under a strong electric field, leading to the spontaneous creation of particle-antiparticle pairs. This phenomenon, known as the Schwinger effect, is one of the few non-perturbative results in quantum field theory, initially derived by Sauter and later by Schwinger in 1951. [1] It predicts the decay rate w of the false vacuum in d+1 dimensions. While many, including Schwinger, equated the vacuum decay rate with the pair creation rate Γ, this equality has remained controversial. Starting with Nikishov in 1970 [2], several authors have demonstrated through direct calculations of Γ that the relation w=Γ holds only at low fields. [3,4]

The Schwinger instability, requiring electric fields around 1018 V.m-1, was long considered experimentally inaccessible. A breakthrough occurred in 2023 when it was demonstrated that a mesoscopic variant of the Schwinger effect in 1+1 dimensions spontaneously manifests in high-mobility graphene under large bias. [5] In this poster, I will elucidate how this experimental setup provides empirical evidence to address the Schwinger-Nikishov controversy, supporting Schwinger's initial interpretation in the context of graphene. I will also discuss the insights this approach offers into the theoretical discrepancy.

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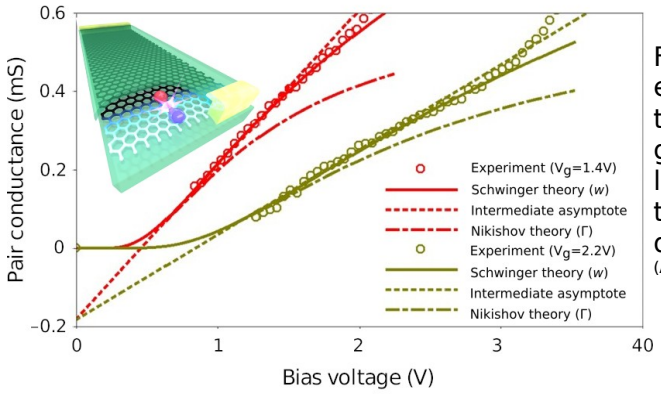

Figure 1: Comparison between the electron-hole pair creation conductance in the mesoscopic Schwinger effect in graphene according to Schwinger (full line), Nikishov (dashed-dotted line), and the experimental high-mobility graphene differential conductance (hollow circles).

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Poster

TOWARDS QUANTUM ANOMALOUS HALL PHASE IN WSE_2-GRAPHENE-$CR_2GE_2TE_6$ 2D HETEROSTACKS

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In the past few years, the solid states physics community managed to synthetize 2d magnetic topological (meta)materials that exhibit perfectly conducting 1d chiral edge states eventhough no external magnetic field is applied[1,2], so-called Quantum Anomalous Hall (QAH) effect. Thanks to theses materials, the chiral edge states of the quantum Hall effect are more easily accessible, relaxing the constraint of a strong external magnetic field, and allowing easier device integration and combination.

In this poster, I will present our attempt to be the first to demonstrate QAH effect in monolayer graphene proximitized by a transition metal dichalcogenide (WSe_2) and a 2d magnetic insulator ($Cr_2Ge_2Te_6$)[3]. The combination of the proximity-induced spin-orbit coupling and magnetic exchange, respectively from the WSe_2 and the $Cr_2Ge_2Te_6$ layers, is predicted to give rise to QAH effect[4]. We used low-temperature magnetotransport measurements to characterize our WSe_2-graphene-$Cr_2Ge_2Te_6$ heterostack and evaluate how close we are to the QAH phase.

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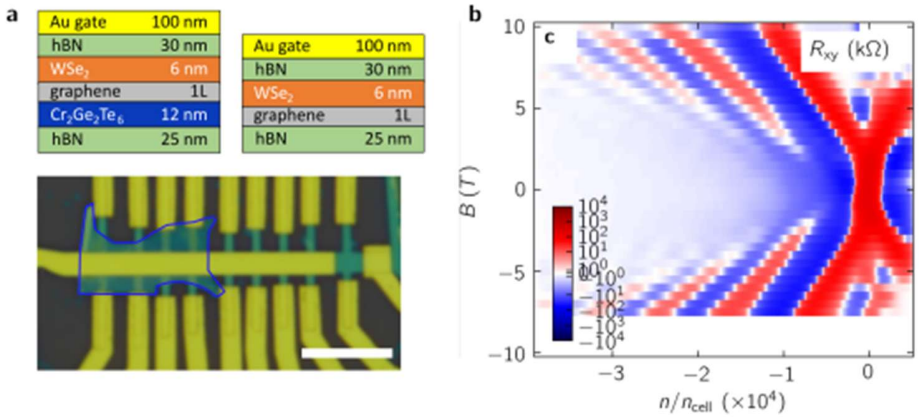

Figure 1: **a**. Top: Sketch of the heterostack layers in the region with and without $Cr_2Ge_2Te_6$. Bottom: optical microscope image of the heterostack, with $Cr_2Ge_2Te_6$ flake highlighted in blue. Scale bar 10 µm. **b**. Hall resistance variations fan diagram of the $Cr_2Ge_2Te_6$ region.

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Poster

MOLECULAR CRYSTALS DOPED WITH GRAPHENE QUANTUM DOTS

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Graphene quantum dots (GQDs) are emerging as a promising platform for the development of single photon sources tailored to quantum technologies, particularly in integrated photonics. Their high quantum yield (~90%) and structural tunability (size, shape, functional groups) endow them with excellent optical properties [1].

This work focuses on stabilizing the emission of individual GQDs at cryogenic temperature and achieving lifetime-limited spectral line. For that, GQDs are embedded in self-assembled molecular crystals, used as host matrices to minimize emitter-environnment coupling. A controlled synthesis method has been developed to tune both the crystal size and the GQDs concentration precisely.
The first studie on small crystals revealed single photon emission at room (fig 1, 2) and cryogenic temperature but we showed spectral jitter at cryogenic temperatures, attributed to fluctuations in the local electromagnetic environment [2]. To reduce this effect, two strategies were explored : increase the size of the crystal or applying a dielectric coating on a small crystal. In larger crystals, at low temperature (~5K) narrow emission lines were observe, limited by the spectrometer resolution, with no detectable spectral fluctuations. The next step will involve implementing a high-resolution photoluminescence excitation technique to determine whether the observed linewidths are truly lifetime-limited.

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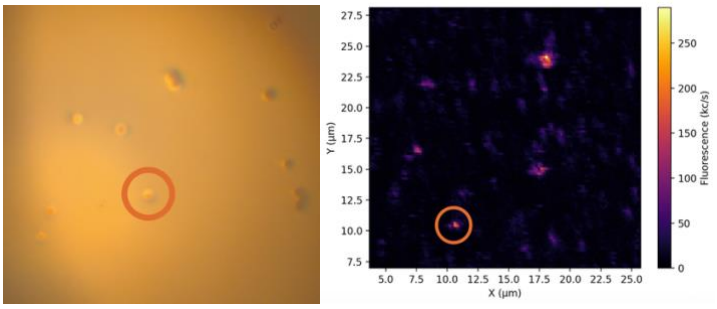

Figure 1 : Wide field image of a molecular crystal (left), and confocal map (right) of the same crystal (highlighted by the orange circle) at room temperature.

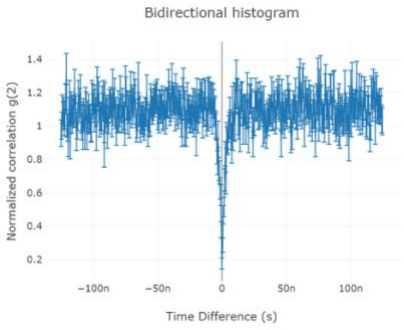

Figure 2 : Second order correlation function of the crystal shown in Fig1, demonstrating single photon emission.

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OPTICAL PROPERTIES OF 1D HYBRID CARBON NANOTUBES

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Abstract

The one-dimensional structure of single-walled carbon nanotubes (CNTs) allows the absorption of electromagnetic waves in the visible range and emission in the near infrared (thanks to van Hove singularities). Encapsulating dyes in these host nanotubes makes it possible to create hybrid nanosystems with tunable optoelectronic properties. To date, we have confined different types of chromophores,1-6 capable of absorbing at short wavelengths in the optical range (400/500 nm) for tetracyanoquinodimethane (TNCQ) and its derivatives F4TCNQ), quaterthiophenes (4T) and tetramethyl-paraphenylenediamine (TMPD) derivatives, or at longer wavelengths (700 nm) for phthalocyanine (MPc). In addition, these dyes can be either electron donors (4T, TMPD) or acceptors (TNCQ, F4TCNQ), enabling charge transfer between the two subsystems.
In this study, we are interested in both the macroscopic and individual scales, as well as the electronic and optical properties of hybrid nanosystems using Raman and photoluminescence spectroscopy.

Photoluminescence experiments clearly demonstrate changes in emission properties after encapsulation. Intensities can be increased or reduced depending on the nature of the confined chromophores (electron donor or acceptor) and the diameter of the CNT.

Raman measurements reveal a significant charge transfer from the confined dye to the nanotube. The main relevant parameters governing charge transfer are the diameter of the nanotube and the nature of the chromophores (electron donor or acceptor).
Therefore, Raman and photoluminescence experiments strongly suggest charge transfer between confined molecules and nanotubes, leading to a shift in the Fermi level that governs the efficiency of radiative de-excitation.

*Speaker

Annual meeting 2025 of the GDR and IRN HOWDI
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Poster

Generation of boron vacancy by ion implantation in ultrathin layers of hBN for quantum sensing application

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Negatively charged boron vacancies (V_B^-) in hexagonal boron nitride (hBN) have become promising quantum defects for the development of room temperature quantum sensors embedded in 2D materials. [1] A key challenge, however, lies in creating these defects in ultrathin hBN flakes, to benefit from atomic scale proximity between the sensor and the sample to probe.

Ion implantation appears to be a simpler method to create defects than the commonly used technique based on neutron irradiation. However, it is not known whether the creation of V_B^- in very thin layers is possible, as current studies are limited to thick layers. [2] The lack of reliable simulations for such thin flakes forces us to use a strictly experimental method. We thus investigated ion implantation as a scalable and controllable alternative to create V_B^- centers in ultrathin hBN layers (<8 nm). By systematically varying the implantation parameters (ion species, energy and dose), optimal conditions are identified through the use of various optical spectroscopy techniques, and the creation of stable V_B^- defects is proven.

These results demonstrate the feasibility of controlled ion implantation in ultrathin layers of hBN, paving the way for the realisation of integrable 2D quantum sensors.

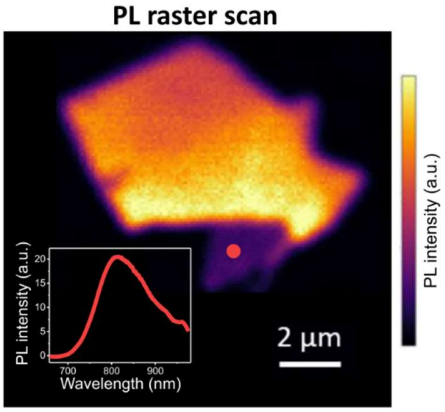

Figure 1 : Photoluminescence (PL) mapping of an implanted hBN flake. Insert shows the PL spectrum of the thinner part.

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Poster

FAST ATOMISTIC COMPUTATION OF OPTICAL PROPERTIES OF CARBON-BASED 2D MATERIALS IN THE VISIBLE AND UV, THANKS TO THE DADI MODEL

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In this poster, results will be presented on absorption, scattering and polarization properties of several reduced graphene oxide flakes, using a model inspired by both the static Atomic Dipole Interaction (ADI) model of Applequist and coworkers [1] and the Discrete Dipole Approximation (DDA) mesoscopic continuum optics model of Purcell and Pennypacker. This model, named Dynamic Atomic Dipole Interaction (DADI) [3], requires as inputs the positions of the atoms in the scattering and absorbing system and the frequency-dependent *atomic* polarizabilities [4]. The latter are obtained by fitting frequency dependent *molecular* polarizabilities computed using the TD-DFT code Octopus [5].

Thanks to new results obtained for oxygen atoms in various neighborhoods, the influence of the type of oxygen containing chemical functions on the optical properties of various reduced graphene oxide flakes is studied. It is worth noting that the DADI calculations of the optical properties of 2D materials are much less computationally demanding than, e.g., TD-DFT methods. They thus give the opportunity of characterizing the influence of finite width and length, and/or of defects in large carbonaceous structures.

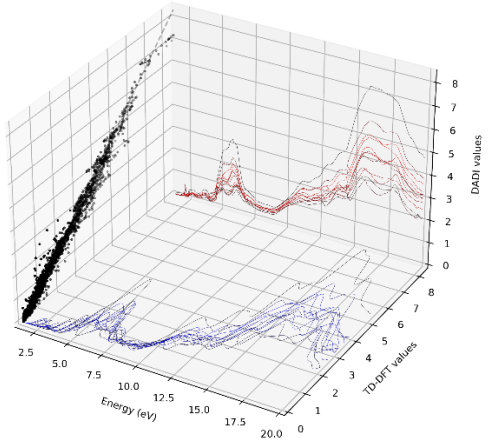

Figure 1: Illustration of the quality of the fit for carbon hydrogen and oxygen frequency-dependent polarizabilities. Bottom panel: absorption spectra of various organic molecules containing oxygen, computed by TD-DFT; right panel: same computed by the DADI model after fitting the atomic polarizabilities; left panel: correlation plot between these 2 quantities

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Poster

EXPLORING THE QUANTUM PROPERTIES OF SPIN DEFECTS IN 2D SEMICONDUCTORS

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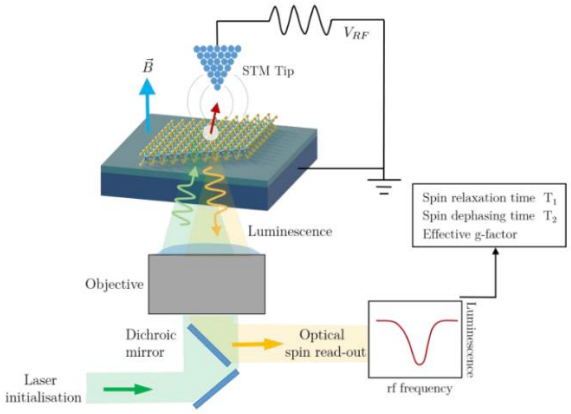
The OneSPIN project aims to unlock the coherent control of single electronic spins in two-dimensional (2D) semiconductors such as MoS_2 and WSe_2, leveraging their unique spin-valley coupling and optical addressability. These monolayer materials host point defects—particularly chalcogen vacancies—that act as quantum-dot-like centers capable of emitting single photons with spin-selective characteristics inherited from the host monolayer. Unlike excitons, which suffer from ultrafast (~ps) spin-valley relaxation, these localized states are predicted to exhibit microsecond-scale spin coherence, making them promising candidates for quantum information applications [1, 2, 3].

We propose a novel methodology that combines scanning tunneling microscopy (STM) with optical detection of magnetic resonance (ODMR) to probe and manipulate individual spins with atomic precision. This technique enables measurement of key quantum parameters and allows direct correlation of spin coherence with atomic-scale structure. A central element of the project is the optical readout of spin resonance from a localized state under RF and static magnetic fields (**Figure 1, left**) [4, 5]. This optical approach circumvents limitations of magnetized-tip ESR, operating under low magnetic fields and broad temperature ranges, and offers a transformative route for quantum material exploration and device engineering. Currently our team is working on the implementation of the STM in an optical cryostat (**Figure 1, right**), being the basis of promising future experiments.



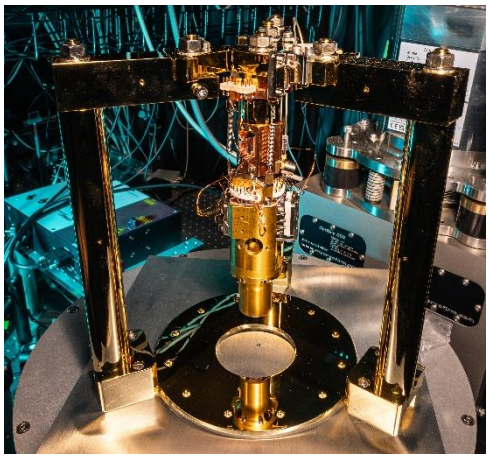


Figure 1: (Left) Principle of the experimental approach proposed in OneSPIN. A localized electron spin (red arrow) is excited by a laser (green arrow) and undergoes coherent precession under the influence of both an external, static out-of-plane magnetic field B and a radiofrequency electric field generated in the tip-sample junction just above the spin. The optical detection of this single spin resonance is achieved by analyzing the photoluminescence (yellow arrow) as a function of the frequency of the driving field. The exact shape of the obtained curve allows for a determination of the longitudinal spin relaxation time T_1 and the spin coherence time T_2 (in addition to the spin g-factor), which are expected to be highly dependent on the spin's atomic and electric environment. **(Right) STM head holded by three pillars on the cryostat basis.**

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Poster

Broadband optical properties of intrinsic monolayer $PtSe_2$

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Two-dimensional (2D) Transition Metal Dichalcogenides (TMDs) are great candidates for opto-electronic applications due to their high electronic mobility, and also due to the strong light–matter interaction. Platinum diselenide ($PtSe_2$) thin films stand out for their remarkable bandgap tunability, ranging from 1.3 eV for a single layer crystal, to zero as the thickness increases [1].

Our previous measurements on monolayer PtSe2 showed the existence of a small and unexpected absorption peak 0.5eV below its bandgap. To investigate if its origin is intrinsic to the material, we fabricated a high-quality monolayer $PtSe_2$ sample obtained via Au-assisted mechanical exfoliation technique, and encapsulated with boron nitride (hBN). Raman was employed to check the stacking [2]. Optical measurements were performed at room temperature within the visible and IR range (400 nm – 1600 nm) of two points: a substrate reference (sapphire plus hBN) and another one with the sample.

We find that hBN encapsulation brings additional richness to the RTA measurements, as opposed to plain $PtSe_2$ samples measurements in which both *T* and *R* brings the same information on the real optical conductivity, leaving the imaginary part inaccessible. The interference effects in the heterostructure bring different information that can be leveraged to fully reconstruct the complex optical conductivity.

Finally, we were able to observe the absorption of the 1L–$PtSe_2$ [3] and then compare the experimental data with an adapted Transfer-Matrix Method [4]. Using the simulated heterostructure, we could recover both differential reflectance and transmittance susceptibility as observed in the experiment, which allow us to reconstruct completely the complex 2D optical conductivity of the investigated crystal.

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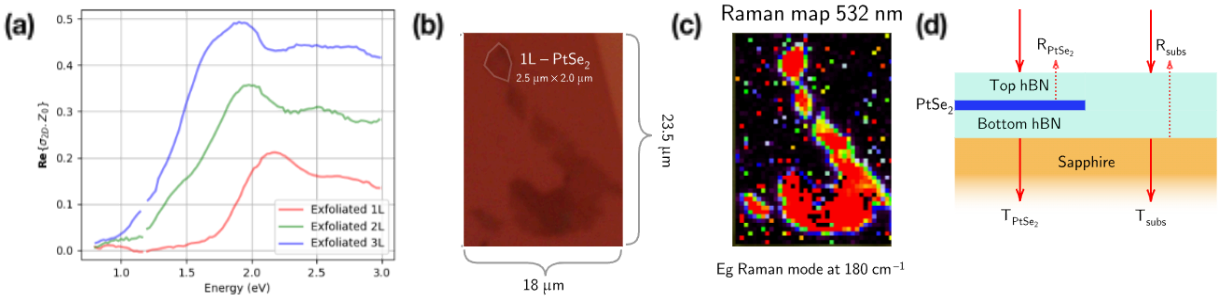

Figure 1: (a) Real surface optical conductivity as function of energy from IR (0.5 eV) up to the blue (3.0 eV). All curves show an unexpected bump in the IR. **(b)** Optical image of the hBN-encapsulated $PtSe_2$ under 80× magnification. The area in evidence shows the target flake of 1L-PtSe2 crystal. **(c)** Raman intensity map of the sample of the E_g peak at 180 cm^{-1} under 532 nm excitation wavelength. **(d)** Diagram of the cross section of the sample and the measured light in the experiment. Top/bottom hBN: 68 nm / 67 nm.

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Poster

Non-Radiative energy transfer between boron vacancy and other 2D materials

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The discovery of the negatively charged boron vacancy (V_B^-) center in hexagonal boron nitride (hBN) has attracted increasing attention as it shows promising optical and spin properties, making it a good candidate for the development of two-dimensional atomic-scale quantum sensor[1]. Additionally, hBN is widely used as a protective or spacer layer in van der Waals heterostructures, making this sensor easily integrable and allowing in-situ sensing in van der Waals devices [2].

However, integrating these defects in ultra-thin hBN layers, in contact with other materials, raises concerns about non-radiative energy transfer to nearby absorptive materials that may limitate the sensitivity of the sensor. In this work, we study the V_B^- photoluminescence (PL) intensity quenching resulting from non-radiative Förster resonance energy transfer (FRET) in monolayer graphene/V_B^- hBN heterostructures.

Our results show that significant PL quenching occurs only for ultra-thin hBN flakes (< 4 nm-thick). This limited impact of the Förster coupling is attributed to the low quantum yield of the V_B^- center. By combining PL intensity mapping and time-resolved PL (TRPL) measurements, we based our analysis on a theoretical model to estimate the radiative decay rate of the center.

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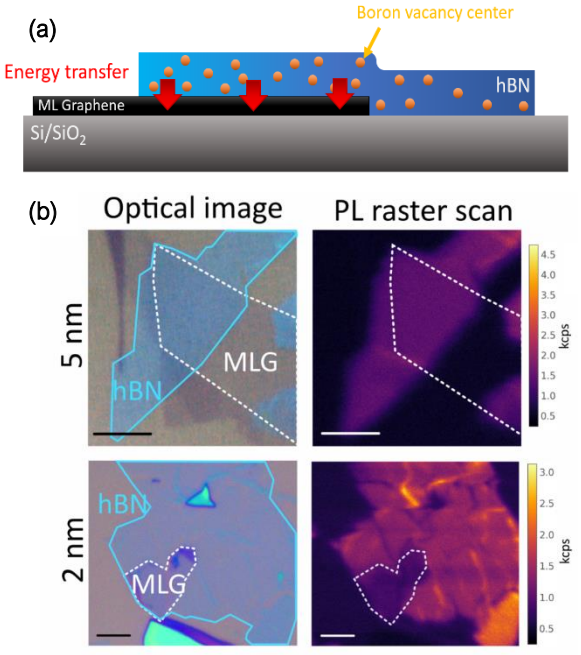
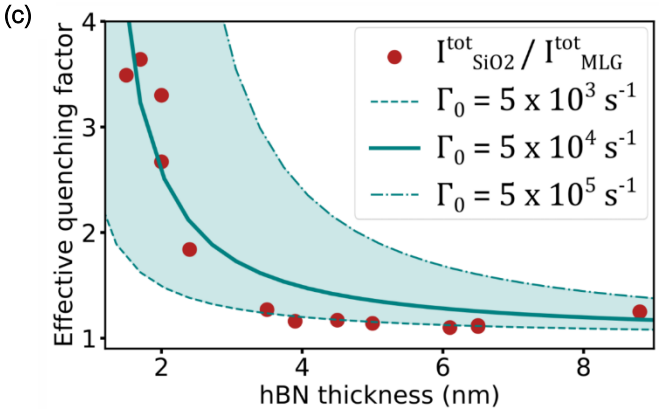


(a) Diagram of the studied structure
(b) (left) Optical images and (b) corresponding PL maps of two different samples with hBN thicknesses of 5 nm and 2 nm.
(c) Effective quenching factor as a function of the hBN flake thickness. The red dos represent the experimental data and the blue curves the simutaionsfor various radiative rate values



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HOWDI Low dimensional van der Waals heterostructures

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Poster

HIGH-THROUGHPUT SCREENING OF 2D RASHBA SEMICONDUCTORS

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Spintronic devices are seen as part of the next generation of microelectronic technology. Many of them rely on the spin-orbit effects. Thus, research on two-dimensional (2D) materials with large spin-orbit coupling (SOC) and specific spin textures is both necessary and fascinating. Among different types of spin-orbit coupling materials, the Rashba type attracts attention for the design of novel spintronic devices. Based on the Materials Cloud Two-Dimensional Structure Database (MC2D), we built a database of potentially large Rashba type SOC nonmagnetic semiconductor monolayer materials. Using point group classification and atom site symmetry, we identify monolayers with intrinsic Rashba effects, whether conventional or hidden. Furthermore, we screen materials containing heavy elements and study their atomic site environments to propose simple descriptors of Rashba magnitude, such as the maximum atomic number at non-centrosymmetric atomic sites.

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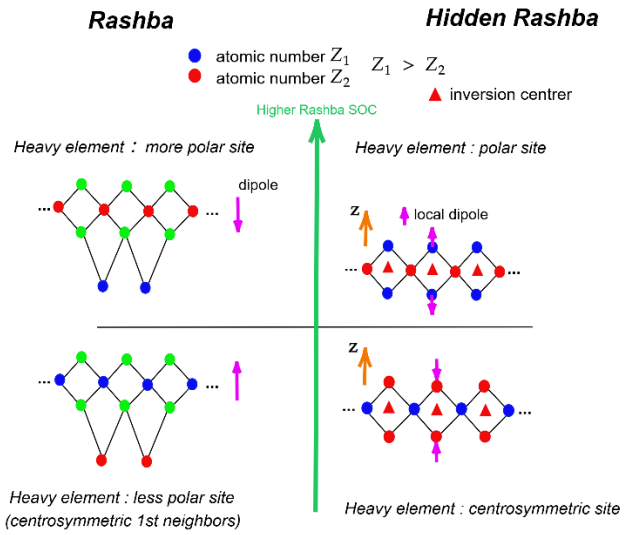

Figure 2: The atomic site of a heavy element correlates with Rashba SOC strength. A site that provides a more polar potential or asymmetric charge distribution is favorable for the heavy atom to induce stronger Rashba SOC.

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Poster

1D NANOHETEROSTRUCTURES FOR OPTOELECTRONICS FROM CHROMOPHORES ENCASPULATED INTO CARBON NANOTUBES

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In nanoelectronics and photonics, obtaining high-performance devices requires efficient optical-to-electrical transduction. In this regard, single-walled carbon nanotubes (SC-NTs) are prime candidates due to their combination of exceptional electronic properties (e.g., high carrier mobility, low capacitance) and unique optical response (direct bandgap, tunable optical transitions, high polarization) associated with their 1D nature. They pave the way for flexible electronic and photonic devices. In addition, SC-NTs exhibit optical absorption and emission in the near-infrared, which is particularly interesting for biological (biological window) and technological (telecommunications) applications. The functionalization of SC-NTs emerged early on as an interesting way to improve the optical properties of nanotubes while adding new functionalities. In this project, we propose to study at a fundamental level the optoelectronic properties of new individual hybrid nano-objects consisting of specifically designed dyes confined inside SC-NTs with a controlled structure. These systems provide a unique model for studying the fundamental optoelectronic properties of chromophores under 1D confinement and their coupling with those of the host nanocontainer. The objective is to engineer the electronic bands of hybrid NTs in order to create (1) nano-light absorbers based on charge transfer (exciton dissociation at the interface) and (2) electroluminescent emitters based on energy transfer (exciton transfer between the two subsystems.

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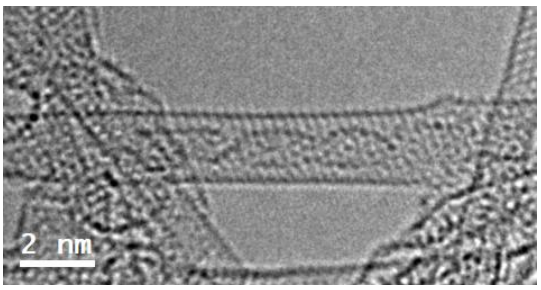

Figure 1: TEM image of dye inserted in a single wall carbon nanotube.

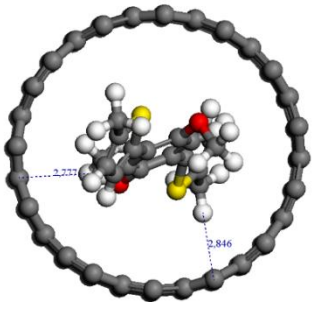

Figure 2: Modelization of dye inserted in a single wall carbon nanotube

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Poster

TOWARDS CONTROL OF SIC(0001) SUBLIMATION PARAMETERS TO STUDY THE INFLUENCE OF BUFFER LAYER AND SIC TERRACES MORPHOLOGY ON GRAPHENE PROPERTIES

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The buffer layer (BL) and the morphology of silicon carbide (SiC) under the graphene influence their properties (optical, electrical, etc.) [1-2]. In this study, we propose to study the influence of graphene growth parameters by sublimation of SiC(0001) in order to have access to reproducible and varied samples. In the case of the SiC substrate, we study the presence of hydrogen in the recipe on step bunching process. Samples of monolayer graphene 1LG (80%) (figure1) are obtained on straight and wide SiC (0001) terraces, which can reach 12 µm on average, with a height of less than 2.5 nm [3]. In the case of BL, studies on its hydrogenation with or without graphene layer above, would allow accessing to samples of 1 or 2 LG directly on SiC. Different groups have already used it successfully to obtain 1LG directly on SiC(0001). Generally, the intercalation is done under a purely H_2 environment [4]. In our case, the intercalation is successfully performed under a mixed environment (H_2/Ar; 20/80). Regarding the properties of the samples produced, the Raman characterizations revealed a low intensity D band on our samples (1LG/SiC(0001)) indicating a low rate of defects. Regarding the electrical properties, 1LG/SiC(0001), was the subject of extensive measurements and analyses. The measurements carried out revealed that this sample was p-type with a Hall mobility, at 300 K, around 1410 $cm^2V^{-1}s^{-1}$. More interestingly, after annealing at 575 K, the evolution of resistivity as a function of temperature could be described by a model suggesting the opening of a gap.

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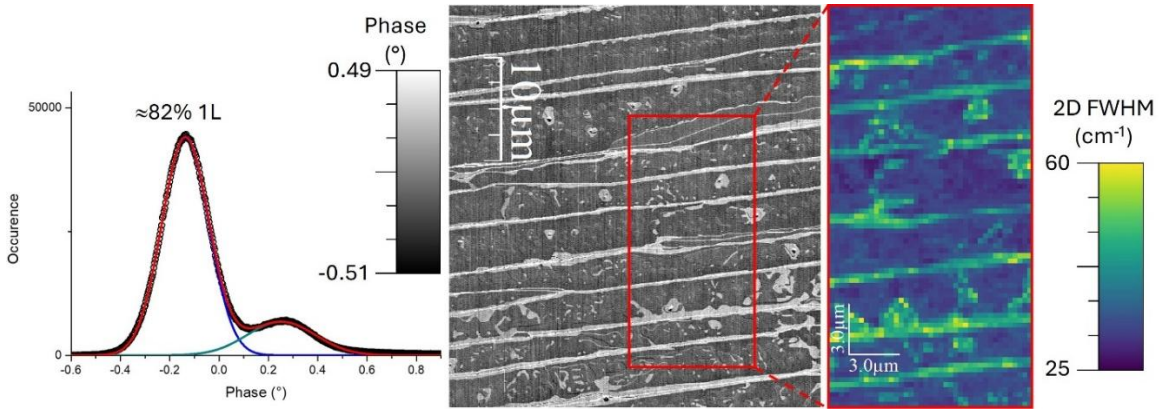

Figure 1: Graph of the occurrence as (°) from the gray AFM image in phase mode. 2D FWHM Raman map was done at the same location than AFM measurements (red rectangle). Complementary technics estimate 80% of 1LG.

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Poster

ATOMIC-SCALE EXCITONIC LUMINESCENCE NANOSCOPY OF MOIRÉ SUPERLATTICES IN VAN DER WAALS HETEROSTRUCTURES

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The optical and electronic properties of van der Waals (vdW) heterostructures are highly sensitive to their nano- and atomic-scale structure. In twisted or lattice-mismatched systems, the formation of moiré superlattices introduces periodic potentials that spatially modulate excitonic luminescence, reshape electronic bands, and give rise to localized quantum states. Understanding how excitonic phenomena evolve across these complex landscapes requires techniques capable of probing light-matter interactions with ultimate spatial resolution.

Conventional optical spectroscopy averages over nanoscale inhomogeneities due to diffraction-limited resolution (~1 µm), obscuring critical insights into local exciton physics. Scanning tunneling microscopy (STM), by contrast, resolves atomic-scale features such as moiré patterns and interfacial defects with sub-nanometer precision. STM-induced luminescence (STML) bridges this gap by using the STM tip as a localized nanoscale excitation source, providing optical access to excitonic properties with high spatial and energy resolution [1].

Here, we employ cryogenic STML (< 7 K, ultra-high vacuum) to investigate exciton behavior in vdW heterostructures assembled under inert conditions using a motorized transfer system inside an argon-filled glovebox. This ensures cleaner interfaces and preserves intrinsic optical properties. In monolayer (ML) and bilayer (BL) $MoSe_2$ on few-layer graphene (FLG), we resolved moiré features and detected excitonic emission, including neutral excitons, trions, and possible low-energy defect states. Complementary scanning tunneling spectroscopy (STS) revealed subtle electronic modulations along the moiré lattice. These combined measurements demonstrate the feasibility of performing spatially resolved exciton mapping across extended nanoscale regions, forming a basis for exploring more complex moiré systems.

Our current focus centers on high-quality, near-aligned TMD/TMD (Transition Metal Dichalcogenide) heterobilayers, such as WSe_2/WS_2, in which long-lived interlayer excitons (IXs) exhibit out-of-plane dipole moments and are highly sensitive to the strong underlying moiré potential [2]. By tuning the twist angle toward zero degrees, we generate larger moiré wavelengths (~8-10 nm) [3] to study how IX localization, recombination dynamics, and potential landscapes evolve across the superlattice. Furthermore, the controlled introduction of atomic-scale defects, via techniques such as argon ion bombardment, offers a pathway to probe defect-bound excitons and investigate the impact of moiré modulation on their optical properties. Ultimately, these studies aim to uncover the microscopic mechanisms behind complex excitonic phenomena in vdW heterostructures and advance the frontiers of nano-optical probing in moiré systems.

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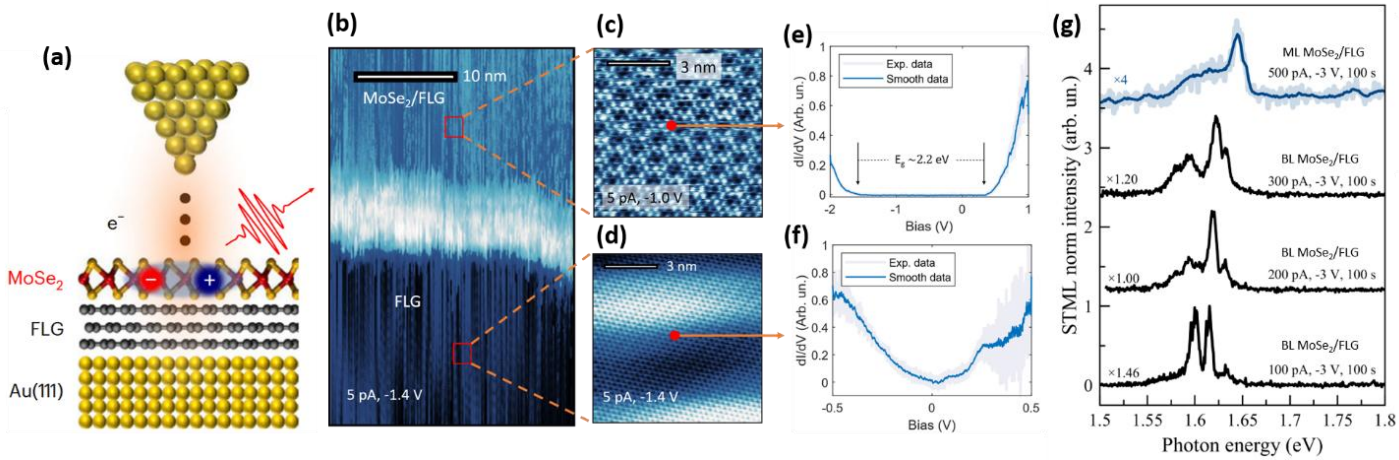

Figure: **(a)** Sketch of STML experiment. STM imaging of **(b)** $MoSe_2$-FLG boundary, **(c)** $MoSe_2$/FLG moiré superlattice, **(d)** FLG lattice. dI/dV spectroscopy of **(e)** $MoSe_2$/FLG, **(f)** FLG. **(g)** STML spectra recorded on atomically resolved ML and BL $MoSe_2$/FLG.

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Poster

MAGNETIC PHASES AND ZONE FOLDED PHONONS IN A BULK FRUSTRATED VAN DER WAALS MAGNET

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Two-dimensional (2D) magnetic materials have attracted extensive research interest due to their potential applications in fields such as nanospintronics and optospintronics [1], and because of their importance in fundamental physics. For instance, on-lattice frustration can result in a variety of magnetic phases, which can be investigated by varying the temperature, magnetic field, or hydrostatic pressure.

In such materials, magnetoelastic interactions allow to use magneto-optical spectroscopies to follow the phase diagram. In this context, magneto-Raman spectroscopy has emerged as the method of choice. It has been particularly useful in probing magnetic transitions and couplings in 2D antiferromagnets such as $MnPS_3$ [2,3] or $FePS_3$ [4].

CrOCl is a frustrated 2D antiferromagnet with a rich magnetic phase diagram and its magnetic transitions are visible in its Raman spectra: as a magnetic field is applied, low-intensity Raman modes appear and disappear as transitions occur between magnetic phases.

In this study, we used density functional theory (DFT) based methods to calculate the phonon modes and their Raman intensities. These calculations allowed us to gain insight into the Raman spectra of CrOCl and its magnetic phases. We showed that different magnetic orders induce small lattice distortions that change the size of the unit cell, effectively resulting in multiples of the primitive cell size. In this context, we showed that the low intensity lattice vibrations that appear or disappear in the Raman spectra are directly related to changes in periodicity of the magnetic phases. Finally, we have used an “unfolding” theoretical procedure to find the connection between the low intensity modes and the phonon band structure of the paramagnetic phase [5].

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Poster

SCREW DISLOCATIONS GIVE AN ADDITIONAL TWIST TO GRAPHENE

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We want to share with the HOWDI community two recent reports on helicity for two type of screw dislocations in graphene. Although it seems trivial, the awareness of Moiré Physics deriving from inter-layer dislocations allow to rationalize many observed features within a well established framework we proposed half a decade ago [1]. Additional guidelines could also be proposed using well-established dislocation concepts.

We recently further characterized such inter-layer dislocations in twisted bilayer graphene. These dislocations where believed to be of pure screw character (due to the twist) while we show in our last EML paper [2] that they are mixed with edge loops thus giving rise to an helical mixed dislocation (panels a-b). This peculiar property drives a large corrugation in the bilayer system that have strong impact on the electronic and superconducting property of the system [3]. Also, the identification of an helical dislocation behind the peculiar Moiré of tBLG ends the debate between dislocations and solitons. Indeed there is no helical solitons while helical dislocations have been understood more than seven decades ago!

Interestingly, intra-layer screw dislocations that are genuinely helical in graphite, have been recently report in CVD grown graphene [4] where they adopt an amazing double helix structure as in DNA [5] as schematized in panel c.

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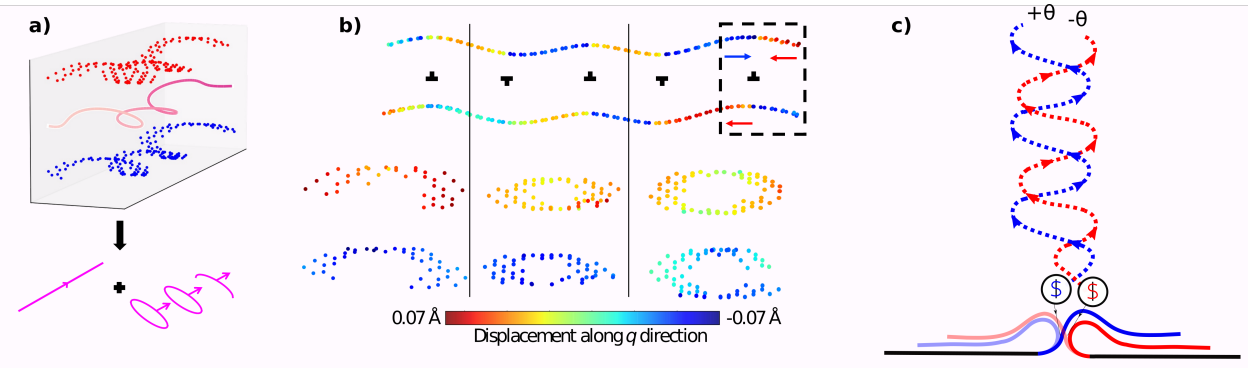

Figure 1: (a,b) inter-layers screw dislocation between two layers of graphene rotated of 1.08° in the (-,-) bending mode [2]. (c) schematics of the double-helix screw dislocation [5] emerging from a tear created by the collapse of a single layered graphene wrinkle [4].

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Poster

GRAPHENE QUANTUM DOTS AS PROMISING BRICKS TO TAILOR SUPER(SUB)-RADIANCE IN COUPLED QUANTUM EMITTERS

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Solid-state quantum emitters are a promising platform in the search for novel photon sources. In particular, Graphene Quantum Dots (GQDs) have been proven to be efficient single-photon sources with quantum yields close to unity [1]. Their bottom-up chemical synthesis provides excellent control on the size, shape and symmetry of the structure, which enables tailoring the optical properties of the GQDs for different applications [2-5].

We designed a new family of elongated GQDs with linear transition dipoles up to 16 Debye, which may be well suited to achieve super- and sub-radiant emission through dipole-dipole coupling. Super- or sub-radiant entangled states only appear when the coupling energy is greater than the detuning between emitters, which is typically on the order of a few 100s of GHz in similar emitters [6]. In the literature, control of the entanglement degree of pairs of molecules coupled by dipole-dipole interaction at low temperature has been demonstrated by actively tuning the emitters through Stark effect [7] or laser-induced tuning [8]. Here, we present some simulations showing how these new GQDs' large transition dipole help reduce the constrain on the detuning between emitters.

Coupled solid-state emitters face an additionnal challenge posed by dephasing effects. While these effects can be managed by working at low temperature (few K), this significantly increases the complexity of experiments, making them harder to scale. A more quantitative understanding of the influence of dephasing on experimental observables could help find a threshold on the acceptable amount of dephasing. For that purpose, we present simulations and analytical results on the impact of dephasing on steady-state and time-resolved observables.

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Poster

HALL EFFECT FINITE-ELEMENT SIMULATION : APPLICATION TO GRAPHENE

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Even though the Hall effect has been discovered in conducting materials almost 150 years ago[1], it led to the development of a great number of applications still used nowadays where low cost magnetic field measurements are needed under ambient or extreme conditions, especially since the rise of semiconductor technologies. In this context, graphene, as a zero bandgap semiconductor, appears as a particularly promising material, thanks to a magnetic field sensitivity higher than the one observed in current sensors[*e.g.* 2].

The linear relationship between the transverse voltage, V_H, and the applied electrical current and magnetic field, I and B, ($V_H=K_H IB$) with the Hall coefficient, $K_H = 1/ne$, are well known (where n is the 2D charge carrier density and e the elementary charge). Nevertheless, they hide numerous effects which could influence strongly the measurements, such as the shape of the device[3], the size and position of the contacts, the anisotropy of conductivity, the disorder[2], or the coexistence of different charge carriers.

In this work, simulation results based on the free finite-element modeling software *FreeFem++*[5] are presented. They allow to precisely account for the behavior of real devices in the presence of a magnetic field (*cf.* Fig1 & Fig.2). The equations used, their variational form and the finite-element methodology using *FreeFem* will be detailed. Preliminary results, applicable to any isotropic 2D material with one type of carrier, allow to take into account the influence of : electrostatic doping, sample geometry, metallic contacts, and geometrical defects. The prospects of this work is to implement a two-carrier model accounting for the effect of thermal activation and of realistic spatial disorder in graphene[2,4] in an open, free access simulation tool.

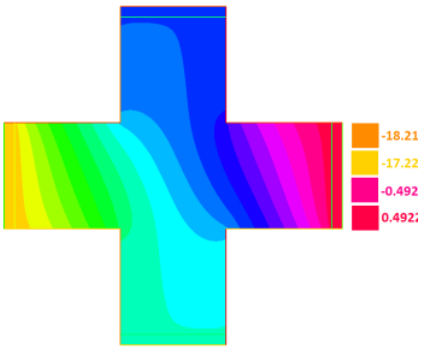

Figure 1: Simulated potential line distribution of a graphene Hall cross (1cm x 1cm) supplied with I =1 mA under a B = 1 T magnetic field. Length/Channel Width, L/W = 3.

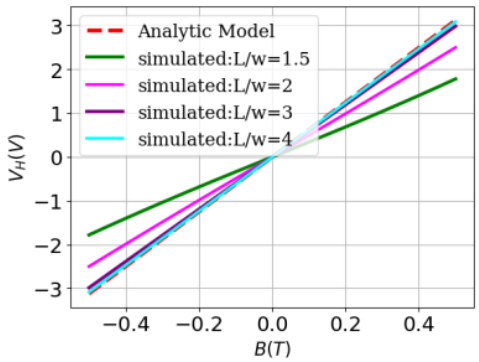

Figure 2: Deviation of the measured Hall voltage V_H from the expected value for various L/W ratio of a L = 1 cm Hall cross.

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Poster

Graphene–β-carotene hybrid phototransistors

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Hybrid 2D photodetectors are devices that combine the properties of heterodimensional materials in order to take advantage of the two fundamental mechanisms involved in light detection: photon absorption and photon conversion into charges. Some recent works use the sensitive electronic properties of graphene to collect charges generated by photon absorption, for example, in PbS quantum dots [1]. In our proposal, we designed a concept hybrid device to explore the electronic properties of graphene and the singlet fission process that occurs in natural chromophores found in plants [2]. Singlet fission is a phenomenon in which one photon excites a high-energy singlet exciton which is converted into correlated triplets, producing two pairs of electrons and holes out of a single photon. Although hybrid devices that use the singlet fission process have been demonstrated [3], the efficient transfer of these triplet excitons is still elusive.

In this context, we propose a graphene-β-carotene hybrid device in which we simultaneously recorded a combination of Raman spectroscopy and electronic transport measurements. Our group applied the same methodology in previous works and demonstrated selective photogating in hybrid devices composed of carbon nanotubes and metalloporphyrins [4], in which the Raman spectra of carbon nanotube is not only downshifted and enhanced, but also reveals an extra peak under illumination in the absorption band of the metalloporphyrin. In the preliminary results of the current work, we characterize the photogating effect in the graphene hybrid upon illumination.

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GROWTH OF FREE-STANDING Mn- AND Nd-BASED NANOMETALLENES

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Abstract

Metallenes, a novel class of two-dimensional (2D) materials composed solely of metal atoms in a single atomic layer, exhibit unique electronic, magnetic, and structural properties due to their high surface atom exposure, flexibility and mainly due to quantum confinement. Despite their promising attributes, the synthesis and isolation of stable, free-standing 2D metals remains a significant challenge due to their thermodynamic instability and the difficulty in characterizing their properties at the atomic scale.

This work presents a viable growth approach of 2D Manganese and 2D Neodymium using monolayer graphene as a substrate within a Transmission Electron Microscope (TEM), where an electron beam induces atomic rearrangements and facilitates the formation of 2D metal structures. Key steps include graphene cleaning via cyclohexane-assisted transfers rather than traditional PMMA assisted transfer to ensure minimal contamination, followed by metal deposition and in situ observation of nanoparticle formation and evolution into 2D metallenes (Figure 1).

Preliminary results for both Mn and Nd reveal the successful formation of metal structures confined within the graphene pores, as evidenced by high-resolution TEM images (Figure 1). Fast Fourier Transform (FFT) analysis confirms the absence of underlying graphene signals, supporting the formation of free-standing metal layers. Electron Energy Loss Spectroscopy (EELS) is underway to verify the elemental purity and atomic composition of the observed metallenes. These findings demonstrate a promising route to stabilize and study atomically thin metals, enabling a new class of 2D functional materials.

*Speaker

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Poster

VAPOR PHASE INFILTRATION FOR SWCNT FILLING

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Single-wall carbon nanotubes (SWCNTs) are renowned for their exceptional charge carrier mobility, along with outstanding optical, thermal, and mechanical properties [1]. Combining these features with their nanometer-scale diameter makes them highly promising for the development of (opto)electronic devices, where the challenge lies in achieving miniaturization without compromising performance. In addition to their intrinsic properties, SWCNTs possess a hollow core that can be filled with various molecules, resulting in unique one-dimensional hybrids that integrate the characteristics of the nanotube with those of the encapsulated species [2].

This study presents the design of a novel reactor and a new methodology based on vapor-phase infiltration for the controlled formation of hybrid molecule@nanotube systems. As a proof of concept, we investigate the encapsulation of dicyanodistyrylbenzene (BDCS), an organic dye used here as a model molecule. BDCS exhibits enhanced fluorescence in its solid state, an effect known as aggregation-induced enhanced emission (AIEE) [3], which arises from specific molecular stacking arrangements. This property makes BDCS particularly suitable for probing encapsulation, as the confined environment within SWCNTs is expected to alter its stacking behavior, thereby offering a direct optical signature of successful filling and molecular organization.

These approaches aim to propose a solvent-free route for nanotube filling and enable improved control over the encapsulation process, opening new possibilities for fine-tuning SWCNT doping levels and enhancing their photosensitization or reactivity under visible light.

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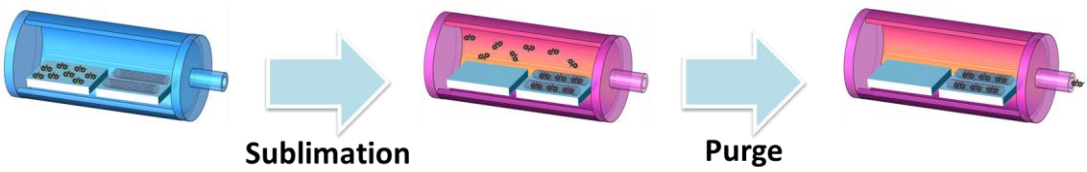

Figure 1: Scheme of the VPI process

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Poster

NANSOCALE ENGINEERING OF DIELECTRIC ENVIRONMENT: TOWARDS ARRAYS OF QUANTUM EMITTERS IN $MOSE_2$

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Engineering the exciton potential landscape in 2D materials is crucial for advancing optoelectronics and nanophotonics[1]. In particular, the ability to confine excitons is key to generating quantum emitters. Various strategies have emerged to achieve this, including defect implantation[2,3], strain engineering[4,5], moiré trapping[6], and electrostatically controlled confinement potentials[7,8]. Precise control over the emitter positions is especially important for realizing ordered arrays, enabling the study of collective phenomena and the development of quantum photonic integrated circuits (PICs) based on 2D materials. Despite relatively high yields in these approaches, accurate spatial localization remains a major challenge. Defect-based methods rely on stochastic implantation, while strain and electrostatic techniques—although effective for creating self-assembled emitters—face intrinsic limitations in emitter density, as large strain gradients or doping profiles are difficult to implement at the nanoscale.

In this work, we present an alternative strategy based on tailoring the dielectric environment of excitons in $MoSe_2$. By nano-structuring surrounding materials such as GaN or TiO_2, we can modulate the excitonic potential landscape with spatial resolutions on the order of tens of nanometers. Building on recent studies[9] of how the high- and low-frequency dielectric constants influence exciton energies, we estimate the resulting confinement potentials and calculate the corresponding eigenstates as a function of nanostructure geometry. Based on these principles, we fabricate a device with the monolayer TMD experiencing a varying dielectric environment, and present results from its spectroscopic analysis in the emission.

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Poster

Quantifying the sp^3/sp^2 ratio in functionalized graphene

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A major challenge in graphene nanoscience is quantifying the concentration of molecules or atoms grafted onto the graphene surface. Raman spectroscopy, a non-contact optical technique, is well-suited to achieve this purpose. However, calibration becomes challenging at low coverage due to the weak signal, and at high coverage due to local fluctuations and large regions that yield no Raman response with visible light excitation. In this work [1], we propose a tailored continuous model that enables accurate quantification of the concentration of covalently bonded molecules or atoms and incorporates input parameters from quantum chemistry calculations that account for surface modifications. We analyze the intensity ratio of the defect-induced D band over the primary G band, along with their broadenings. This approach is validated through the comparison with both our experimental observations [1] and previously published results [2] on various adatom coverage rates. Good agreement is found for both low coverage rates, where the sizes of distorted and activated regions are derived from calculations, and high coverage rates, where sp^3-hybridized, Raman-inactive regions are included. A detailed analysis of the electronic modifications induced by chemisorbed atomic hydrogen on the graphene surface enables a non-empirical approach to quantify the coverage rate.

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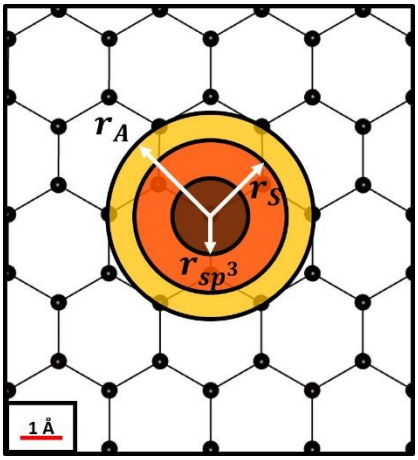

Figure 1: Schematic representation of the three regions affected by a sp^3-type point defect in graphene

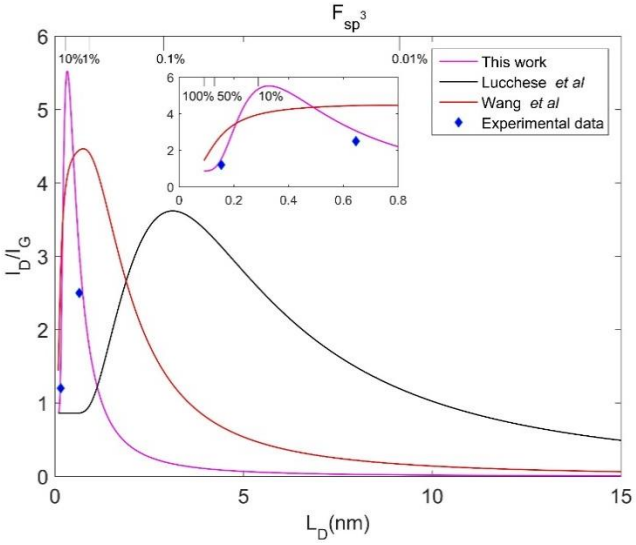

Figure 2: Intensity ratio of the D band over the G band (I_D/I_G) as a function of the average distance between the sp^3-type point defects (L_D) for our model and two models from the literature compared with experimental data from the literature.

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Poster

TILTED ELECTRON DIFFRACTION FOR PROBING STACKING POLYMORPHS IN PTSE2 BILAYERS

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Layered 1T-$PtSe_2$ exhibits extraordinary properties that depend strongly on both the number of layers and the stacking configuration. The material is a semiconductor with a bandgap of approximately ≈1.2 eV in the monolayer limit, gradually transitioning to a semi-metallic state as the thickness increases from multilayer to bulk [1]. Additionally, a wide range of stacking phases has been reported, characterized by different band gaps and possessing distinct electronic and optical properties [2]. $PtSe_2$ therefore exhibits high carrier mobility in its semi-metallic form and strong absorption in the infrared and near-infrared regions, making it highly attractive for optoelectronic applications [3].

This tunability enables exciting opportunities for material design but also results in strong variations in the structural, electronic, and optical properties of synthesized polycrystalline films due to inevitable phase mixing [4]. A clear methodology to characterize the various staking phases is still difficult to delineate, as Raman spectroscopy does not provide a clear signal for their distinction [1]. High-resolution scanning transmission electron microscopy (HR-STEM) can resolve slight differences in in-plane atomic configurations, but can only probe small regions and doesn't allow a statistical analysis of the stacking geometries.

Our work aimed to develop a methodology that enables the systematic mapping of different stacking polymorphs over large areas, crucial for understanding the experimentally measured optoelectronic properties. We employed 4D-STEM (4D Scanning Transmission Electron Microscopy) in a tilted geometry, the tilt introduces a projection of out-of-plane atomic configurations into the diffraction pattern recorded at each scanned position, allowing the retrieval of out-of-plane stacking information. Through numerical simulations, we were able to reconstruct the diffraction signals associated with the different stakings. This preliminary step has allowed us to optimize the tilting condition and clearly distinguish not only the different staking geometries but also inverted domains. Through this protocol, insightful observations are demonstrated on MBE-grown polycrystalline PtSe2 bilayers, such as a statistical analysis of the incidence of various stakings and mapping of the grain boundaries and inversion domains boundaries.

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Poster

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