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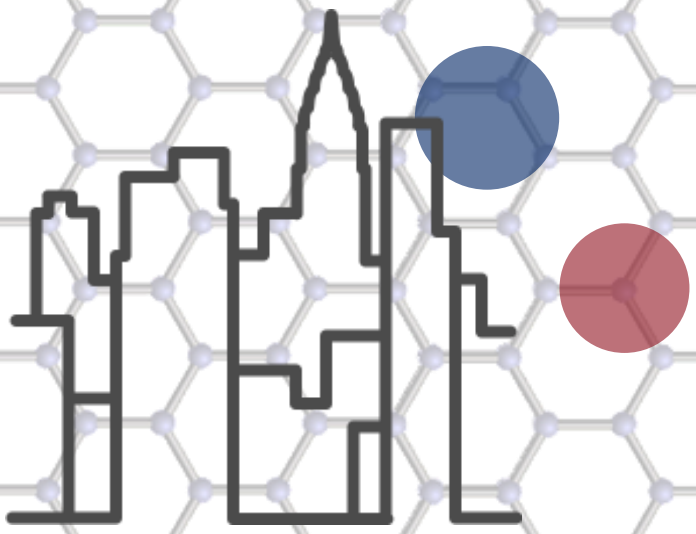

ABSTRACTS BOOK

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FOREWORD

On behalf of the Organising Committee we take great pleasure in welcoming you to New York for the third edition of the **GrapheneforUS** 2020 International Conference.

A plenary session and thematic workshops with internationally renowned speakers will feature current and future "Graphene and 2D Materials" developments.

GrapheneforUS 2020 will bring together, from a global perspective, scientists, researchers, end-users, industry, policy makers and investors in an environment of cooperation and sharing towards the challenges of Graphene and 2DM commercialization.

We truly hope that **GrapheneforUS** 2020 serves as an international platform for communication between science and business.

We are also indebted to the following Scientific Institutions and Companies for their help and/or financial support: PennState (Materials Research Institute) / Center for 2-Dimensional and Layered Materials (2DLM), Rensselaer, Honda Research Institute USA, Millipore (Sigma-Aldrich), Columbia University, The Graduate Center and The Advanced Science Research Center (ASRC) of City University of New York.

We also would like to thank all the exhibitors, speakers and participants that join us this year.

One thing we have for granted: very few industries, one way or another, will escape from the influence of Graphene and 2D Materials and the impact on businesses is here to stay.

Hope to see you again in the next edition of **GrapheneforUS** to be held in 2021.

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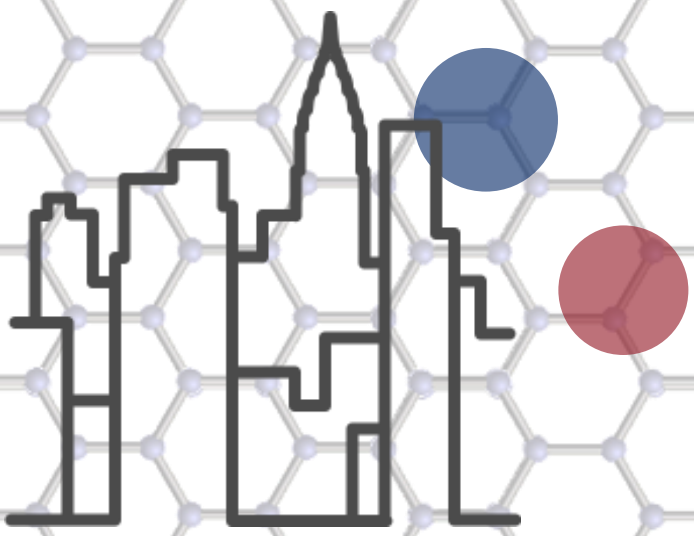

KEYNOTE SPEAKERS

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Hybrid Metasurfaces for Enhanced Light-Matter Interactions and Extreme Polariton Manipulation

In this talk, we discuss our recent efforts in the context of hybrid metasurfaces formed through nanophotonic engineering of metasurfaces [1-6], 2D materials and their combinations, reporting our recent theoretical and experimental results in the context of hyperbolic polariton manipulation, valley exciton control, sorting and steering, and twisted bilayers for polariton canalization and extreme dispersion engineering. During the talk, we will discuss the highly unusual light-matter interactions and potential opportunities for nanophotonic devices.

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Figure

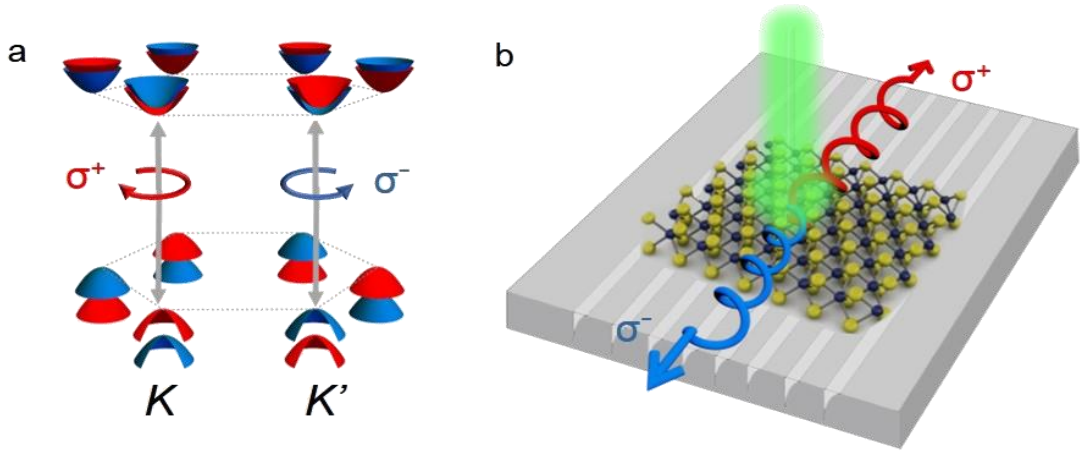

Figure 1: (From [5-6]) Valley exciton sorting and routing using hyperbolic metasurfaces with asymmetric grooves.

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Plasmonic Nanostructures

In this talk I will discuss recent experiments on nano-imaging of plasmon polaritons in graphene-based nanostructures. The focus will be on controlling nano-optical phenomena with the electric field. We implemented several variants of photonic crystals for plasmon polaritons [Xiong et al. Nature Communications 10, 4780 (2019) and Science 362, 1153 (2018)]. I will also discuss recent progress in multi-messenger nano-imaging recently implemented in our laboratory (Nature Materials 2020 https://doi.org/10.1038/s41563-019-0533-y).

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An epigraphene platform for coherent 1D nanoelectronics

Exceptional edge state ballistic transport, first observed in graphene nanoribbons grown on the sidewalls of trenches etched in electronics grade silicon carbide even at room temperature, is shown here to manifest in micron scale epigraphene structures that are conventionally patterned on single crystal silicon carbide substrates. Electronic transport is dominated by a single electronic mode, in which electrons travel large distances without scattering, much like photons in an optical fiber. In addition, robust quantum coherence, non-local transport, and a ground state with half a conductance quantum are also observed. These properties are explained in terms of a ballistic edge state that is pinned at zero energy. The epigraphene platform allows interconnected nanostructures to be patterned, using standard microelectronics methods, to produce phase coherent 1D ballistic networks. This discovery is unique, providing the first feasible route to large scale quantum coherent graphene nanoelectronics, and a possible inroad towards quantum computing.

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Solution-Processed 2D Materials for Next-Generation Lithium-Ion Batteries

Efficient energy storage systems represent a critical technology across many sectors including consumer electronics, electrified transportation, and a smart grid accommodating intermittent renewable energy sources. Arguably, the most important advance in energy storage over the past three decades is the lithium-ion battery, which was recognized with the 2019 Nobel Prize in Chemistry. However, despite its many successes, issues related to safety, energy density, charging time, and operating temperature range have hindered the large-scale adoption of some of the most revolutionary lithium-ion battery technologies such as electric vehicles and grid-level storage. Nanostructured materials were once thought to present compelling opportunities for next-generation lithium-ion batteries, but inherent problems related to high surface area to volume ratios at the nanometer-scale (e.g., undesirable surface chemical interactions between electrodes and electrolytes) have impeded their adoption for commercial applications. This talk will explore how the chemical inertness and solution processability of select two-dimensional (2D) materials are driving a resurgence in nanostructured lithium-ion battery materials [1]. For example, conformal graphene coatings on lithium-ion battery cathode powders mitigate surface degradation and minimize the formation of the solid electrolyte interphase, thus improving cycling stability. In addition, the high electrical conductivity of graphene reduces cell impedance, resulting in enhanced kinetics that enable high-rate capability and low-temperature performance down to –20 °C [2]. On the other hand, ionogel electrolytes based on ionic liquids and hexagonal boron nitride nanoplatelets enable safe, high-rate operation at high temperatures up to 175 °C, which represents the highest operating temperature to date for solid-state lithium-ion batteries [3].

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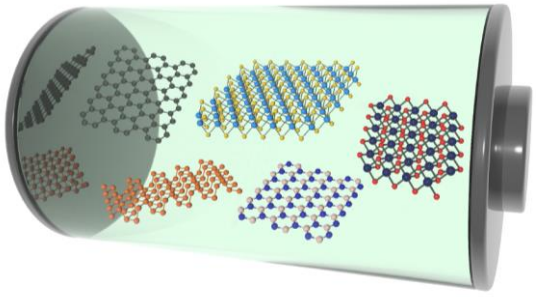

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Mixed-dimensional stackable electronics enabled by freestanding 2D/3D materials

2D material-based devices have received great deal of attention as they can be easily stacked to obtain multifunctionality. With their ultrathin thicknesses, such multifunctioning devices become so flexible and conformal that they can be placed onto any 3D featured surfaces. However, 2D heterostructures are typically demonstrated as stacked flakes where single or few devices can be fabricated due to lack of strategies for layer-by-layer stacking of 2D materials at the wafer scale. In this talk, I will discuss about our unique strategy to isolate wafer-scale 2D materials into monolayers and stack them into a heterostructures by using a layer-resolved splitting (LRS) technique [1]. This technique enables my group at MIT to explore unprecedented wafer-scale 2D heterodevices including integrated photonics, 3D neuromorphic computing, and microLEDs, which will be introduced in my talk.

While 2D heterostructures promise interesting futuristic devices, the performance of 2D material-based devices is substantially inferior to that of conventional 3D semiconductor materials. However, 3D materials exist as their bulk form, thus it is challenging to stack them together for heterostructures. Obviously, conformal coating of such single-crystalline bulks on 3D features is impossible. My group at MIT has recently invented a 2D materials-based layer transfer (2DLT) technique that can produce single-crystalline freestanding membranes from any compound materials with their excellent semiconducting performance [2-4]. This technique is based on remote epitaxy of single-crystalline films on graphene followed by peeling from graphene. Stacking of freestanding 3D material membranes will enable unprecedented 3D heterostructures whose performance is expected to be superior to that of 2D heterostructures. I will talk about our group's effort to apply single-crystalline freestanding membranes for flexible, conformal electronics as well as for 3D heterostructures.

Finally, I will conclude my talk by discussing perspectives of coupling 2D-3D freestanding membranes for 2D-3D mixed heterostructured devices that can be enabled by our LRS and 2DLT techniques [5,6].

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Synthesis of Two-dimensional Materials via Chemical Vapor Deposition

In recent years, tremendous efforts have been devoted to the research on two dimensional materials. Their unique structures and remarkable properties have offered great potential for a wide range of applications in electronics, optoeletronics, valleytronics, catalysis, etc. The synthesis of high quality large area mono- and few-layer 2D materials is highly desirable for their applications. In this talk I will present our further understanding regarding the chemical vapor deposition (CVD) synthesis (Fig. 1) process in monolayer MoS2 [1], and our development of other novel 2D materials [2, 3].

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Figures

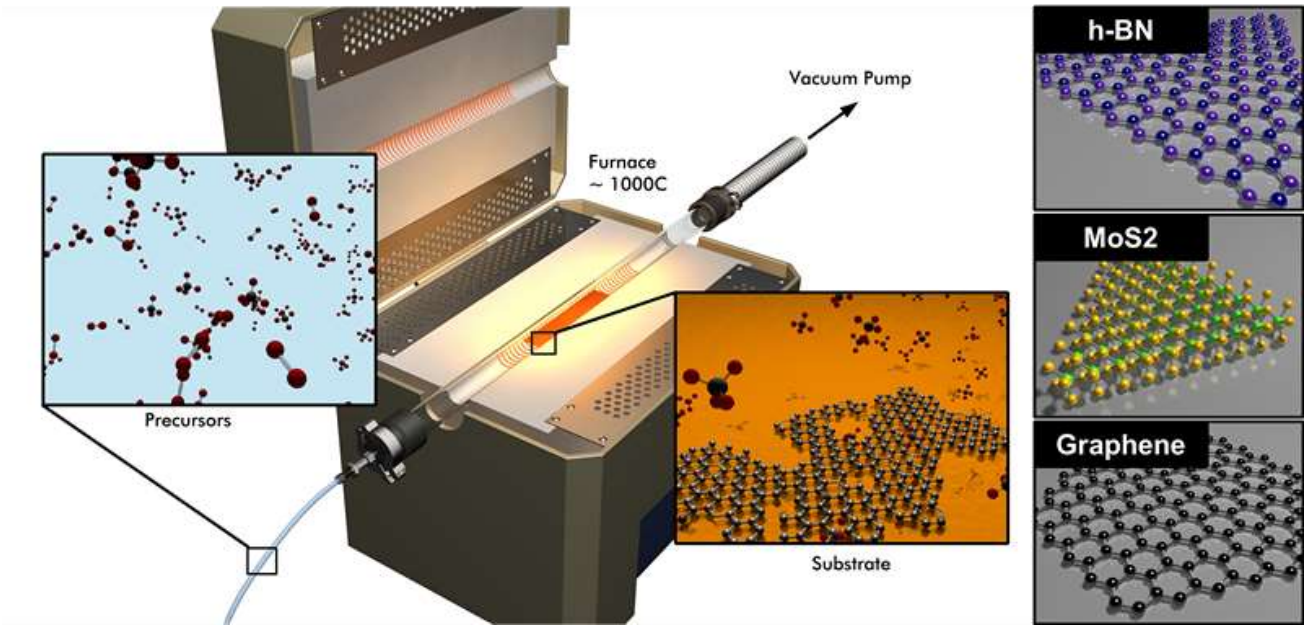

Figure 1: Schematic illustration of the Chemical Vapor Deposition synthesis process for 2D materials.

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Stacking and twisting 2D materials for quantum nano-optoelectronics

We discuss 2D-material heterostructures as a novel toolbox for controlling light and electrons at the atomic scale. In particular, we will show nano-optoelectronic devices that demonstrate the exciting properties of 2D polaritons1,2,3,4,5, such as plasmon, phonon and exciton polaritons. We challenge the limits of quantum light-matter interactions and study the fundamental limits of optical field confinement and optical non-linearities and topological properties down to the length-scale of single atoms2. In addition, quantum confined status can be probed through intersubband transitions in few-layer semi-conducting 2D materials5.

We will also present studies on twisted bilayer graphene using scanning near-field optical microscopy. Twisted bilayer graphene near the magic angle (MABG) exhibit strongly correlated phases have been observed, including superconductivity and the Mott-like insulating state6,7. We studied plasmon excitations associated to vertical transitions between the flat bands and the first excited bands close to the K point of the Moiré lattice Brillouin zone8.

Some device applications, such as detectors for infrared and THz light will also be discussed9.

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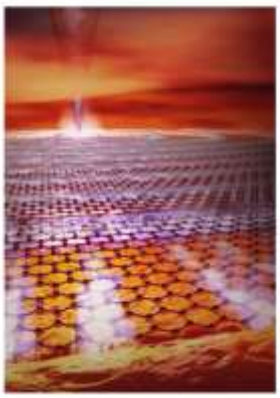

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Pushing the fundamental limits of 2D plasmons

Plasmon with large confinement is attractive for various applications such as bio- and gas- sensing, infrared detectors, and beamforming. Various nanophotonics would also benefit from non-reciprocal devices without the application of a magnetic field. In this talk, I will discuss strategies in realizing 2D plasmons with large confinement and non-reciprocity.

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Control of light-matter interaction in van der Waals materials

Abstract
Two-dimensional (2D) van der Waals materials have emerged as a very attractive class of optoelectronic material due to the unprecedented strength in its interaction with light. In this talk I will discuss approaches to enhance and control this interaction by integrating these 2D materials with microcavities, and metamaterials. I will first discuss the formation of strongly coupled half-light half-matter quasiparticles (microcavity polaritons) [1] and their spin-optic control [2] in the 2D transition metal dichacogenide (TMD) systems. Following this I will discuss the formation of polaritons using excited states (Rydberg states) to enhance the nonlinear polariton interaction. Recent results on electrical control [3] and realization of a polariton LED based on 2D TMDs [4] will also be presented. Finally, I will talk about strain activated room temperature single photon emission from hexagonal boron nitride (hBN) [5] which can be integrated with microresonators on silicon photonic platform.

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Metals at the Atomic Limit

The last decade has seen an exponential growth in the science and technology of two-dimensional materials. Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting that can be grown over large scales for a variety of electronic devices and quantum technologies, such as topological quantum computing, quantum sensing, and neuromorphic computing. In this talk I will discuss our pioneering work in confinement heteroepitaxy (CHet) that enables the creation of 2D forms of 3D materials (e.g. 2D-Ga, In, Sn) and *decouples* the growth of the metals from other 2D layers, thereby enabling a new platform for creating artificial quantum lattices (AQLs) with atomically sharp interfaces and designed properties. As a specific example, we synthesize plasmonic layers that exhibit >2000x improvement in nonlinear optical properties, and 2D-superconductors combined with topological insulators as the building block of next generation "2D" topological superconductors. Confinement heteroepitaxy opens up avenues for enabling a virtual "legoland" of hybrid quantum materials.

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2D Esaki junctions, Schottky-barrier and tunnel field-effect transistors, and the path to applications

The path to applications of two-dimensional (2D) semiconductors is being paved by synthesized materials [1]. 2D transition metal dichalcogenides are advancing for electronics applications, particularly as channel materials for field-effect transistor (FETs) and tunnel field-effect transistors (TFETs) [2]. Steady progress in synthesized materials has led to the development of batch fabrication processes, atomic layer deposition of gate dielectrics, p-n junction formation, and realization of 2D Esaki tunnel junctions [3]. Careful study of transistor transport has yielded experimentally-validated Schottky-barrier FET models that account for the measured transport from subthreshold to saturation [4]. This presentation will highlight recent findings.

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Figures

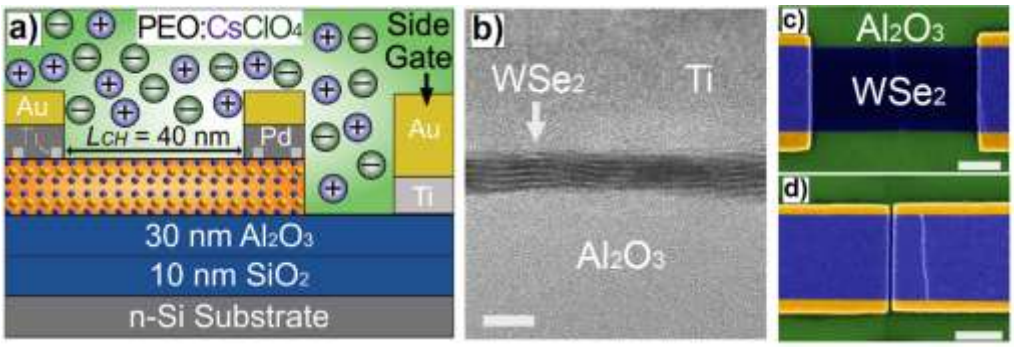

Figure 1: (a) Schematic cross section of an electric-double layer WSe_2 FET used to induce a 2D Esaki tunnel junction. (b) Transmission electron microscope cross section in the contact region. The MBE-grown WSe_2 epilayer is 6 monolayers thick; the scale bar is 5 nm. (c) False-colored scanning electron microscope top view of a 2 μm-long WSe_2 FET prior to PEO:$CsClO_4$ coating; the scale bar is 500 nm. (d) WSe_2 FET with source-drain separation of ~60 nm, scale bar of 500 nm.

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Spin-orbit proximity phenomena and tunable spin-to-charge conversion in graphene

Graphene has emerged as a centerpiece for future spintronics, owing to its tunable electronic properties and ability to transport spin information over very long distances [1]. For active devices, however, spin manipulation remains an open challenge. Such a challenge can be resolved with spin-orbit coupling (SOC) induced by proximity effects. Here, I will discuss our recent experiments on proximity-induced SOC and spin-to-charge interconversion (SCI) in stacks of graphene and transition metal dichalcogenides (TMDC) [2,3]. I will show that key information can be obtained from the spin-lifetime anisotropy, as it is determined by the preferential direction of the spin-orbit fields that cause the spin relaxation. Even though the spin-lifetime in graphene on SiO_x is isotropic, it becomes strongly anisotropic in bilayers comprising graphene and a TMDC. Indeed, the spin-lifetime varies over one order of magnitude depending on the spin orientation and is largest for spins pointing out of the graphene plane, even at room temperature [2]. This suggests that the strong spin-valley coupling in the TMDC is imprinted in graphene and felt by propagating spins. I will further demonstrate that the proximity-induced SOC leads to strongly enhanced room-temperature SCI [3]. By performing spin precession experiments in appropriately designed Hall bars, we are able to separate the contributions of the spin Hall effect (SHE) and the spin galvanic effect (SGE). Remarkably, their corresponding conversion efficiencies can be tailored by electrostatic gating in magnitude and sign (Fig. 1), peaking near the charge neutrality point with an equivalent magnitude that is comparable to the largest efficiencies reported to date.

References

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Figures

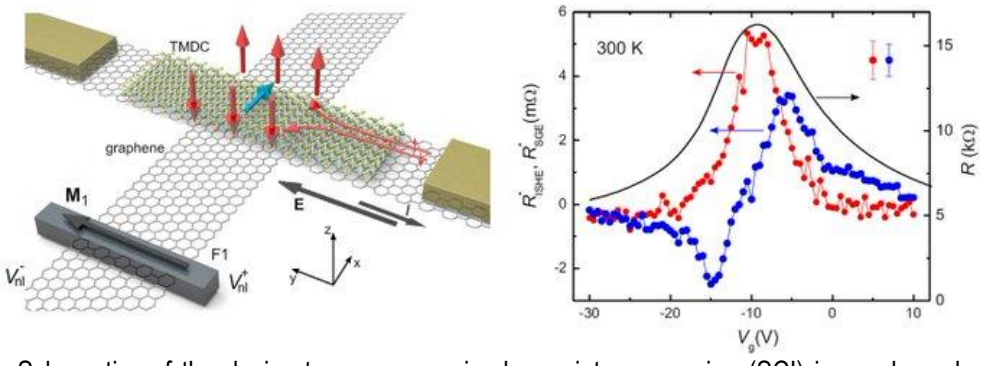
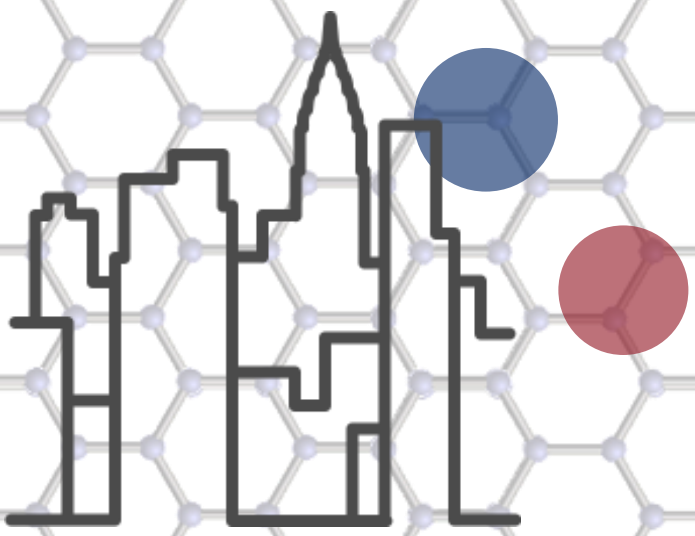


Figure 1: Left: Schematics of the device to measure spin-charge interconversion (SCI) in graphene by proximity of a TMDC. A current *I* generates a transverse spin current owing to the SHE (red arrows) and an in-plane spin density due to the inverse SGE (blue arrow). **Right:** Tunable SCI as a function of carrier density, modulated by the gate voltage V_g.



INVITED SPEAKERS

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Viscous electronics in graphene

Electron–electron (e–e) collisions can impact transport in a variety of surprising and sometimes counterintuitive ways. Despite long-time interest, experiments on the subject proved challenging because of the presence of momentum-relaxing scattering sources (e.g. phonons or impurities). Only recently, sufficiently clean electron systems in which transport dominated by momentum-conserving e–e collisions have become available, enabling the study of electron transport governed by interactions.

In this talk we will see that interacting electrons in graphene can behave as a very viscous fluid. It will be shown that the flow of electron fluid resembles that of classical liquids, such as oil, and is accurately described by the theory of hydrodynamics [1-4]. We will discuss how to measure the viscosity of electron fluids and talk about the applications of viscous electronics.

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2D Materials for Magnetic Tunnel Junctions

Spin-based electronics is at the heart of widely distributed applications (such as sensors, hard drives read heads, MRAMs…), and has recently been highlighted as a main contender for post-CMOS approaches (spin logics, stochastic, neuromorphic and quantum computing). In this context, 2D materials have opened novel exciting opportunities in terms of functionalities and performances for spintronics devices. To date, it is mainly graphene properties for efficient spin transport which have been put forward. Here we will present experimental results on another venue: 2D materials integration in the prototypical spintronics device, the magnetic tunnel junctions (MTJ).

We will first present experiments based on a large-scale low temperature catalyzed chemical vapor deposition (CVD) step to integrate graphene directly on ferromagnetic spin sources [1]. We will show that the graphene passivation layer can prevent the oxidation of a ferromagnetic spin source, in turn enabling the use of novel humid/ambient low-cost processes (such as ALD) for spintronics. Importantly, the use of graphene on ferromagnets allows to preserve a highly surface sensitive spin current polarizer/analyzer behavior and adds new enhanced spin filtering property that will be discussed [2]. We will then present results concerning 2D materials beyond graphene for MTJs. Characterizations of complete spin valves making use of 2D insulator h-BN as a tunnel barrier grown by CVD on Fe or Co will be discussed. Observed strong spin signals and inversion of the spin polarization will be presented (with ab-initio calculations in support) in light of h-BN hybridization with ferromagnetic metal in contact [3]. We will finally show our most recent experiments making use of 2D semiconductors, highlighting fundamental interfacial spin polarization processes [4]. These experiments unveil the strong potential of 2D materials for spintronics.

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Control of quantum light emission from 2D materials

Photonics based on two-dimensional (2D) materials has made incredible progress in the last years and currently sets the state of the art for a number of applications in optoelectronics and optics. Recently, 2D materials have also begun to impact the field of semiconductor quantum optics through the demonstration of stable quantum emitters in semiconductor transition metal dichalcogenides (TMDs) and hexagonal boron nitride (hBN). Despite the great promise of this system, a few challenges still need to be tackled before promoting this system for real quantum applications.

In this work, we focus on the quantum emission from atom-like defects in 2D hBN with particular attention to the broad inhomogeneous spectral distribution. Our experiments were able to link this multicolor emission to variations of the electromagnetic environment with the development of a method to actively tune the emission energy by externally modifying strain. This fabrication process produces a tunable ultra-bright room-temperature single photon source with the advantages of 2D materials, including transferability, stretchability, heterogeneous device assembly and straightforward integration with photonic circuits.

In the second part of the talk, we present our current research aimed at the investigation of the vibronic states in hBN molecules for enhanced quantum efficiency of the single-photon emission. Our photoluminescence excitation experiments show that light absorption is more efficient when mediated by in-plane optical phonons. Enhanced absorption results in higher quantum efficiency when emitters are excited by non-resonant pumping with detuning in the range 150-200 meV. By interfacing our experimental results with theoretical calculations of the phononic modes of hBN and simulations based on DFT methods, we are making progress towards the understanding of the nature of active structural defects in hBN.

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New Mechanism for the Growth of 2D Materials

The role of additives in facilitating the growth of conventional semiconducting thin films for cutting-edge electronics is well established. Apparently, their presence is also decisive in the growth of two-dimensional transition metal dichalcogenides (TMDs), yet their role remains ambiguous. Current dominant model suggest that the salt additives promote the growth by lowering the melting points of the refractory metal oxide precursors. In this work we will show that the growth of TMD monolayers enabled by a salt additive is governed by a surfactant-mediated mechanism. Specifically, we discovered that when using sodium bromide as an additive to molybdenum dioxide precursors, the sodium atoms chemically passivate the edges of the growing molybdenum disulfide monolayer crystals, relaxing in-plane strains so as to suppress 3D islanding and promote monolayer growth. Furthermore, pre-deposited salt on substrates acts as a removable template for patterned growth of monolayers aiming at lithography-free device fabrication. This finding provides a strategy for the synthesis of new TMD monolayers on various surfaces with desirable patterns.

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Janus Monolayer-Induced Abnormal Interlayer Coupling in 2D Heterostructures

Janus transition metal dicalcogenide (TMD) is a newborn of the two-dimensional (2D) materials family. Its structure is similar to TMDs such as MoS_2, but one layer of chalcogen is different from the other layer, one example being MoSSe. Due to the unique crystal structure of Janus TMD, unconventional phenomena have been theoretically predicted, including out-of-plane piezoelectricity and exciton disassociation by the intrinsic out-of-plane dipole moment. In this talk, I will introduce our recent work on the fundamental phonon properties of Janus monolayer MoSSe and interlayer coupling of MoSSe/MoS_2 heterostructures. Interlayer breathing and shear modes of high-symmetry 2H and 3R heterostackings are probed by low frequency Raman spectroscopy. Unintuitively, interlayer coupling strength in the heterostructures is stronger than their pure MoS_2 counterparts possibly due to the compressive (tensile) strain in MoSSe (MoS_2) introduced during synthesis. Difference in high frequency modes between MoSSe/MoS_2 and pure MoS_2 supports the strain hypothesis. These spectroscopic features can serve as a fingerprint of stacking configurations, interlayer coupling in heterostructures, and degree of selenization in the fabrication process from TMDs to Janus TMDs.

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Democratizing Two-Dimensional Materials

Two-dimensional (2D) materials remain important tools for researchers. Scientists and engineers from a variety of disciplines routinely take advantage of the unique mechanical and electronic properties of 2D materials. However, production methods used to synthesize layered crystalline materials and processing techniques used to delaminate them are complex and often require specialized equipment. We will discuss some of the high quality ready to use 2D materials that MilliporeSigma offers and how your research may benefit from them. Additionally, our partnerships with leaders in the field ensure our products are made with the expertise required to give scientists and engineers access to ready to use 2D materials.

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Pressure-induced Formation of an Ultra-Hard 2D Diamond Structure from Graphene and h-BN

The quest for materials with exceptional mechanical properties is the long-time focus of major efforts in the material science community. The study of the nanomechanical behavior of atomically thin graphene has led to the discovery of attractive mechanical properties, such as its outstanding in-plane stiffness and out-of-plane flexibility, although its hardness and transverse stiffness are inferior to those of diamond. Here we explore the elastic properties of supported 2D films of graphene by modulated Å-Indentation, an Atomic Force Microscopy (AFM)-based technique capable of achieving sub-Å indentations depths during force-indentation measurements. We experimentally demonstrate that at room temperature and under localized indentation pressure, a single layer of graphene on top of a carbon interface layer (buffer layer), both epitaxially grown on the Si-face of a SiC(0001) substrate, exhibits transverse stiffness superior to that of CVD bulk diamond, it is resistant to perforation by a diamond indenter and shows a reversible change in electrical conductivity upon indentation. Density functional theory (DFT) calculations indicate that the 1+buffer layer graphene film undergoes a pressure-induced reversible phase transformation to a new ultra-stiff, ultra-hard 2D diamond structure, named diamene, followed by sp2-to-sp3 chemical bond transitions. DFT calculations also show that the transition to a 2D diamond structure is facilitated by the presence of the interfacial buffer layer, that strongly interacts with the reactive Si-terminated face of the SiC substrate, and that does not require the presence of adsorbates to stabilize the film surface in contact with the indenter. This finding casts light on the importance of the physics of the interface between graphene and the substrate in the emergence of the hardening effect. Recent experiments indeed demonstrate the absence of the graphene-diamene transformation in exfoliated graphene films of any thickness on SiO2.
Besides graphene, other 2D materials possess the structural characteristic necessary for sustaining a similar pressure-induced sp2-to-sp3 phase transition. In particular, hexagonal boron nitride (h-BN) may be converted to a stable cubic phase (c-BN) under pressure. Our most recent Å-indentation experiments demonstrate that 2-layer h-BN flakes, mechanically exfoliated on a SiO2 substrate, consistently exhibit a transverse elastic modulus almost two times bigger than that of the bare substrate. This stiffening effect is observed only for flakes of thickness between 2 to 5 atomic layers, but not in single- nor multilayer (> 6-layer) h-BN. MD simulations also show that the transition is not uniform but it starts in nuclei under and around the tip-sample contact..

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Introducing FLLTER, a division of Grafoid Inc for economical, sustainable, and scalable graphene-based water treatment.

FLLTER Inc. is a privately-owned water filtration technology company launching its global operations in 2020. Headquartered in Kingston, Ontario (Canada) within the Grafoid Global Technology Centre, we are a growing business that is scaling up our manufacturing capacity of disruptive graphene-based materials for use in our flagship water filtration products called the M1 FLLTER ™ and G1 FLLTER ™. Our production quality and output scale will meet market demands for consumer products, industrial opportunities, and municipal treatment systems while making a positive and cost-effective impact on the global socioeconomic challenges surrounding clean water purification and water security. FLLTER Inc. relies exclusively on the unique material production methods developed and patented by Grafoid for our source of Mesograf ™ and Graphene Oxide raw materials, which we subsequently process further into the M1 FLLTER ™ and G1 FLLTER ™ formulations that are added directly into conventional water treatment devices that would similarly hold a loose material such as granular activated carbon (Figure 1). This presentation will primarily highlight the technical performance of the M1 FLLTER ™ and G1 FLLTER ™ formulations for specific application verticals within the water treatment industry. This presentation will additionally highlight case studies and continued product research and development initiatives ongoing at FLLTER Inc. that will solidify our position as an industry leading organization for graphene-based water treatment technology in the years to come.

Figures

Figure 1: Overview of the materials within a standard FLLTER ™ product. Each material labelled within the above image is currently undergoing NSF certification testing for compliance with international standards surrounding water treatment.

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Superconductivity in Graphene Induced by the Rotated Layer

Recent discoveries in graphene bilayers have revealed that when one of the layers is rotated by a specific angle, superconductivity emerges. We provide an explanation for this phenomenon. We find that due to the layer rotations, the spinors are modified in such way that a repulsive interaction becomes attractive in certain directions.
We also find that due to rotations the nodal points become angle dependent. The spinor in layer $ i=2 $ depends on the twisting angle in contrast to the spinor in layer $i=1$.
As a result, the physics in the two layers depends on the twist and is identified with a twisted phase. In order to observe the twist we use an interaction term which changes sign.
The change from a repulsive interaction to an attractive one gives rise to a one dimensional charge-density-wave. Due to tunneling between the two layers, the proximity of layer $i=1$
induces superconductivity in the charge-density-wave phase in layer $i=2$. This result is obtained by following a sequence of steps: when layer 2 is rotated by an angle θ, this rotation is equivalent to a rotation of an angle $-\theta$ of the linear momentum. Due to the discrete lattice, in layer 1 the Fourier transform conserves the linear momentum $modulo$ the hexagonal reciprocal lattice vector. In layer 2, due to the rotation, the linear momentum is conserved $modulo$ the $Moire$ reciprocal lattice vector. Periodicity is achieved at the $magic $ angles obtained from the condition of commensuration of the two lattices.

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Atomic Defects in 2D Semiconductors - From Chemical Doping to Quantum Technologies

Chemical doping is a vital technology to tune the conductivity and optical properties of semiconductors. While dopants in bulk materials usually create shallow states that can contribute mobile charge carriers, the electronic states of dopants in 2D materials exhibit much more localized wavefunctions and higher binding energies. This offers exciting possibilities to engineer atomic quantum systems by chemical design rules.

In this talk I will give an overview on the recent progress in understanding the physical properties of single impurity atoms in 2D semiconductors and its implications for devices based on 2D materials.

Individual point defects in pristine and intentionally doped semiconducting transition metal dichalcogenides (TMDs) were studied by means of high-resolution scanning probe microscopy. We directly resolve the discrete electronic spectrum of single dopants in a charge neutral or ionized state and map out their associated defect orbitals [1-4]. Different types of defects reveal the interplay between chemical impurity states [1,3], multi-valley hydrogenic bound states [4], and electron-phonon coupling [3,5] at reduced dimensions.

Furthermore, tip-induced hydrogen desorption of CH-doped WS_2 is demonstrated, creating reactive surface sites with atomic control [5] and offering new avenues for atomic precise functionalization of 2D manifolds.

We also show electrically driven photon emission from individual defects [6]. Atomically resolved luminescence maps from single sulfur vacancy defects are presented. The widely tunable optical emission generated by charge carrier injection into localized defect states in a 2D material is a powerful platform for electrically driven single-photon emission.

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Single photons, phonons and spins in atomically thin WSe2

Monolayer transition metal dichalcogenides (TMDs), such as WSe2, are atomically thin semiconductors with a "valley" degree of freedom, which can be optically addressed, thus opening up exciting possibilities for quantum "valleytronics". Recently, naturally occurring single quantum emitters, believed to be excitons trapped in shallow potentials, were reported in TMDs [1]. They seem to inherit the valley degree of freedom from the host TMD and owing to their longer lifetimes, appear promising for quantum information processing applications.
In this talk, I will begin by highlighting some unique properties of TMDs excitons which result from the off-Gamma-point origin of the constituent single particle electronic states. After describing the basic properties of quantum dots in TMDs, I will present evidence for quantum entanglement between chiral phonons of the 2D host and single photons emitted from the quantum dots [2]. I will also present evidence for optical initialization of single spin-valley in WSe2 FET devices [3]. Finally, I will discuss our future plans for implementing a dynamically tunable array of qubits in pristine TMDs which can serve as an ideal platform for quantum information processing applications and also for understanding fundamental many-body physics.

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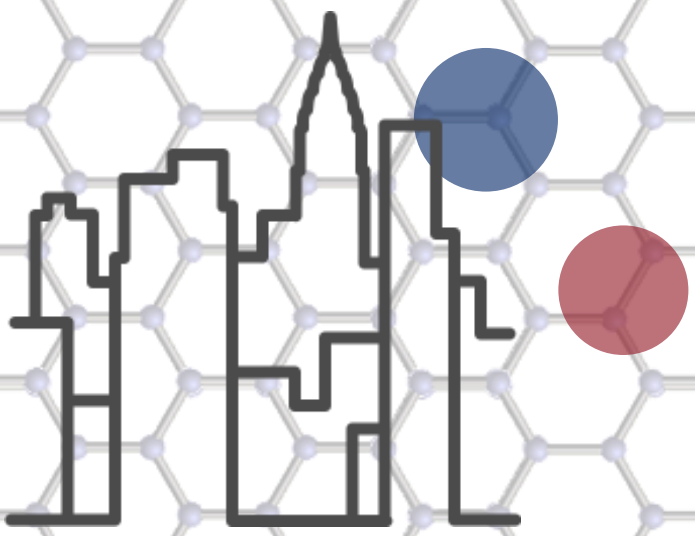
Graphene and the Analog Landscape

Graphene has been around since 2004, yet the path to integration with standard semiconductor flow stays elusive. This talk will cover the potential for graphene in a predominantly analog company like TI, attempts towards integration and issues faced in the process.



ORAL CONTRIBUTIONS

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Using Novel Properties of Graphene for Designing Efficient Infrared Photodetectors

Graphene has unique electronic and optical properties that makes it suitable for use in optoelectronic devices such as photodetectors. A high carrier mobility exhibited by graphene allows it to be used for building efficient high-speed charge carrier collector. Graphene also shows highly controllable charge transport properties that can be leveraged for dynamic control of electrical characteristics in a device. Ultrafast carrier multiplication has also been observed in monolayer and bilayer graphene recently [1]. Using these novel features of graphene, we propose two designs of photodetectors where graphene is coupled with standard photosensitive materials, which can form the starting points for a new generation of high performance photodetectors. We propose a graphene-PbSe infrared photodetector, structure shown in Fig. 1(a), that can be operated in three different modes (schematic shown in Fig. 1(b)): a) high mobility collector, b) controllable Schottky barrier based photo-rectifier, and c) Graphene PhotoFET [2]. These different operating modes depend on the insulator material thickness that is inserted between the graphene-PbSe interface during device fabrication. We also propose a novel bilayer graphene|CdTe|HgCdTe photodetector whose schematic is shown in Fig. 1(c). This design uses photon-trapping micro-holes [3] and the carrier multiplication in graphene (schematic illustration shown in Fig. 1(d)) to increase the efficiency of photon absorption for higher performance. Using first-principles based calculations and semi-analytical models we demonstrate the feasibility and superiority of these detector designs. Using these designs the dark current can be decreased by an order of magnitude while the photo current can be increased by a few orders in comparison to standard photodetectors.

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Figures

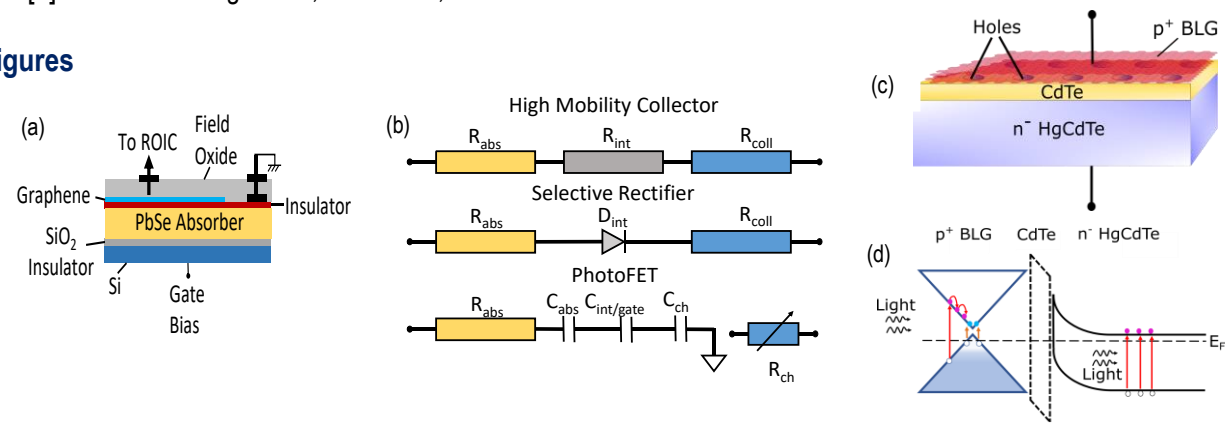

Figure 1: (a) schematic of graphene-PbSe photodetector, **(b)** circuit schematic of different operation modes of graphene-PbSe photodetector, **(c)** bilayer graphene|CdTe|HgCdTe photodetector with micro-holes, and **(d)** band diagram of the bilayer graphene|CdTe|HgCdTe photodetector demonstrating carrier multiplication process and light absorption regions.

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Gate-tunable spin anisotropy in graphene – WS_2 heterostructures at room temperature

When graphene is in proximity to a transition metal dichalcogenide (TMDC), it acquires an enhanced spin orbit interaction (SOI) together with a complex spin texture with out-of-plane and winding in-plane components [1]. Among the relevant consequences of this unique type of SOI, we have unambiguously demonstrated spin to charge (StC) conversion in graphene by proximity of WS_2 at room temperature with high electrical tunability [2]. Notably, StC conversion is accompanied by anisotropic spin dynamics with spin lifetimes that vary orders of magnitude depending on the spin orientation [2]. Such anisotropic features indicate that the strong spin–valley coupling in the TMD is imprinted in the heterostructure and felt by the propagating spins [3].

In this talk, I will present an unprecedented electric-field tunability of the spin dynamics in graphene-WS_2 heterostructures at room temperature. The characteristic spin relaxation varies from highly anisotropic to nearly isotropic when the applied displacement field *D* changes from 0.5 V/nm to -0.5 V/nm (Figure 1) [4]. This finding is unexpected and may indicate the presence of defects or impurities as responsible for the SOI enhancement.

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Figures

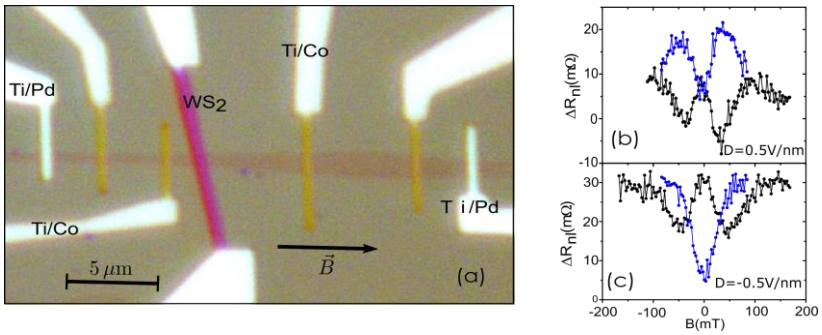

Figure 1: Figure 1: (a) Optical image of a typical spin device, which includes a graphene – WS2 device and two reference pristine graphene devices enclosing it. (b), (c) spin precession response in the graphene–WS2 device for parallel (black) and antiparallel (blue) configuration of the spin injector and detector with in-plane ***B***. (b) For *D* = 0.5 V/nm the maximum (minimum) signal is observed around *B* = 50 mT, which indicates that the out-of-plane spin lifetime is much larger than the in-plane one. (c) For *D* =-0.5 V/nm the maximum (minimum) spin signal is obtained at *B* = 0, a consequence of the nearly isotropic spin relaxation (see [3]).

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Large Scale LiC_6 for Electronic Applications

Electronic devices operating at GHz frequencies have rapidly become an integral component of modern technology. As their applications continue to develop, electromagnetic interference could severely degrade performance. In this work, we explore the use of LiC6, a graphite intercalation compound used in battery technology, as a shielding material for prevention of electromagnetic interference. LiC6 exhibits metallic behaviour at room temperature with high reflectivity in the microwave regime and reasonable optical transparency in the visible spectrum [1]. We present preliminary results on the fabrication and characterization of large-scale, stable LiC6 films.

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Tools for precise shaping and non-invasive contacting of 2D materials

NanoFrazor (thermal scanning probe) lithography has recently entered the market as the first true alternative to electron beam lithography (EBL) [1]. Core of the technology is a heatable probe tip that is used for both patterning and simultaneous inspection of complex nanostructures. The heated tip can pattern very high-resolution (< 10 nm half-pitch) nanostructures by locally evaporating resist materials. The structures are inspected by the cold tip in parallel with the patterning process, enabling stitching and markerless overlay with sub-5 nm accuracy [2]. The technique is compatible with all the common pattern transfer processes [3,4,5].

Shaping 2D materials into narrow ribbons, Hall bars etc. is often required in order to study their properties. Another challenge is formation of high-quality electrical contacts on them. Predominant fabrication process - i.e. EBL followed by etching or lift-off of metal – has its resolution limited by proximity effects, may require complex overlay procedures and typically yields poor quality non-ohmic metal contacts with high Schottky barriers and large contact resistances [6]. Here, we show that NanoFrazor lithography can be used for shaping 2D materials with very high precision (Figure 1a-b) [7] and for forming high-quality metal contact electrodes on them (Figures 1 c–d) [5]. The fabricated devices exhibit vanishing Schottky barrier heights (around 0 meV, Figure 1d), record-high on/off ratios of 10^{10}, no hysteresis, and subthreshold swings as low as 64 mV per decade.

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Figures

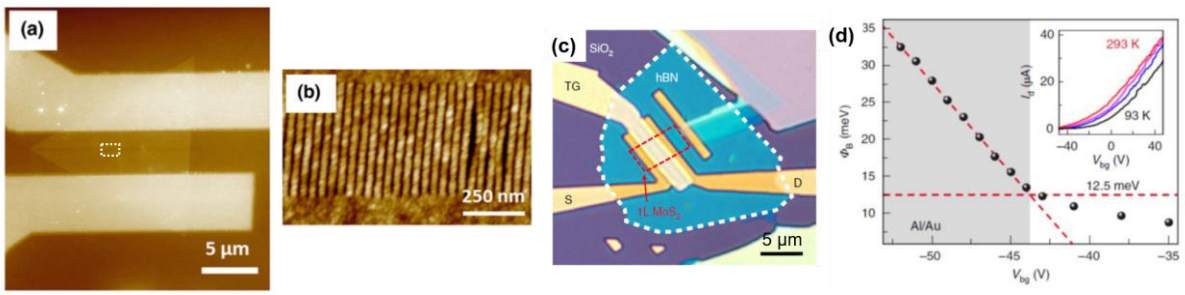

Figure 1: (a) AFM image of 18-nm half-pitch 1L MoS_2 nanoribbon array patterned along the zigzag direction. (b) A close-up of the region marked with a white dashed box in (a). Figures (a) and (b) from Ref [7]. (c) Optical image of a 1L MoS_2 FET with a h-BN gate dielectric where the source, drain and top-gate electrodes have been patterned with a NanoFrazor. (d) Gate voltage dependence of Schottky barrier height of a 1L MoS_2 FET with Al/Au contacts (V_{ds} = 2 V). The deviation from the linear response at low V_{bg} (dashed red line) defines the flat band voltage and the SBH. Inset, corresponding temperature-dependent transfer curves (V_{ds} = 2 V). Figures (c) and (d) from Ref. [5].

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Mass production of CVD graphene, reliable transfer, and co-integration with TMDs

Although graphene has been maturing in university laboratories for over 15 years, further research effort is still required to implement graphene in real-world applications. Besides the great progress made so far, there remains grand challenges on the way to the industrial manufacturing of 2D materials-based electronic and optoelectronic devices. These challenges include (i) the large-scale cost-effective production of ''electronic grade'' graphene, (ii) the development of a non-destructive, clean, reliable and scalable transfer method, and (iii) the co-integration of graphene with other 2D materials. This talk presents the latest developments in our laboratory to facilitate the transition of graphene from academia to functional technologies.

First, we show how the chemical vapor deposition (CVD) method can offer flat, highly crystalline, single-layer graphene with a high throughput. The mass production is achieved by using a series of closely-packed vertically-standing 3-inch wafers coated with a thin Cu film [1]. Thin Cu films evaporated on C-plane sapphire substrates provide a flat and smooth template for the synthesis of graphene and mitigate the formation of wrinkles and cracks [2].

Then, we present how the catalytic substrate surface morphology influences the reliability of the transfer process and graphene physical properties once transferred on a device compatible substrate. We demonstrate that regardless of the selected transfer approach, the Cu template morphology is one of the major sources for the formation of tears and wrinkles as well as non-uniform electrostatic doping and mechanical strain in the transferred graphene sheet [3].

Finally, we present experimental data regarding the formation of 2D heterostructures by direct MOCVD growth of WSe_2 on graphene [4]. Our results reveal that triangular WSe_2 crystals (with a lateral size exceeding 1 micrometer) exhibit an in-plane orientation matching with the underlying graphene. The WSe_2 seeding density is also found to depend on the number and the stacking order of the underlying graphene layers.

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Kinetic Ionic Permeation and Interfacial Doping of Supported Graphene

Due to its outstanding electrical properties and chemical stability, graphene finds widespread use in various electrochemical applications. Although the presence of electrolytes strongly affects its electrical conductivity, the underlying mechanism has remained elusive. Here, we employ terahertz spectroscopy as a contact-free means to investigate the impact of ubiquitous cations (Li^+, Na^+, K^+, and Ca^{2+}) in aqueous solution on the electronic properties of SiO_2-supported graphene. We find that, without applying any external potential, cations can shift the Fermi energy of initially hole-doped graphene by ~200 meV up to the Dirac point, thus counteracting the initial substrate-induced hole doping. Remarkably, the cation concentration and cation hydration complex size determine the kinetics and magnitude of this shift in the Fermi level. Combined with theoretical calculations, we show that the ion-induced Fermi level shift of graphene involves cationic permeation through graphene. The interfacial cations located between graphene and SiO_2 electrostatically counteract the substrate-induced hole doping effect in graphene. These insights are crucial for graphene device processing and further developing graphene as an ion-sensing material.

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Figures

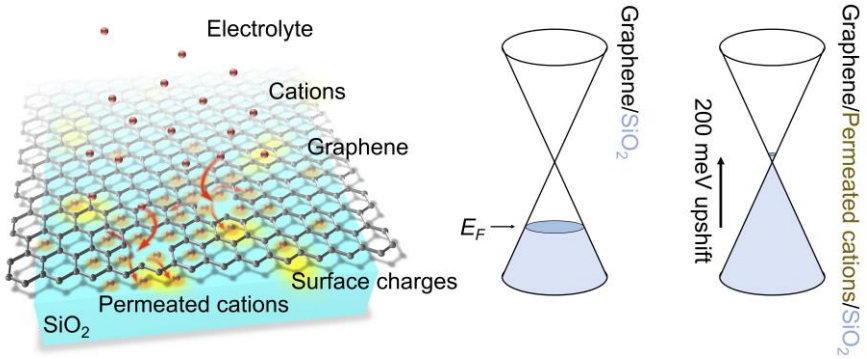

Figure 1: Illustration of cation permeation through the graphene sheet to the graphene-SiO_2 interface. Graphene is initially hole-doped due to the presence of negative surface charges (indicated in yellow) on the SiO_2 surface. Intercalated cations lead to a shift of the Fermi level of graphene toward the Dirac point.

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First-Principles Study of 2D Materials for Photochemical/Electrochemical Applications

Based on first-principles calculation, we show that a non-Janus MoSSe/WSSe heterobilayer can be much more advantageous than Janus heterobilayer for the photocatalytic reduction of CO_2 to CO or HCOOH due to the absence of vertical polarization.[1] Also will be described is a series of recent collaborations with a sophiscated experimental group for photocatalytic/electrocatalytic water splitting and CO_2 reduction on 2D materials. First, combined experimental and theoretical effort is described for efficient photoelectrochemical water splitting of *p*-GeAs/*n*-Si and *p*-GeP/*n*-Si heterojunctions based on the band edge positions obtained from band structure calculation.[2,3] Second, our calculation on the activation barrier of Volmer-Heyrovsky reaction gives deep insight into our experimental results, which have shown that the 1T'-phase guest-intercalated MoS_2/WS_2 nanosheets synthesized by one-step hydrothermal reaction exhibit excellent catalytic activity toward hydrogen evolution reaction (HER).[4-6] Third, another calculation on the Gibbs free energy along the reaction path for Se-rich $MoSe_2$ and Ru,Co-coped MoS_2 also lead us to understand their chemical structures as well as their excellent catalytic activity toward the HER and CO_2 reduction under both acidic and basic conditions.[7,8]

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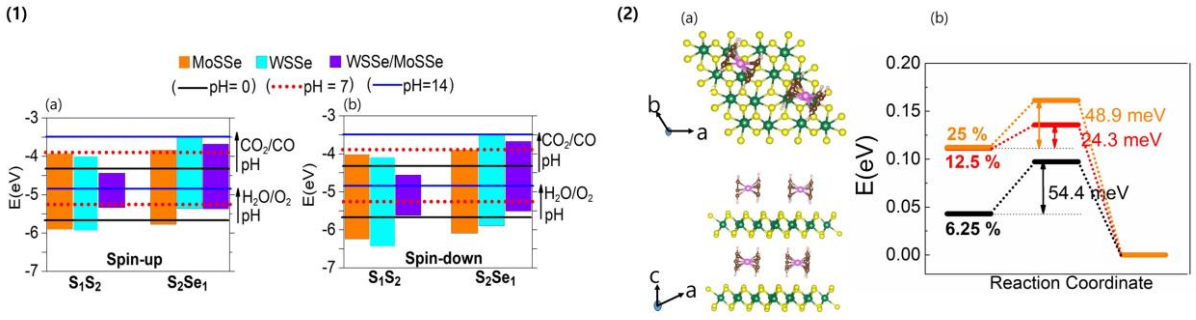

Figure 1: (a) Spin-up and (b) spin-down components of the band edge positions of the MoSSe and WSSe monolayers as well as those of the WSSe/MoSSe heterobilayer in non-Janus (S_2Se_1) and Janus (S_1S_2) configurations.
Figure 2: (a) Structure of 1T' phase (4×4) $2WS_2$-$CoCp_2$-4 (at 12.5%) in top and side views, where $CoCp_2$ is cobaltocene. (b) Comparison of the activation barrier of Heyrovsky reaction at various concentration of $CoCp_2$.

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Engineering valley coherence in van der Waals heterostructures

Abstract:

Of particular interest recently is the exciton in two dimensional transition metal dichalcogenides (TMDCs). In these systems, the exciton has been shown to have a large binding energy on the order of hundreds of meV. Interestingly, electronic bandstructure of monolayer TMDCs consists of two inequivalent yet degenerate valleys (K and K') in $k-$space for which the optical selection rule is sensitive to the helicity ($\sigma_{\pm}$) of the exciting photon. This selection rule is inherited by excitons associated with these two valleys when Coulomb interaction is taken into account. There have been several proposals to use this ``valley degree of freedom" for the development of optoelectronic devices analogous to those in the field of spintronics.

In order to harness this valley degree of freedom in TMDCs, it is important to be able to actively control the coherence between excitons in the two valleys. In this work, we demonstrate how this valley coherence can be achieved by creating a heterostructure of the TMDC with other two dimensional materials. In this talk I will discuss some general results on exploring the parameter space of optical conductivity tensor of such a heterostructure which will lead to the highest values of valley coherence and coherence times. This analysis will help the community in designing the appropriate 2D heterostructures with the optimal optical conductivity tensor for maximum valley coherence. Subsequently we will present our recent results on applying this technique to show tunability of the coherence using certain commonly available 2D semiconductor heterostructures.

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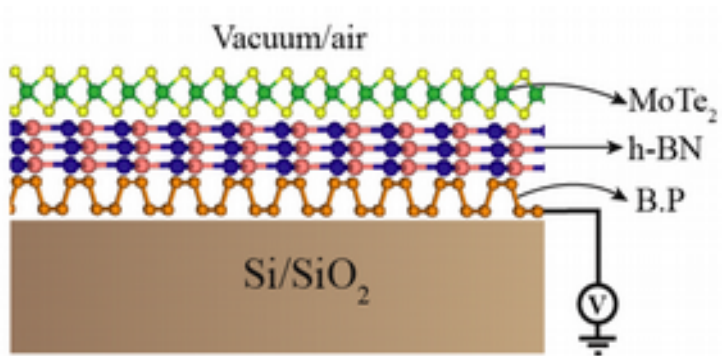

Figure 1: Schematic of the proposed device for achieving valley coherence

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Elasticity Measurements of Ultra-hard, Ultra-stiff Graphene Films via Atomic Force Microscopy Modulated Å-Indentation

The ability to characterize and manipulate materials down to the atomic scale for tuning their mechanical and physical properties is the cornerstone of material science. Here we explore the elastic properties of supported 2D graphene films by the use of modulated Å-Indentation, a novel Atomic Force Microscopy (AFM)-based technique capable of achieving sub-Å indentation depths during force-indentation measurements. In conventional nanoindentation experiments, the indentation depths are usually in the order of units of nanometers, which hinder the possibility of studying ultra-thin films (<10 nm) and atomically thin 2D materials supported on substrates. By using extremely small amplitude oscillations (<<1 Å) at high frequency, achievable by combining a commercially available lock-in amplifier and AFM, we show how Å-Indentation enables non-destructive local accurate measurements of the contact stiffness and out-of-plane elastic moduli of ultra-thin ultra-stiff films, including CVD diamond films (thus even up to TPa range stiffness), as well as the transverse moduli of supported graphene and other 2D materials (<1 nm thickness). Å-Indentation thus obtains in-situ indentation curves combining superior resolution and indentation depths as small as 0.3 Å (Fig.1) with AFM nanoscale topographical imaging. Thanks to this technique, we experimentally demonstrate that at room temperature and under localized indentation pressure, a single layer of graphene on top of a carbon interface layer (buffer layer), both epitaxially grown on the Si-face of a SiC(0001) substrate, exhibits transverse stiffness superior to that of CVD bulk diamond (Fig.1). Backed by density functional theory (DFT) calculations, these results indicate that the 1+buffer layer graphene film undergoes a pressure-induced phase transformation to a new ultra-stiff, ultra-hard diamond structure, named *diamene*, followed by a sp^2-to-sp^3 chemical bond transitions. Furthermore, we find that the formation of ultra-stiff *diamene* is exclusive of 1-layer epitaxial graphene plus buffer layer films grown on SiC(0001), and it is not observed in the buffer layer alone, nor in thicker epitaxial graphene (2-layer or more – see Fig.1), nor in exfoliated graphene films of any thickness on SiO_2 substrate. Extending the capabilities of the Å-indentation technique to the analysis of other 2D materials, our ongoing studies explore the possibility of similar pressure-induced phase transition in hexagonal boron nitride (h-BN). Recent experiments demonstrate that 2-layer h-BN flakes, mechanically exfoliated on SiO_2 substrate, consistently exhibit a transverse elastic modulus almost two times larger than that of the bare substrate. This stiffening effect thus appears to be related to the conversion of h-BN to cubic BN (c-BN) induced by the pressure applied through the indenter.

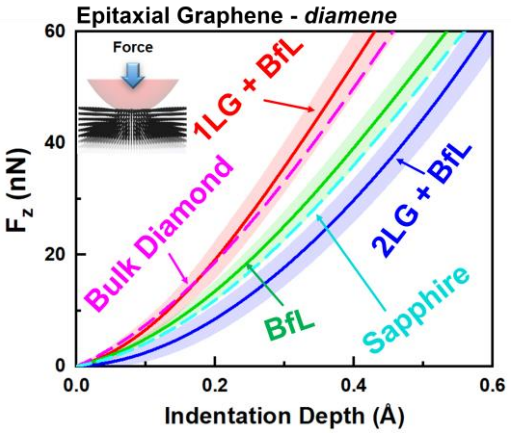

Figure 1: Experimental force vs indentation curves showing that *diamene* (1-layer graphene + buffer layer) exhibits stiffness larger than CVD bulk diamond. The ultra-high stiffening effect is not obserbved for 2-layer graphene + buffer layer.

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Functionalization of graphene

Different ways of functionalization in graphene have been explored. This includes, deposition of atoms or molecules, intercalation, substitutional doping, creation of intrinsic defects and several others. In this talk, I will present a brief overview of different approaches we have used to modify the electronic properties of graphene such as nanostructuration of graphene into graphene nanoribbons [1], preparing a well ordered buffer layer graphene [2,3], introducing a superperiodic potential by growing graphene on a vicinal noble metal substrates [4].

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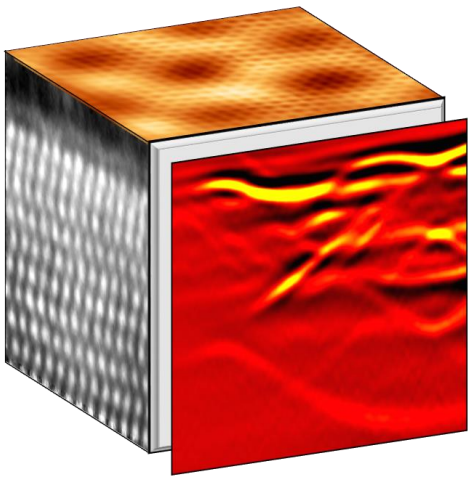

Figure 1: ARPES, STM and scanning transmission electron microscopic view of buffer layer graphene

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Atypical quantized resistances in millimeter-scale epitaxial graphene *p-n* junctions

We have demonstrated the millimeter-scale fabrication of monolayer epitaxial graphene *p-n* junction devices using simple ultraviolet photolithography [1], thereby significantly reducing device processing time compared to that of electron beam lithography typically used for obtaining sharp junctions. This work presents measurements yielding nonconventional, fractional multiples of the typical quantized Hall resistance at v = 2 ($R_H \approx 12906\ \Omega$) that take the form: $a/b*R_H$. Here, *a* and *b* have been observed to take on values such 1, 2, 3, and 5 to form various coefficients of R_H. Additionally, we provide a framework for exploring future device configurations using the LTspice circuit simulator as a guide to understand the abundance of available fractions one may be able to measure. These results support the potential for simplifying device processing time and may possibly be used for other two-dimensional materials.

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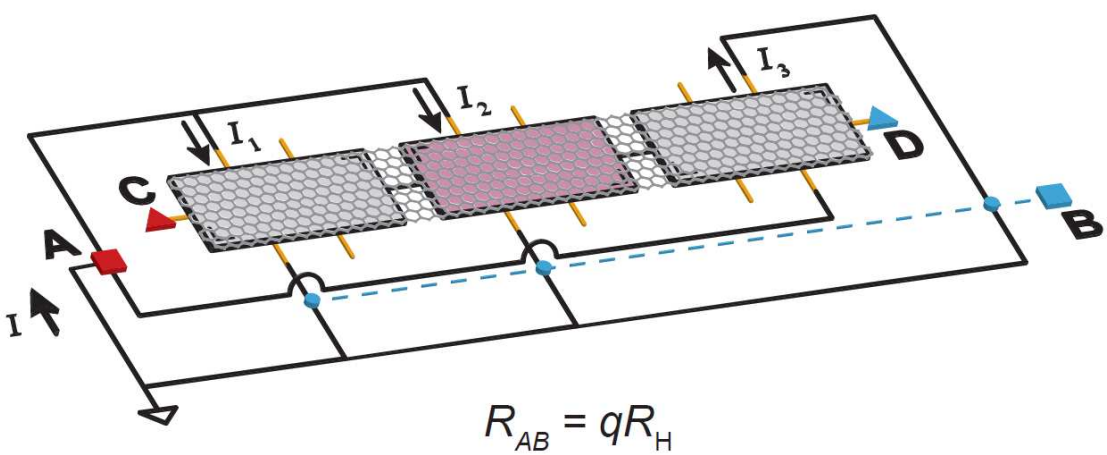

Figure 1: An illustration of the circuit model implemented by the spice circuit simulator is shown. A total current (*I*) of 1 μA is used and split among up to three distinct injection points on the device, shown as I_1, I_2, and I_3. Though only one example is shown here, the measured resistances of several different configurations of current injection yield nonconventional multiples of R_H.

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Optimal transport and colossal ionic mechano-conductance in graphene crown ethers

Directly interrogating the mechanism of ion transport in sub-nanoscale pores is challenging as several processes contribute to ion translocation: van der Waal repulsion, dehydration, electrostatic interactions, structural fluctuations, etc. Biological ion channels, for example, balance electrostatic and dehydration effects to yield large ion selectivity alongside high transport rates. These macromolecular systems are often interrogated through point mutations of their pore domain, limiting the scope of mechanistic studies. In contrast, using all-atom molecular dynamics simulations, we demonstrate that graphene crown ether pores afford a simple platform to directly investigate optimal ion transport conditions, i.e., maximum current densities and selectivity. We show that small pore strains (1%) give rise to a colossal (100%) change in conductance. This process is electromechanically tunable, with optimal transport in a primarily diffusive regime, tending toward barrierless transport, as opposed to a knock-on mechanism. These observations suggest a novel setup for nanofluidic devices while giving insight into the physical foundation of evolutionarily optimized ion transport in biological pores.

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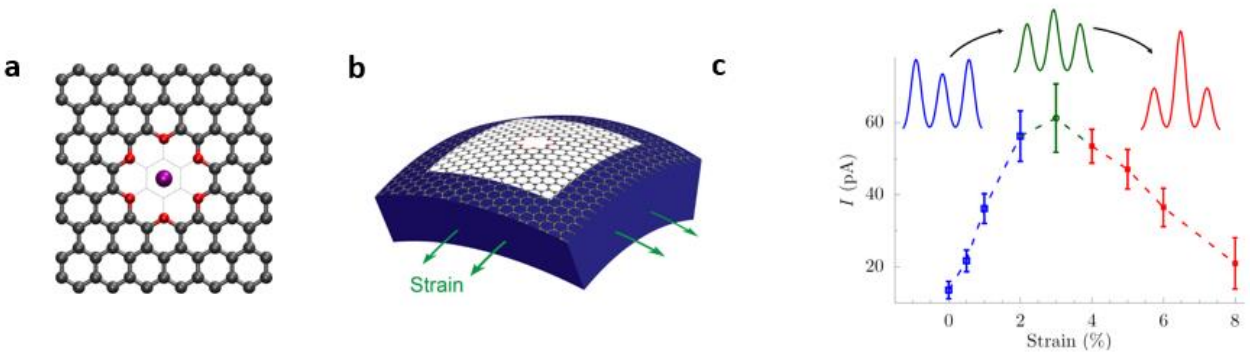

Figure 1: Optimal transport in graphene crown ether pore. a) K^+ ion (purple) in an 18-crown-6 pore embedded in graphene. b) Schematics of potential experimental setup. c) MD results of current versus strain, showing a colossal rise in the current at small strains, optimal transport around 3 % strain, and subsequent drop in the current at large strain. The insets show the schematics of the free-energy profile in each regime.

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Plasmons in 1D Periodic Graphene Structures: S-Matrix Retrieving and T-Matrix Model Verification

We present a comprehensive study of graphene plasmon eigenmodes in 1D periodic structures formed by plasmonic junctions of different types. Transmission and reflection coefficients composing scattering matrix of a junction are obtained directly from numerical solutions of equations describing the plasmons in the considered structures. The obtained results for the single junctions are in perfect agreement with analytical formulas for the cases when they are available. Using our method as a reference, we analyze the limitations of the semi-phenomenological transfer matrix approach applied to the calculation of reflection from the double-junction structures. Our results can be useful in designing and calculating graphene plasmon resonators, waveguides, switches, etc.

Figures

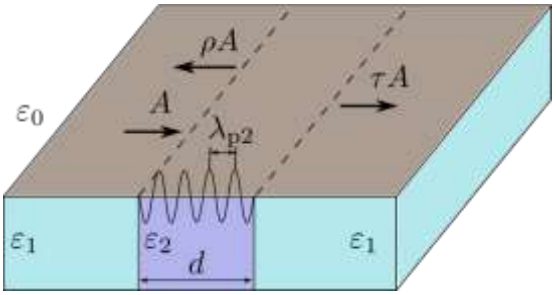

Figure 1: Schematic view of the graphene plasmon double-junction supported by a wafer with discontinuously changed dielectric permittivity.

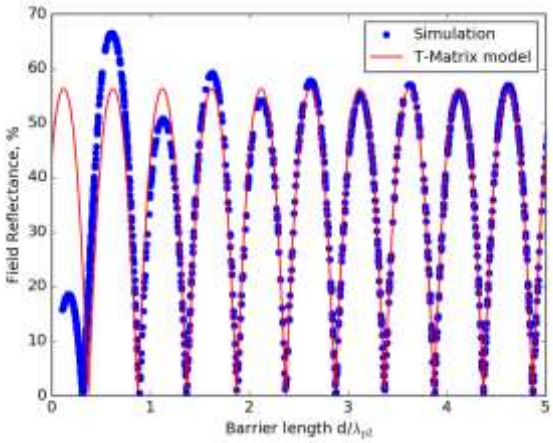

Figure 2: Absolute value of the reflection coefficient of a plasmon in graphene scattered on a barrier formed by the two junctions versus its normalized length. Solid line shows the reflectance predicted by a transfer matrix model, and circles are calculated with our numerical analysis.

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Dry Transfer of van der Waals Crystals for Nanoscale Characterization of Buried Interfaces

The synthesis and characterization of two dimensional (2D) transition metal dichalcogenides have attracted much attention in recent years due to their potential optoelectronic applications. However, due to the fact that they are synthesized mostly on insulating substrates, their characterization at a fundamental level has not been straightforward for as-grown crystals. Usually, they are transferred to noble metal substrates such as gold through exfoliation or polymer-assisted transfer, but these methods suffer from contamination of the crystal surface. Here, we present a simple method for clean, dry, and residue-free transfer of CVD-grown crystals to gold, which allows for easy and comprehensive nanoscale surface characterization using techniques such as Scanning Probe Microscopy (SPM) and Raman spectroscopy [1]. In particular, the combination of the two techniques enable tip-enhanced Raman scattering (TERS), leading to nanoscale Raman mapping at spatial resolutions better than 20 nm. Further, scanning Kelvin probe microscopy allowed for high resolution imaging of the surface potential, which provided key insights on the charge transfer between the crystals and the noble metal substrate. Thus, the transfer procedure demonstrated here is expected to enable robust optical and electronic characterization of a variety of different 2D materials. This is expected to be of particular importance in understanding metal contacts as well as buried interfaces in engineering devices based on 2D materials.

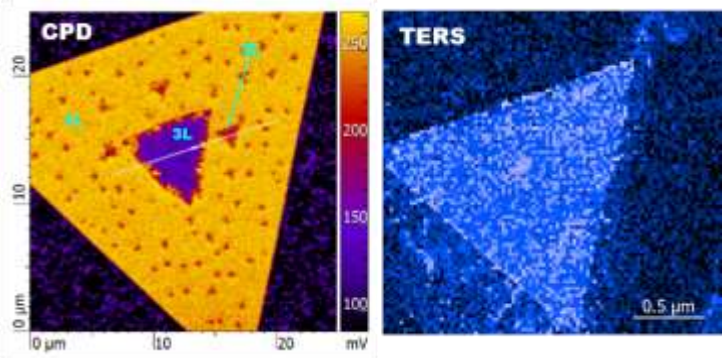

Figure 1: Scanning Kelvin Probe image (left) showing contact potential difference (CPD) and TERS image (right) of the 2-layer part (2L), measured from the buried layer of a CVD-grown WSe_2 crystal transferred to gold.[1]

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International Interlaboratory Comparison of Raman Spectroscopy for CVD-grown Graphene

There is an urgent requirement for reliable, reproducible, accurate and consistent measurements of Graphene to enable this growing industry, which is now producing large-scale quantities of material. To this end, several measurement standards are underdevelopment within the Nanotechnologies committees of ISO and IEC. To develop high quality international standards, protocols must be developed and verified, with the associated uncertainties determined.

Towards this effort, we report the procedure and the initial results of a VAMAS interlaboratory study conducted under TWA 41 Project 1 (Graphene and Related 2D Materials) for Raman spectroscopy of chemical vapour deposition (CVD) grown graphene. This project will directly support the development of the ISO/IEC standard "*PWI 21356-2 - Nanotechnologies - Structural Characterisation of CVD-grown Graphene*". This interlaboratory study gathered data from 15 participants across academia, industry (including instrument manufacturers) and National laboratories. This study investigates the measurement uncertainty contributions of both instrumentation and data analysis, with all the participants performing measurements on a commercially-supplied CVD-grown graphene sample using the same measurement protocol.

By comparing reported Raman metrics with the measurements of the same regions made by the lead participant, variations in the reported peak intensity ratios and peak fits could be explored. While many of the reported measurements were relatively consistent, significant and meaningful outliers were observed due to differences in both the instrumentation and data analysis. These variations ultimately resulted in inconsistent reports of the coverage of single layer graphene and must be understood to provide reproducible and comparable measurements for the growing graphene industry worldwide.

Figures

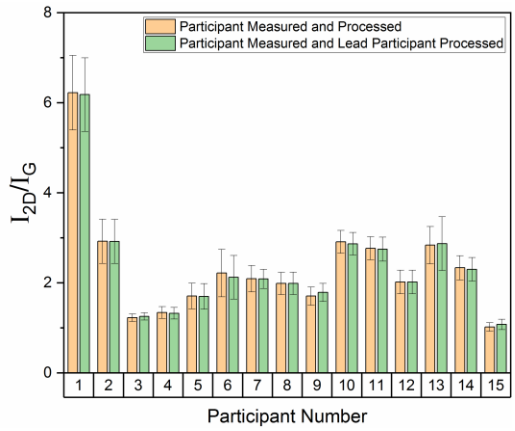

Figure 1: I_{2D}/I_G Raman peak intensity ratios reported by the VAMAS participants. Differences in peak intensity ratios due to the data analysis being performed by the participants (green) and one lead user (orange) are also shown.

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Soliton signature in the phonon spectrum of twisted bilayer graphene

The discovery of unconventional superconductivity in slightly-misaligned bilayer graphene [1] has triggered an important enthusiasm from the scientific community. While the electronic properties of such a system have already been carefully examined by the means of the theoretical approaches, its vibrational properties have yet to be fully-explored. In this work, we investigate the phonons for a set of 692 twisted bilayer graphene structures, combining force field and an unfolding scheme in order to unravel the numerous phonon modes of the considered systems. The emergence of phonon side bands at the high-symmetry points of the graphene Brillouin zone is highlighted, especially for small mislignement angles between the layers. Those side bands are rationnalized with the introduction of the Nearly-Free Phonon Model, which can be understood as the counterpart for phonons of the Nearly-Free Electron model [2], where the electrons and the nucleus potential have been respectively replaced by the phonons and the soliton network potential.

References

[1] Y. Cao, V. Fatemi *et al.*, Nature **556** (2018)
[2] K. M. Rabe, Physics Today **55**, (2002) 61

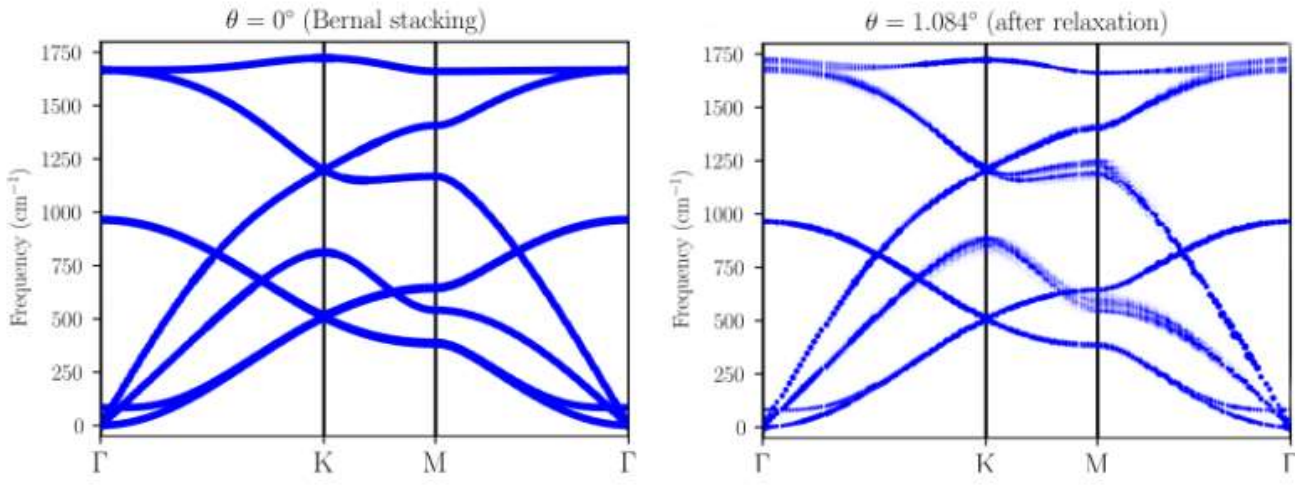

Figure 1: phonon band structure of (left) aligned bilayer graphene and of slightly-misaligned bilayer graphene (unfolded on the Brillouin zone of the graphene bottom layer). Side bands emerge at the high-symmetry points of the Brillouin zone.