Abstract Book

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'From physics of graphene to graphene for physics'

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Graphene-based heterostructures

Kostya Novoselov

The physics of a vacancy in the graphene lattice

Eva Y. Andrei
Rutgers University

Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries and to the promise of important applications. I will discuss new and surprising phenomena that emerge when the perfect honeycomb lattice of graphene is disrupted by single atom vacancies as revealed by scanning tunneling microscopy and spectroscopy. These include i) the ability to charge the vacancy site into the supercritical regime where atomic collapse leads to the formation of an artificial atom[1]; ii) the the appearance of a local magnetic moment at the vacancy site and its Kondo screening.

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Graphene for Metrology

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Metrology guarantees the worldwide uniformity of all measurements and most countries have accepted the SI system (International System of Units) as the basis for accurate measurements. Four base units (meter, second, kilogram and Ampere) fix all units in mechanics and electricity. Surprisingly, quantum phenomena in super- and semiconductors (Josephson and quantum Hall effect) are the driving forces for a revolutionary change of our SI system expected for 2018. Magneto transport measurements on graphene play an important role in this development, not only for electrical standards but also for the kilogram.

Already the first graphene publication in 2004 [1] demonstrated the observation of the quantum Hall effect in this nearly ideal two-dimensional system. The outstanding electronic properties of this material (high mobility, large cyclotron gaps at relatively small magnetic fields, extremely wide quantum Hall plateaus for graphene on SiC with efficient thermal contact to the substrate) qualifies this material as the preferred quantized Hall resistance standard if the stability and reproducibility of the devices can be guaranteed. A first prototype for a compact table-top turnkey system has been presented for industrial application.

The presentation will summarize the expected changes in our international system of units where quantum standards and especially graphene play a crucial role for the realization of a new SI system based on fundamental constants [2].

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WEDNESDAY 6 SEPTEMBER
Andrea Ferrari

Light Scattering and Emission from Hetero-structures

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Heterostructures based on layers of atomic crystals have a number of properties often unique and very different from those of their individual constituents and of their three dimensional counterparts. The combinations of such crystals in stacks can be used to design the functionalities of such heterostructures. I will show how Raman spectroscopy can be used to fingerprint such heterosctructures, and how these can be exploited in novel light emitting devices, such as single photon emitters, and tuneable light emitting diodes.

Ballistic transport and Aharonov-Bohm interference in graphene

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The recent technological advances in encapsulating graphene by hexagonal boron nitride forming artificial van-der-Waals heterostructures allows the fabrication of graphene devices with unique electronic properties. Outstanding charge carrier mobilities and mean free paths with more than 25 micrometer are now accessible making this material stack interesting for studying ballistic transport. By further structuring the graphene-hBN based heterostructures mesoscopic devices can be fabricated on which phase coherent ballistic quantum transport can be studied.

Here, I will present low-temperature magneto-transport measurements on both (i) graphene quantum point contacts and (ii) high mobility graphene rings encapsulated in hexagonal boron nitride. Our experiments allow to extract information on quantized conductance, renormalized Fermi velocities close to the charge neutrality point as well as the co-existence of weak localization, Aharonov-Bohm (AB) oscillations and universal conductance fluctuations in graphene rings. In particular, I show signatures of magnetic focusing effects at small magnetic fields confirming ballistic transport in mesoscopic graphene devices and I report on the observation of the AB conductance oscillations in the quantum Hall regime at reasonable high magnetic fields, where we find regions with enhanced AB oscillation visibility with values up to 0.7%. These oscillations are well explained by taking disorder into account allowing for a coexistence of hard and soft-wall confinement.

Topological defects and topological electronic phases in 2D materials

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Grain boundaries and dislocations are intrinsic topological defects of all polycrystalline materials, including the two-dimensional materials such as graphene and monolayer transition metal dichalcogenides (TMDs) [1]. In my talk, I will discuss the structure of topological defects and their effect on the charge-carrier transport with a focus on ballistic transmission across periodic grain boundaries. In graphene such regular defects are predicted to give rise to tuneable transport gaps [2] and valley-polarized charge carriers [3,4]. Strong spin-orbit interactions in monolayer TMDs further allow producing spin-polarized charge carriers upon transmission across line defects [5]. In the final part of my talk, I will cover some recent results on the 1T'-phase monolayer dichalcogenides of Mo and W that were predicted to host the topological quantum spin Hall (QSH) phase [6]. In particular, I will discuss the robustness of QSH phase [7] as well as the properties and experimental signatures of one-dimensional topological states at the edges and interfaces of 1T'-phase monolayer TMDs [8].

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Quantum devices in 2D materials

Klaus Ensslin

2D crystals are ideal systems for the realization of strongly confined quantum structures. Many experiments have focused on etched graphene quantum devices because of the missing band. Most devices were dominated by localized states along the graphene edges, which are difficult to control on the atomic scale.

In this talk I will present two solutions to this problem. In bilayer graphene a bandgap arises for vertical electric fields. We demonstrate that a split-gate arrangement can be used to define a narrow 1D ballistic channel. An additional well positioned top gate allows to pinch off the channel. Furthermore a series of plateau-like features occurs when the channel is opened. An interesting level scheme arises in particular for high magnetic fields.

Another approach is based on MoS2 encapsulated between layers of BN to obtain best electronic quality. At low magnetic fields we observe a degeneracy of 6, which is explained by the 3-fold valley degeneracy in the conduction band of MoS2 plus a factor of 2 for spin-degeneracy. In a quantum point contact again conductance pinch-off and quantization is observed. 2D materials have improved to an extent, that novel electronic quantum devices can be realized with great promise.

Higher-than-ballistic conduction in viscous flows of electrons

Leonid Levitov

Valley-momentum locking in a graphene superlattice with Y-shaped Kekulé bond texture

Carlo Beenakker, Instituut-Lorentz, Leiden University

Recent experiments on a graphene-copper superlattice have revealed an unusual Kekulé bond texture in the honeycomb lattice — a Y-shaped modulation of weak and strong bonds with a wave vector connecting two Dirac points. We show that this socalled "Kek-Y" texture produces two species of massless Dirac fermions, with valley isospin locked parallel or antiparallel to the direction of motion. In a magnetic field B the valley degeneracy of the B-dependent Landau levels is removed by the valley-momentum locking — but a B-independent and valley-degenerate zero-mode remains.

Dirac Fermions in confined geometry

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We describe here our recent theoretical work on Dirac and massive Dirac Fermions in confined geometry - in quantum dots in 2D crystals. The goal is to both understand the role of e-e interactions and design nanostructures with the three functionalities of a quantum circuit: electronics, photonics and spintronics, in a single material and at the nanoscale[1]. The design tools include size, shape, type of edge, sublattice symmetry, topology, number of layers and carrier density in graphene quantum dots [1-9]. In particular, size engineering leads to optical gaps from THz to UV, shape engineering leads to a degenerate exciton spectrum allowing for the generation of entangled photon pairs via XX-X cascade[7,8] and sublattice engineering allows design of magnetic moments tunable with voltage and light. Geometry and e-e interactions allow for the integration of topologically protected states of matter into carbononics[9,10]. Experiments on colloidal graphene quantum dots [6-8] as well as massive Dirac Fermions in bilayer graphene qdots and 2D crystals of transition metal dichalcogenite [11-13] will be discussed.

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Electron and phonon confinement in graphene nanoribbons

Vincent Meunier

In this talk I will review the effect of quantum confinement on the electronic and vibrational properties of one-dimensional carbon nanoribbons. The talk will present research conducted at the interface between theory and experiment where a combination of disciplines is found to lead to an atomistic understanding of measurable properties of low-dimensional structures.[1-3] Inspired by the recently developed capability of assembling nanostructures from the bottom up with atomic precision, the field devoted to the detailed understanding of the physics of carbon nanostructures is poised to offer an unprecedented test-bed for predictions of quantum confinement. In particular, the emergence of magnetic states, tunable electronic properties, vibrational (and thermal) properties is now being exploited as a real possibility to develop carbon-based devices of the future, with higher density of information and processing power. I will use specific examples to illustrate that as we venture into a new regime of material science research where the position of each atom is known precisely, theoretical description is found to face new challenges that are not apparent in defective materials.

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Spin-orbit-coupling and topology in 2D: topological insulators, interfacial skyrmions, graphene and TMD

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The recent years have seen the emergence of unprecedented phenomena and novel properties induced in 2D-electronic systems by spin-orbit coupling (SOC), symmetry breaking and topology effects. First example, the 2D electronic states at the surfaces/interfaces of topological insulators or at Rashba interfaces present a locking between spin and momentum that permits an efficient conversion between spin and charge currents of real potential for spintronic devices. Equally the chiral spin interactions induced by SOC and symmetry breaking at the interface between magnetic and heavy metals can be used to generate topologically protected magnetic solitons that are called skyrmions and at the base of several types of devices.

Can such interesting properties of 2D systems be also obtained by introducing SOC into graphene?

After a review of the interesting properties of topological insulators, Rashba interfaces and skyrmionic systems, I will present recent advances on SOC effects induced into graphene by proximity with another material: spectroscopic results, experiments of spin to charge conversion, chiral spin interactions at the interface between graphene and magnetic thin films, SOC effects in heterostructures of graphene with TMD…

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New opportunities for spintronics with graphene and other 2D materials

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Spintronics is a paradigm focusing on spin as the information vector from quantum information to fast and ultra-low-power non-volatile devices such as the new STT-MRAM memory. Beyond its widely distributed application in data storage it aims at providing more complex architectures for beyond CMOS. The discovery of graphene has opened novel exciting opportunities in terms of functionalities and performances for 2D materials in spintronics devices. We will present experimental results on the potential of 2D materials such as graphene for spintronics. While highly efficient spin information transport can occur in graphene, with large spin signals and macroscopic spin diffusion lengths highlighting graphene's interest as a platform for spin transport[1], new potentials can emerge for spintronics. For example a thin graphene passivation layer can prevent the oxidation of a ferromagnet [2] enabling its use in novel wet/ambient low-cost processes for spintronics devices such as Atomic Layer Deposition (ALD) already used intensively in micro-electronics industry but absent from spintronics [3] or prospect in molecular spintonics. We will show that graphene coating doesn't spoil the highly surface sensitive spin current polarizer/analyzer behavior, but more importantly adds a new enhanced spin filtering property [2,3]. We will show extension from graphene to other 2D materials leading to a new type of 2D-MTJs [4].

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Recent theoretical advances in graphene spintronics

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Graphene has been heralded as the ideal material to achieve long spin propagation and further control the spin degree of freedom, in the quest of advancing non-charge-based information processing and computing, and for creating a new generation of active (CMOS compatible) spintronic devices together with non-volatile low energy MRAM memories. However, despite ultralow intrinsic and Rashba spin-orbit couplings (SOC) in clean graphene (μeV range), measured spin lifetimes remain in the range of several nanoseconds. This is orders of magnitude shorter than initially predicted, but already enough to envision disruptive non-charge-based room-temperature applications [1].

Besides, the physics of graphene "*can be enriched and manipulated*" by harvesting the large amount of possibilities of proximity effects with magnetic insulators, strong SOC materials, topological insulators, etc. One challenge is to endow a sizable charge-to-spin current conversion efficiency by enhancing spin-orbit interaction (up to meV). Claims have been made that very large spin Hall effect could be generated by using chemical functionalization with hydrogen or Au/Cu ad-atoms, or interfacing graphene with WS_2 substrate [2]. Those results are however fiercely questioned [3] while the theoretical understanding of spin dynamics for Dirac fermions in presence of enhanced SOC remains elusive, and often based on phenomenological arguments or semi-classical spin diffusion treatment which fail to capture the complex spin dynamics of Dirac fermions.

In this talk, I will discuss the fundamentals of spin transport for Dirac fermions propagating in graphene, scrutinizing the effect of substrate and interfaces, as well as impurities and ad-atoms. The role of "pseudospin" in driving spin dephasing and relaxation will be unveiled in the ultraclean limit and the impact of proximity effects on spin lifetime anisotropy will be discussed [4]. Second, I will show how chemical functionalization (fluorine, gold and thallium ad-atoms) and proximity effects with other 2D materials can generate spin-dependent phenomena such as spin filtering, quantum spin Hall and tunable spin Hall effects.

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Recent progress in experimental graphene spintronics

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Graphene has great potential as a building block for new spintronic applications. Room temperature spin relaxation lengths of over 30 micrometers have already been achieved, enabling the transport of spin information over long distances. Spin filtering effects and the demonstration of enhanced perpendicular magnetic anisotropy in cobalt-graphene structures are both promising for magnetic random access memory applications. Furthermore, the combination of spin transport with spin manipulation, which is possible in graphene by inducing magnetic correlations or large spin-orbit coupling by proximity with suitable materials, may pave the way to disruptive spintronic technologies based on "all-graphene" devices [1]. In this talk I will start with an overview of the experimental state of the art and describe our understanding of the basic spin relaxation mechanism in graphene, which is the key to achieve full control of the spin degree of freedom. I will introduce the main theoretical models that are currently being considered, which are unique to graphene and involve either resonant scattering with magnetic centers or spin-pseudospin coupling and Rashba spin-orbit interaction. I will then discuss recent experimental efforts aiming at highlighting their peculiarities; in particular, at verifying whether the spin relaxation is anisotropic, which would be the hallmark of the presence of a dominant spin orbit field [2,3]. These experimental efforts can also provide valuable information of spin-orbit proximity effects and spin Hall effects [4,5]. In the last part of the talk, I will discuss the generation, propagation and detection of hot carriers in graphene using purely electrical means. I will show that because typical carrier cooling times can be similar to spin lifetimes, it is possible to implement nonlocal hot-carrier injection and detection methods analogous to those used for spin [6]. In addition, I will present evidence that the spin propagation can be reinforced (suppressed) by the presence of hot electrons, suggesting that the remote spin accumulation can be controlled using temperature gradients.

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FRIDAY 8 SEPTEMBER 2017

Graphene hybrid architectures: squeezing the best out of graphene

Jurgen Smet

Plasmonic Properties of Graphene

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In this talk we review the concept of surface plasmon-polaritons (SPP's) in graphene, considering the cases of a single graphene layer, a double-layer graphene, and a metalspacer-graphene. The effect of hybridisation of SPP's with the surface phonons of the substrate will also be discussed. We show that double layer graphene supports two types of SPP's: acoustic (anti-symmetric) and optical (symmetric) modes. On the contrary, the metal-spacer-graphene only supports the acoustic (anti-symmetric) mode. With the emergence of hBN, it became possible to have a single monolayer of this material separating graphene from the metal. Using this possibility we show that one can confine mid-IR electromagnetic radiation down to an atom thick cavity. We show that this type of extreme confinement can be achieved and the mode can be excited using a metallic grating, separated from graphene by a single sheet of hBN. The role of non-locality in the optical response on graphene will also be discussed. Graphene is also known to exhibit strong Faraday rotation in the THz spectral range. We show that using a metallic grating the resonances in the Faraday rotation angle can be controlled and explored for molecular detection. We will also discuss the problem of a graphene-protected metallic grating, which can support spoof plasmons. We show that in the THz spectral range, the dispersion of this type of plasmons can be controlled using a graphene layer.

FRIDAY 8 SEPTEMBER 2017

Graphene (*or how to reinvent engineering with extreme materials*)

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Graphene and other Van der Waals materials show extreme and unique properties, which make them ideal for a wide variety of applications. This talk will review some of these applications in the field of electronics and microsystems.

Some of the applications will not change the world, but could solve problems of significant technological relevance. For example, the perfect structure of graphene makes it an ideal membrane, through which not even helium can go through. This can be used for the development of new passivation materials to protect more conventional semiconductor devices from oxygen and other impurities, and increase their reliability without sacrificing operating frequency. Other applications of these materials, on the other hand, may allow us to redefine what microsystems are can do. For example, the atomic-level thickness of these new materials confers them with unsurpassed flexibility, which makes them ideal for the development of a new generation of microsystems that resemble biological cells in their shape, size and some of their functionality. At the same time, the recent progress on 3-D printing techniques, and roll-to-roll growth and fabrication represents the first steps towards the use of these materials in large area distributed electronic and sensing applications embedded on everything, from airplanes to highways. Finally, the ability of these materials to be transferred to any arbitrary substrate, offers an unprecedented new degree of freedom to tune each material to specific applications. This can be used to enable ultrasensitive photodetectors, new sensors for neuro-science applications, or novel transistor structures.

The progress on the use of two-dimensional materials in engineering applications is definitely accelerating, however it is also important to remember Prof. Herbert Kroemer's "Lemma of New Technology". It says that "The principal applications of any sufficiently new and innovative technology always have been—and will continue to be—applications *created* by that technology". This statement has never been more true than in the case of graphene and other Van der Waals materials. It is therefore critical to understand the qualitatively new properties that two-dimensional materials bring, and keep the eyes open to catch, at the right time, the revolution they will enable.

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Tuning quantum non-local effects in graphene plasmonics

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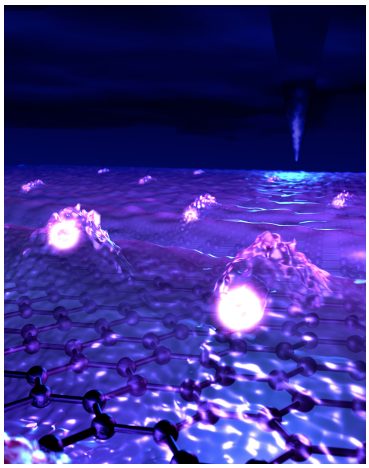
The control of polaritons are at the heart of nano-photonics and opto-electronics. Two-dimensional materials have emerged as a toolbox for in-situ control of a wide range of polaritons: plasmons, excitons and phonons. By stacking these materials, heterostructures can be designed with control at the atomic scale, while maintaining extremely high quality and clean interfaces. In this talk, we will show several examples of 2d material heterostructure devices with novel ways of exciting, controlling and detecting polaritons [1,2,3]. We challenge the limits of quantum light-matter interactions [5,6] as well as extremes in propagating plasmon confinement, down to the scale of a few nanometers. More recently, we used propagating grapheme plasmons, together with an engineered dielectric–metallic environment, to probe the graphene electron liquid and unveil its detailed electronic response at short wavelengths. The near-field imaging experiments reveal a parameter-free match with the full theoretical quantum description of the massless Dirac electron gas, in which we identify three types of quantum effects as keys to understanding the experimental response of graphene to short ranged terahertz electric fields. We demonstrate how, in principle, our experimental approach can determine the full spatiotemporal response of an electron system.



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Nonlinearity-induced spectral broadening of laser pulses in graphene-covered waveguides

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In recent years the integration of graphene on silicon waveguides has attracted much attention as it allows using well-established CMOS technology for constructing next-generation photonic integrated circuits. However, important challenges need to be overcome regarding the fabrication, patterning and doping of graphene-on-silicon devices. In addition, a more in-depth investigation of the fundamental optical properties of graphene-covered silicon waveguides, and in particular their nonlinear optical characteristics, will be required. In this talk we present a novel approach for local patterning and doping of graphene on top of silicon waveguides, and provide new insights in the nonlinear optical properties of the graphene-on-silicon material platform. The patterning approach that we developed is based on laser ablation and plasma etching, removing the graphene top layer without damaging the underlying silicon material [1]. As opposed to lithographic patterning, our chemicals-free method avoids unintentional modification of graphene's optical characteristics, and can be applied to chips of arbitrary size and shape at low cost. To dope the graphene, we have developed a novel chemical doping technique that fulfils for the first time the requirement of having both a high optical transparency and a low surface roughness, as needed for photonic applications [2]. Our doping approach relies on the electron acceptor F4-TCNQ dissolved in methyl ethyl ketone (MEK), yielding a uniform deposition because of an extraordinary charge transfer interaction between the F4-TCNQ and MEK molecules. Finally, to obtain a better understanding of the Kerr-nonlinear optical process of self-phase modulation (SPM) in graphene-covered silicon waveguides, we have carried out SPM broadening experiments using chirped laser pulses [3]. By comparing the obtained experimental results with our theory for chirped-pulse-pumped SPM, we found that the magnitude of graphene's Kerr nonlinearity is in correspondence with that observed in earlier experiments, whereas its sign turns out to be negative, in contrast to what has been assumed so far. Graphene's negative Kerr nonlinearity strongly impacts how this 2D material should be exploited for enhancing the nonlinear response of photonic integrated devices exhibiting a positive nonlinearity. It also opens up the possibility of using graphene to annihilate unwanted nonlinear effects in such devices, and to develop unexplored approaches for establishing Kerr processes in these components.

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POSTER PRESENTATION ABSTRACTS

WEDNESDAY 6 SEPTEMBER 2017

Disorder and field induced effects on the DC conductivity of twisted bilayer graphene

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Different 2D materials have a plethora of properties, which could be used as building blocks for structures of arbitrary functionality, choosing between metallic, semiconducting or insulating behavior. Their design although, in theory, could produce an infinite set of properties only by stacking different layers, in practice has limitations due to the fabrication processes, and the inability to do large-scale production, but is certainly a promising field still in its infancy.

Bilayer graphene is one of the most studied examples of multilayer structures, which, during the fabrication can result in a small twisting between the layers due to misalignment. The moiré structure produced in such a way affects the electronic and optical properties depending on the angle and gives rise to similar properties as the ones in graphene on top of hBN. Rotated bilayers or twisted bilayer graphene (TBLG) can be produced by growing on the C face of SiC substrate, by CVD, or by folding single graphene sheets. Intentional rotation leads to controllable and diverse electronic and optical properties, such as the Dirac like spectrum, renormalization of the Fermi velocity, the appearance of the low energy van Hove singularities and the localization of low energy states, which are all angle dependent.

We model the TBLG with a real-space methodology and calculate DC transport properties from the Kubo-Bastin formula in the linear response regime, through expansions in terms of Chebyshev polynomials[1]. Starting from a tight-binding (TB) representation we calculated the electronic properties of different structures with small, and large rotation angles, and examined the effects of the electric field. The method itself allows us to easily include different disorder effects such as vacancies or charged impurities. We examine the effects of vacancy induced states on the low energy conductivity and discuss the protection[2] or the breaking of chiral symmetry at the Dirac point.

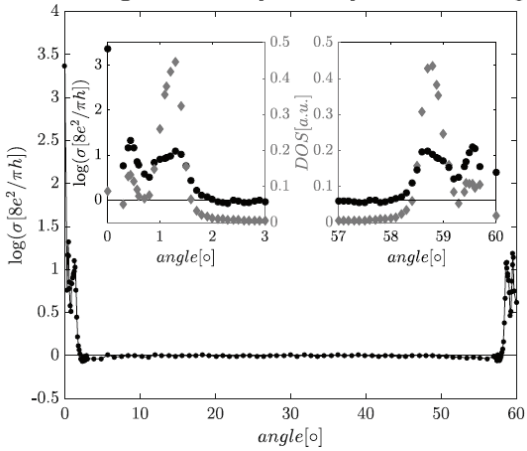

Fig. 1. Conductivity and DOS of TBLG at the Dirac point energy as a function of the rotation angle.

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Excitonic Properties of *h*-AlN-$Mg(OH)_2$ van der Waals Bilayer Heterostructure

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Motivated by recent studies that reported the successful synthesis of monolayer $Mg(OH)_2$ [Suslu *et al.*, Sci. Rep. **6**, 20525 (2016)][1] and hexagonal (*h*−)AlN [Tsipas *et al.*, Appl. Phys. Lett. **103**, 251605 (2013)][2], we investigate[3] structural, electronic, and optical properties of vertically stacked h-AlN and $Mg(OH)_2$, through *ab initio* density-functional theory (DFT), many-body quasiparticle calculations within the *GW* approximation and the Bethe-Salpeter equation (BSE). It is obtained that the bilayer heterostructure prefers the AB′ stacking having direct band gap at the Γ with Type-II band alignment in which the valance band maximum and conduction band minimum originate from different layer. Regarding the optical properties, the imaginary part of the dielectric function of the individual layers and heterobilayer are investigated. The heterobilayer possesses excitonic peaks, which appear only after the construction of the heterobilayer. The lowest three exciton peaks are analyzed in detail by means of band decomposed charge density and the oscillator strength. Furthermore, the wave function calculation shows that the first peak of the heterobilayer originates from spatially indirect exciton where the electron and hole localized at h-AlN and $Mg(OH)_2$, respectively, which is important for the light harvesting applications.

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Electronic and vibrational properties of V 2Cbased MXenes: from experiments to firstprinciples modeling

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In the present work, I focus on the characterization of V2C-based MXene systems and deal with structural, electronic and vibrational properties. Firstly, I describe the pristine bare V2C monolayer (see Fig.1(a)). Using first-principles calculations, I obtain the optimized crystal structure and the relative electronic band structure. Secondly, I calculate the vibrational normal modes thanks to density functional perturbation theory (DFPT) within the harmonic approximation. I discuss the Raman and infrared activity of the modes and compare the former with an experimental Raman spectrum (see Fig.2).

On top of the calculations for the pristine V2C, I perform a systematic analysis of 2D V2CT2 mono-sheets (with T=F,O,OH) (see Fig.1(b)) with the aim to establish the role of surface terminal groups in the electronic and vibrational properties. More specifically, I show the improvement in approximating the experimental Raman peaks positions when considering 2D fully-terminated V2CT2 systems (see Fig.2).

Finally, I present some recent results obtained for systems with mixed terminal groups (see Fig.2). The actual agreement between our experimental and theoretical results is relatively good and some perspectives for reducing the remaining discrepancies are proposed.

All-strain based valley filter in graphene nanoribbons using snake states

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The discovery of graphene brought the possibility of observing interesting phenomena due to its unique band structure, consisting of Dirac cones in points labeled as K and K′ in its first Brillouin zone. In fact, the existence of two inequivalent cones is of special importance, since it enables a new degree of freedom to be explored in novel valley-tronic devices. Several suggestions have been made to harvest valley polarization in graphene, involving *e.g.* specific combinations of armchair and zigzag edges in a monolayer graphene ribbon, [1] or non-uniform substrate induced masses [2]. On the other hand, recent studies have demonstrated that pseudo-magnetic fields can be induced in graphene by specific strain configurations and, since these fields point towards opposite directions in different Dirac cones [3], several suggestions of strain-based valley filters have been proposed in the literature. Most of these proposals involve combinations of the strain induced fields with applied magnetic and electric fields. [4] Indeed, strain based valley filters are specially interesting, because of graphene's ability to withstand large mechanical stress. [5]

In this work, we investigate the electronic transport and valley filtering through a pseudo-magnetic field kink, which can be realized along a graphene nanoribbon using strain engineering. Electron transport along this kink is governed by snake states that are characterized by a single propagation direction. As those pseudo-magnetic fields point towards opposite directions in the K and K′ valleys, snake states end up valley-polarized. In a graphene nanoribbon with armchair edges, this effect results in a valley filter that is based only on strain engineering. We discuss how to maximize this valley filtering by adjusting the parameters that define the stress distribution along the graphene ribbon. [6]

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Multicomponent electron-hole superfluidity and BCS-BEC crossover in double bilayer graphene

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Superfluidity in coupled electron-hole sheets of bilayer graphene is multicomponent because of the conduction and valence bands[1,2]. We investigate the superfluid crossover properties as functions of the equal electron and hole densities and the tunable energy gap between the bands[3]. We determine the momentum dependent multicomponent superfluid gaps, the multicomponent condensate fractions, and the chemical potential.

For small band gaps, we find that interaction driven excitations from the valence band to the conduction band can block the system from entering the BEC regime even at very low densities. For large band gaps Van Hove singularities magnify the ratio Δ/EF and suppress excitations from the valence band. Both these effects push the system toward the strongly coupled BEC regime, the optimal range for high-TC superfluidity.

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Ab-initio quantum transport of polycrystalline graphene

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Out of the different production approaches for two-dimensional materials, chemical vapor deposition (CVD) is presently by far the most viable and industry compatible one. However, CVD materials are found to be polycrystalline in nature and composed of many single-crystal domains separated by grain boundaries (GBs). In graphene, GBs are experimentally observed as one-dimensional line of defects of irregular shapes, constituted of pentagons, twisted hexagons and heptagons, as depicted in Fig.1. The structural defects forming those GBs strongly affect the overall properties of wafer-scale graphene [1]. Additionally, GBs are an important source of scattering that limit drastically the carrier mobility and consequently the performance of graphene-based electronic devices. Only a few ab-initio studies have been performed so far on GBs, mostly with ideal geometries. In the present research, highly-efficient simulations based on density functional theory have been used to explore charge transport in polycrystalline graphene. Firstly, the transmission properties are investigated for simple GB geometries exhibiting two different electronic structures, as formerly described in the literature [2]. Charge transport is also described ab-initio for more complex but highly realistic GB geometries, including thousands of atoms (as illustrated in Fig.1). Afterwards, a perturbation approach is applied on the periodic pattern of an initially charge-reflective system, indicating the existence of leakage currents. Finally, the effect of additional realistic disorder is investigated in the form of vacancies, large scattering regions and out-of-plane buckling for a constant periodicity. In summary, the present research intends to contribute to a more extensive understanding at the atomistic level of the detrimental effect of GBs on electronic transport for progressing towards technological applications of polycrystalline graphene.

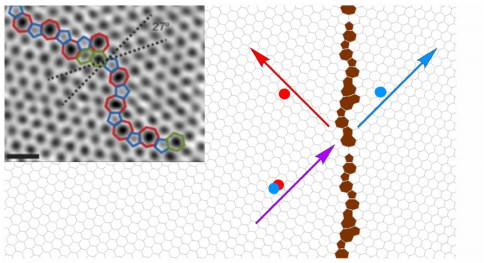

Figure 1. Modeling electronic transport through grain boundaries in polycrystalline graphene. Highresolution TEM image (from Ref[1]) of a grain boundary compared with an atomistic model, based on hexagons, heptagons and pentagons. Colored arrows illustrate both the reflexion and the transmission of traveling electrons with different spin states throughout a realistic grain boundary in graphene.

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Detailed characterization of the third order nonlinearity of graphene with enhanced optical Kerr effect method

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We study the third order optical nonlinearity of graphene on a given substrate with an enhanced version of the optical Kerr effect method coupled to optical heterodyne detection [1,2], using a theoretical description of the optical interactions of light at an interface with a graphene current sheet characterized by its surface susceptibility [3,4]. We measure separately the time response of the two main vector components of the nonlinear susceptibilities, and we show that $\chi_{xyxy} + \chi_{xyyx}$ accounts for the fast birefringent and dichroic contribution to the nonlinear response, in agreement with [5] for the dichroic response, while χ_{xxyy} has a picosecond relaxation time. We also measure the ratio between the real and the imaginary part of the nonlinearity and we validate experimentally the assumption that the out-of-plane tensor components are small. Our method can be applied to other 2D materials, as it relies mainly on the small ratio between the thickness and the wavelength. In addition, the proposed theoretical model could help for the development of numerical simulation tools using sheet currents to model the linear and nonlinear optical response of graphene or other 2D materials [6].

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From Floquet topological insulators to Floquet isolators

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Light-matter interaction is at the heart of intriguing phenomena and has led to many practical applications like, for instance, Raman spectroscopy. But beyond characterization, several studies have gone deeper into actually using light to modify the electrical properties of a material. This can be done, for example, by using light to switch off the conduction in graphene [1,2] (or other materials [3]), thereby allowing to tune the material's response with optical means, or even inducing tunable topological states in materials that would otherwise lack them [1,2,4,5,6,7,8] (i.e. a *Floquet topological insulator* [4]). The latter would expand the playground of topological insulators to a broader set of materials. The recent experimental realization of laser-induced bandgaps at the surface of a topological insulator [3] has added much interest to this area.

Here we provide an overview of our recent works in this field with a focus on the generation of Floquet chiral edge states in graphene [6,9,10], and other materials including topological insulators [8,11], and their Hall response [12]. We also show how light-matter interaction could be used to realize a *Floquet isolator* [13, 14], a system where transmission can occur only between say lead L to lead R.

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MoS_2-based vertical spintronic devices

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Since the discovery of graphene in 2004, 2D materials have attracted a huge attention thanks to their amazing properties at the single layer level. 2D materials encompass compositions including almost all the elements of the periodic table and offer an extremely rich variety of functionalities that cover the whole range of electronic and magnetic properties [1]. More interestingly, a key asset of 2D materials is the possibility of combining the best of their properties altogether in multilayers to obtain new materials with enhanced or new functionalities, making them very appealing for next generation functional devices [2].
Concerning the spintronics field, the large range of properties offered by 2D materials and, most important, their intrinsic two dimensional nature, creates thin, tunable and free of defects barriers with sharp interfaces, that make them perfect candidates to be used as Lego building blocks towards the ultimate miniaturization and engineering of spintronic devices. Despite this great potential, very few results exist up to date on the integration of 2D materials beyond graphene into spintronic devices, even the simplest ones as magnetic tunnel junctions (MTJs) [3]. Moreover, in most of these works, bottom ferromagnetic (FM) electrode has been exposed to the air during the device fabrication process and it is thus oxidized.

In this work we focused on MoS_2 as prototypical 2D material of the transition metal dichalcogenide (TMDC) family. We will first report investigation of vertical transport through mechanically exfoliated MoS_2 flakes on Co/Al_2O_3 ferromagnetic electrode using a local atomic force microscopy (AFM) approach that allows us to investigate transport properties at the local level on the flakes. Then, we will show successful integration of mechanically exfoliated MoS_2 flakes in real devices, as $Co/MoS_2/Co$ MTJs. To do that we adopt an original approach where flakes are exfoliated inside a glove box to prevent bottom ferromagnetic electrode oxidation. Finally, we will show negative magnetoresistance (MR) signal measured in these devices up to room temperature (Figure 1).

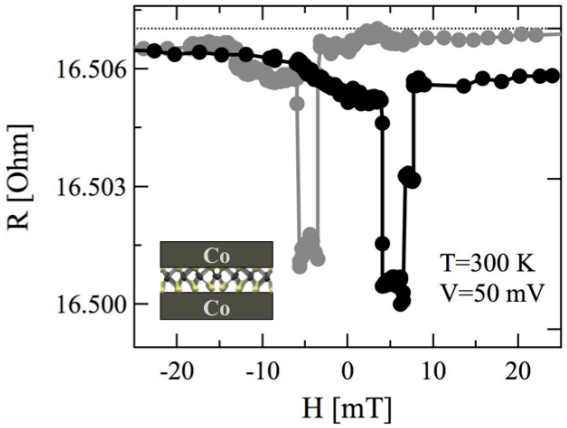

Figure 1: MR signal measured at room temperature in a $Co/MoS_2/Co$ MTJ. (Inset) Schematic of the vertical device.

These findings represent an advance in the understanding of vertical transport mechanisms through MoS_2 thin layers and are an important step forward in the integration of other TMDCs into 2D-based MTJs.

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Beyond Dirac physics: effects of the anisotropic band structure on the spreading of electronic wave packets on MoS_2 sheets

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ABSTRACT Anisotropic band structure of the TMDC materials can cause anisotropies in the transport properties [1]. By a new formulation of the split-operator FFT technique [2] we were able to directly include the *ab-initio* calculated energy dispersion relations into the kinetic energy operator, thus incorporating both the effect of the crystal structure and electronic structure in an *ab-initio* level. For the case of monolayer MoS_2 we calculated the $E = E_n(\vec{k})$ dispersion relation by DFT calculations using the Vienna ab initio simulation package (VASP). Elastic collisions by impurities and other defects can be included by introducing appropriate scattering potentials in the Hamiltonian. Localized wave packets can be injected, for example, onto a 2D sheet by an STM tip. The time development of the **Error! Objects cannot be created from editing field codes.** wave function is computed from the time-dependent 3D Schrödinger equation. By applying a t-E Fourier transform the **Error! Objects cannot be created from editing field codes.**wave function and energy-dependent measurables are also available. In the presence of spin polarization, the valence bands around K and K' points will be equally populated, but with electrons of opposite spins. For each spin, the probability current spreads in a threefold symmetric pattern, but the total current will average to a hexagonal symmetric pattern.

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Massless Fermions in 3D Carbon Structures

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The discovery of massless Fermions in low-dimensional carbon-based nanostructures has strongly impacted condensed matter physics by introducing pseudo-relativistic effects in their electronic properties. Indeed, the linear energy dispersion with the crossing of electronic bands at a particular point, forming the so called Dirac cone, imposes the electrons to behave like massless Dirac Fermions in graphene (2D) and carbon nanotubes (1D). Intense efforts have been realized to extent the tremendous properties of massless Dirac Fermions to the 3D materials family. Recently, massless Fermions have been experimentally evidenced in several 3D materials such as Na3Bi [1], Cd3As2 [2,3] and HgCdTe [4] paving the way towards a new class of materials.

In the present work, we predict the possibility to observe 3D massless Dirac Fermions in a schwarzite structure (Fig.1), a 3D purely carbon-based allotropic form [5]. Carbon schwarzites consist of a graphenic surface in which carbon rings with more than six atoms (heptagons, octagons, etc.) are incorporated to induce negative curvature. By means of density functional theory and tight-binding approaches, the electronic properties of a large gyroidal schwarzite structure are investigated. Fully isotropic and symmetric linear band crossings are evidenced. The corresponding charge carriers are thus expected to behave as 3D massless Dirac Fermions. This schwarzite can thus be considered as a remarkable playground to investigate the physics of these exotic Fermions in 3D materials.

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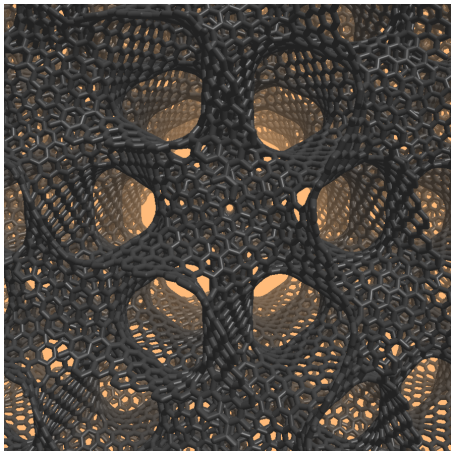

Figure 1: Atomic model of a carbon-based 3D schwarzite structure

Magneto-exciton states in a circular graphene quantum dot

Longlong Li

Abstract: Magneto-exciton states in a circular graphene quantum dot (CGQD) were investigated by means of the configuration interaction method. We found that (i) excitonic effects are very significant in the CGQD ; (ii) two types of excitons (intravalley and intervalley) are present in the CGQD; (iii) the intravalley and intervalley exciton states display different magnetic-field dependencies; (iv) the magneto-exciton ground state in the CGQD undergoes an intravalley to intervalley transition accompanied by a change of its angular momentum; (v) the exciton binding energy does not increase monotonically with the magnetic field; and (vi) the optical transitions of magneto-exciton states are strongly valley-dependent.

Ordered non-covalent functionalization of graphene by controlled formation of 2D supramolecular self-assemblies at the graphene surface forming hybrid vdW heterostructures

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The rise of graphene and related 2D materials makes possible the formation of heterostructures held together by weak interplanar van der Waals (vdW) interactions.[1,2] Periodic potentials naturally occur at the interface, which can significantly change the electronic structure of the individual materials within the stack, thus offering the possibility to build up novel structures with unique properties. Unfortunately, it is quite hard to precisely control the periodic potential in these structures since they are essentially determined by the lattice mismatch between the different materials.[3,4] Also, the fabrication of such inorganic vdW heterostructures is quite demanding in terms of technical efforts and costs. In this context, combining different molecular functionalities in a same graphene heterostructure is highly attractive for several reasons. First, graphene can be doped with a variety of molecules, which can act as nanoscopic potentials and locally modify graphene electronic structure.[5,6] Secondly, crystalline structures with 2D architecture can be formed with a collection of molecules capable of physisorbing on graphene and other 2D materials.[7,8] In this regard, self-assembly of linear alkyl chains is particularly interesting. As a matter of fact, it is now well established that long alkane chains, and related functionalized molecules physisorb on graphite surface, generating highly ordered 2D patterns.[8,9] Besides, periodic modulation with different geometries are predicted to affect the electronic band structure of graphene in very different ways. Namely, an anisotropic propagation of the charge carriers is predicted for graphene sheet in which a 1D potential is applied.[10]

Here, we explore the 1D modulation of graphene properties that is programmed with atomic precision via the exploitation of self-assembled monolayers driven by linear alkyl chains, generating well-organized supramolecular architectures at the graphene surface.[11]

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Combination of graphene-polymer heterostructures and near-zero refractive index metamaterials towards? robust perfect tunable electromagnetic absorption

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The electromagnetic properties of solid materials are directly related to their electrical conductivity. This link remains true for 2D conducting materials such as graphene. The reflectance, transmittance and absorbance of this one-atom-thick carbon layer are analytically derived in this work, generalizing the Fresnel formula to the case of a 2D conducting material inserted between two semi-infinite dielectric media. The stacking several graphene monolayers, separated by a polymer spacer, is a way to control the effective conductivity of a system since the conductivity of N independent layers σ_N is equal to $N\sigma_1$ $\mathrm{N}\sigma_1$, where σ_1 is the 2D conductivity of a monolayer [1]. Via an optimization process based on the Fresnel relations, one may find an optimum number of layers for which the absorption of electromagnetic radiations inside the graphene layers is maximal. Accordingly, the device must satisfy impedance matching conditions. Such graphene-polymer heterostructures have been shown to efficiently absorb GHz electromagnetic radiation up to ~50% [1,2] under these conditions.

Moreover, these structures, once impedance matching conditions are verified, are robust to fabrication process defects (microscopic holes, microscopic embryos of two-layer graphene or domain boundaries) that may occur in graphene samples produced by chemical vapor deposition [2]. Numerical rigorous coupled wave analysis is used to account for the presence of random defects in graphene. We demonstrated that the optimum absorbance of the device does not weaken to the first order in defect concentration. This finding testifies to the robustness of the shielding efficiency of the proposed absorption device.

The analytical relations show that perfect electromagnetic absorption (100%) can be reached if the graphene/polymer heterostructure is laid over a material possessing a refractive index close to zero [3]. This can be achieved using an epsilon-near-zero metamaterial.

Finally, tunability of the proposed absorbers is theoretically worked out by modulating the charge carrier density of graphene. An applied voltage modifies the effective conductivity of the device and a modulation of 40% of absorption/reflectance is shown using a voltage below the breakdown (voltage) of the polymer layers [4].

The proposed strategy can be applied to any kind of 2D conducting materials on epsilon-near-zero metamaterial.

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One-atom-thick membranes with subatomic selectivity

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One-atom-thick crystals are impermeable to all atoms and molecules, but hydrogen ions (thermal protons) penetrate through them even in the absence of structural defects[1]. We show that monolayers of graphene and boron nitride can be used to separate hydrogen ion isotopes. Employing electrical measurements and mass spectrometry, we find that deuterons permeate through these crystals much slower than protons, resulting in a separation factor of ≈10 at room temperature[2]. The isotope effect is attributed to a difference of ≈60 meV between zero-point energies of incident protons and deuterons, which translates into the equivalent difference in the activation barriers posed by two dimensional crystals. In addition to providing insight into the proton transport mechanism, the demonstrated approach offers a competitive and scalable way for hydrogen isotope enrichment[3].

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Electromagnetic properties of multilayered 2D materials: application to graphene.

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The determination of the electromagnetic properties of 2D materials is of primary interest for applications in biosensing, shielding and optronics. Various methods have been proposed to numerically evaluate the electromagnetic response of plane or nanostructured 2D materials. These methods generally model graphene either as an isotropic material with a given thickness or via a surface current.

In the present work, we have explored several models such as the surface current calculation, the rigorous coupled wave analysis and the discrete dipole approximation to study graphene single layer, graphene multilayers and graphene nanostructures. We highlight the role of the layer thickness by comparing it to the skin depth and investigate the effect of the intrinsic anisotropy on the electromagnetic properties of graphene. In particular, we derive the conditions to model a multilayer as a surface current and to model a single layer as a thick slab for numerical application.

Comparing experimental data and theoretical results, we have shown the modification of the Brewster angle when a dielectric substrate is covered with a conducting 2D material. For a multilayer, we prove that the shift of the Brewster angle is proportional to the number of layers. Consequently, the measurement of the shift is proposed as a method to characterize 2D material by optical measurement [1].

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Superconductivity and magnetism in 2D materials: 2H-TaS_2 and LCP

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Graphene [1] is one of the most studied materials due to its unique properties such as hardness, flexibility and high electric and thermal conductivity. However, probably the best quality of graphene is that it has opened the field to many other 2D crystals [2], including phenomena such as magnetism and superconductivity.

In this work, **A)** the synthesis and characterization of metal chalcogenides are discussed. As an example, transport measurements in thin layers of 2H-TaS_2 are presented. It is observed a superconducting temperature (Tc) enhancement by decreasing the number of atomic layers (from 0.6 K in the bulk sample to ca. 2K in a ~3 nm layer, as can be seen in Figure 1) [4]. This behaviour is the opposite of the one reported in other 2D superconductors, as $NbSe_2$ [5]. This effect can be interpreted on the basis of a simple band model and on optical phonons localized in each plane; it shows that the tunneling between the bands decreases the effectiveness of the pairing interaction that in turn is mediated by in-plane phonons.

Moreover, **B)** a new family of magnetic layered coordination polymers (LCP) with different terminal groups are mechanically exfoliated down to the monolayer. Then, thanks to this pre-synthetic approach, it is possible to obtain 2D materials with *defect-free* functionalization and modify at will its surface properties (as the wettability) while the magnetic behaviour remain unaltered.

These results may bring superconductivity and molecular magnetism into the flatland for their future use in magnetic sensors, membranes, gas-sensing or low energy applications.

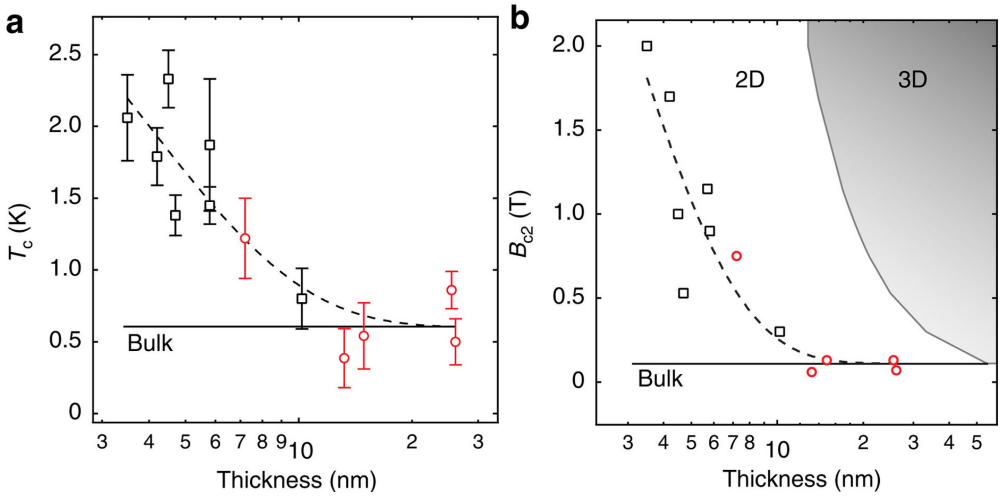

Figure 1: (a) Variation of T_c as a function of the thickness of the 2H-TaS_2 flakes. Devices exhibiting a non-zero residual resistance below T_c are plotted in red. **(b)** Variation of Bc_2 as a function of flake thickness. The red circles mark the same devices in **a** having residual resistance. The black solid line indicates the bulk limit upper critical field of 110 mT. The grey solid line plots the Ginzburg-Landau coherence lengths, calculated from the *y* axis B_{c2} values, and marks the edge of the 2D limit.

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Strain controlled valley filtering in multi-terminal graphene structures

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Mechanical deformations in graphene can lead to the generation of pseudo-magnetic fields (PMFs) that exceed 300 T. The generated PMF has the opposite direction for electrons originating from different valleys. This property can be used in order to separate electrons from the two valleys and obtain a valley-polarized currents - a prerequisite for valleytronics. We show that straining graphene locally into a Gaussian bump by e.g. an STM (scanning tunneling microscopy) tip, it is possible to obtain highly tunable polarized valley currents in two realistic device settings: a two-probe nanoribbon and a Hall bar. The pseudo-magnetic field created by the deformation allows electrons from only one valley to transmit and a current of electrons from a single valley is generated at the opposite side of the locally strained region, as sketched in Fig. 1(a). In Fig. 1(b) we plot the change of the transmission probabilities T_K and $T_{K'}$ together with the polarization $\tau_K = T_K/(T_K + T_{K'})$ with the width of the bump σ. Figure shows that both transmissions decrease with increase of σ up to a certain value after which only T_K increases and τ_K approaches unity. In this regime, valley polarized conduction channels open inside the bump and the system behaves as a valley filter. We show that valley filtering is most effective with bumps of a certain height and width. This is shown in Fig. 1(c) where we plot valley polarization τ_K versus the parameters of the bump. Notice that the valley filtering regime occurs only for $c_1 < \sigma < c_2$, with $c_1 \approx 0.8$ while the upper limit depends on the values of the Fermi energy and width of the collector. Despite the fact that the highest contribution to the polarized current comes from electrons from the lowest sub-band, contributions of other sub-bands are not negligible and can significantly enhance the output current.

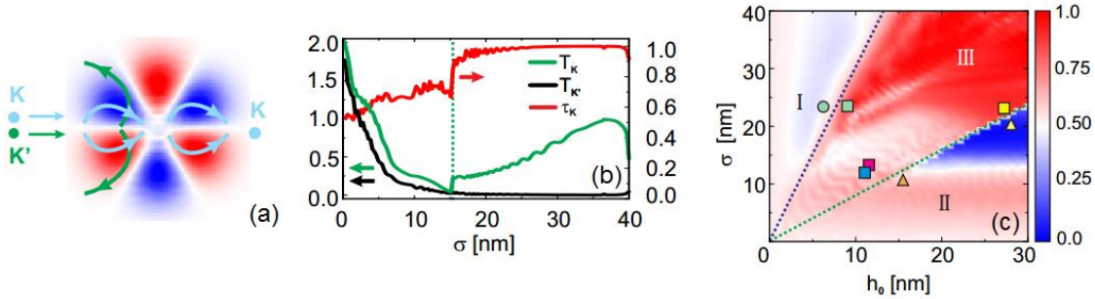

Figure 1. (a) Cartoon drawing of the flow of electrons from different valleys through the bump. (b) Probabilities T_K, $T_{K'}$, and τ_K versus the width of the Gaussian bump using $h_0 = 20$ nm, $E_F = 0.1$ eV and a Hall bar geometry. (c) Contour plot of valley polarization τ_K versus the width and the height of the bump.

Layer-dependent magnetism in atomically-thin CrI3

Authors: Efren Navarro-Moratalla, Bevin Huang, Genevieve Clark, Dahlia R. Klein, Ran Cheng, Kyle L. Seyler, Ding Zhong, Emma Schmidgall, Michael A. McGuire, David H. Cobden, Wang Yao, Di Xiao, Pablo Jarillo-Herrero, Xiaodong Xu

The library of 2D materials has been continuously growing since the discovery of graphene. There is now a large collection of single-layer materials with a variety of optoelectronic properties from which to choose for the fabrication of designer van der Waals heterostructures. However, there was still one conspicuous absence in the 2D materials playground: a magnetic 2D material. Recently, the first 2D material with anti-ferromagnetic order was confirmed by Raman scattering, but the lack of a net magnet moment hindered the direct detection of the magnetic properties and precluded the applications of this material.[1] We focus our study in the isolation of few-layer crystals of chromium triiodide (CrI3), which exhibits a transition to a ferromagnetic phase below 60 K in the bulk. Our magneto-optic Kerr effect experiments show that ferromagnetism prevails down to the monolayer, providing proof of the discovery of the first 2D magnet with spontaneous magnetization made out of a single layer of CrI3.[2] In addition, the field-dependent measurements showcase the dramatic layer dependence of the magnetic ground state in the 2D limit. This work opens new opportunities for exploring low-dimensional magnetism by harnessing the unique features of atomically-thin materials, such as the electrical control for realizing magnetoelectronics or van der Waals engineering for the study of novel spintronic phenomena.

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Spatial design and control of graphene flake motion

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The recent design of particular patterns of structural defects on a graphene surface allows us to propose an alternative approach for controlling the motion of a graphene flake over a graphene substrate. The thermally induced motion of a graphene flake is controlled by engineering topological defects in the substrate. Such defect regions lead to an inhomogeneous energy landscape and are energetically unfavorable for the motion of the flake, and will invert and scatter graphene flakes when they are moving toward the defect line. Engineering the distribution of these energy barriers results in a controllable trajectory for the thermal motion of the flake without using any external force. We predict superlubricity of the graphene flake for motion along and between particular defect lines. The recent design of particular patterns of structural defects on a graphene surface allows us to propose an alternative approach for controlling the motion of a graphene flake over a graphene substrate. The thermally induced motion of a graphene flake is controlled by engineering topological defects in the substrate. Such defect regions lead to an inhomogeneous energy landscape and are energetically unfavorable for the motion of the flake, and will invert and scatter graphene flakes when they are moving toward the defect line. Engineering the distribution of these energy barriers results in a controllable trajectory for the thermal motion of the flake without using any external force. We predict superlubricity of the graphene flake for motion along and between particular defect lines.

Valley filtering and electron optics in polycrystalline graphene systems

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Owing to peculiar electronic structure and outstanding physical properties, graphene has been shown to be an ideal platform for exploring several novel transport phenomena [1,2]. Examples include Klein tunneling, anomalous quantum Hall effect, Berry's phase manifestation, valleydependent transport, optical-like behaviors of charge carriers, etc. Among them, valleydependenttransport and optical-like behaviors, are exceptional phenomena and have attracted a great amount of attention from the scientific community since they are essential ingredients for applications in valleytronics and electron optics devices [2], respectively. Valleytronics lies in exploiting the manipulation of charge carriers in two valleys of graphene to encode data indigital computing. Electron optics exploits the optical-like behaviors of charge carriers to design novel quantum devices with a variety of interference and diffraction effects. Here, we present a new scheme [3] to manipulate simultaneously highly valley-polarized currents and optical-like behaviors of charge carriers in graphene (see Fig.1). Our proposed approach is based on the use of polycrystalline graphene systems containing two misoriented domains (or "grains") separated by a periodic array of dislocations. These two graphene domains generally exhibit different electronic structures (i.e. their Dirac cones can be located at different positions in the momentum space), especially when the system is strained. Such a discrepancy can manifest itself in a strong breaking of the inversion symmetry, and hence can induce a high valley polarization of the electronic currents through the system. Additionally, in analogy to optical systems, these two domains act as different media for electron waves, leading to optical-like behaviors of charge carriers in the system, i.e., offering the possibility to modulate and obtain negative refraction indexes.

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Fig. 1: (a) Schematic of considered graphene systems where the charge transport across the grain boundary is calculated. (b) Diagrams illustrating the strain effects on the band structure of grapheme domains and the momentum conservation rule. (c) Obtained directional currents and valley polarization.

Generalized Dirac structure beyond the linear regime in graphene

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We show that a generalized Dirac structure survives beyond the linear regime of the low-energy dispersion relations of graphene. A generalized uncertainty principle of the kind compatible with specific quantum gravity scenarios with a fundamental minimal length (here graphene lattice spacing) and Lorentz violation (here the particle/hole asymmetry, the trigonal warping, etc.) is naturally obtained. We then show that the corresponding emergent field theory is a table-top realization of such scenarios, by explicitly computing the third order Hamiltonian, and giving the general recipe for any order. Remarkably, our results imply that going beyond the low-energy approximation does not spoil the well-known correspondence with analogue massless quantum electrodynamics phenomena (as usually believed), but rather it is a way to obtain experimental signatures of quantum-gravity-like corrections to such phenomena.

Large-scale alignment of millimetre-sized graphene flakes grown by chemical vapour deposition

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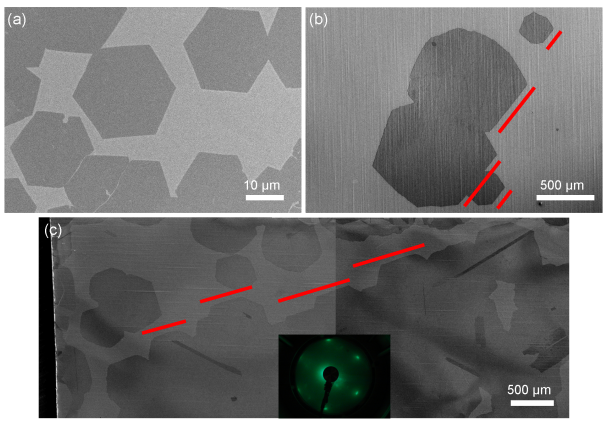
Chemical vapour deposition (CVD) holds great promises for large-scale production of high-quality graphene, more specifically on copper substrates. For many applications, the ideal graphene sheet should be free of domain boundaries at the wafer scale. To reach that objective, one first route consists in growing large single-crystalline isolated graphene flakes. The second avenue involves merging seamlessly aligned graphene domains grown on a single-crystalline substrate.

Here we propose a synergistic method combining the two previous approaches. We take advantage of residual oxygen present in the atmosphere of the CVD furnace to (1) reduce graphene nucleation density and (2) recrystallize the copper foil along the (111) orientation, in a single shot. More precisely, the oxidation of the copper foil followed by reduction in hydrogen proves to greatly accelerate its reconstruction by "abnormal grain growth".

In this way, we produce monolayer millimetre-sized graphene hexagonal flakes aligned with each other at the centimetre scale. These domains are shown to be single-crystalline, of high structural quality, and to grow in epitaxial registry with the copper (111) substrate. See reference [1] for more details about this work.



Scanning electron microscopy images of (a) small-sized, not aligned graphene flakes and (b) large-sized, aligned graphene flakes. (c) Centimeter-scale alignment of large-sized domains. Inset: corresponding low-energy electron diffraction pattern.

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Anisotropic electron-hole superfluidity in double layer phosphorene

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There is currently experimental interest in generating electron-hole superfluidity [1] in double sheets of 2D materials with the expectation of high transition temperatures. Double bilayer and few layer sheets of graphene are expected to access the regime of strong pairing necessary for superfluidity in a range of carrier densities accessible to experiments [2, 3].
We study the possibility of electron-hole superfluidity in coupled phosphorene sheets at zero temperature. The two phosphorene layers are separated by a thin hexagonal boron nitride insulating barrier to prevent tunneling between the carriers. Monolayer phosphorene is known as a material with highly anisotropic band structure. We first generalize the mean-filed equations for the superfluid gap and density to the case of an anisotropic dispersion energy. We show that the electron-hole phosphorene layers exhibits a highly anisotropic superfluidity where the magnitude of the superfluid gap is not only momentum dependent, but also depends on the direction. We demonstrate that the superfluidity is enhanced in one direction while an anisotropic screening suppresses the superfluidity in another. We find that superfluidity is predominately in the strongly-coupled BEC and BCS-BEC crossover regimes, with anisotropic large superfluid gaps with transition temperatures up to 80 K. Our results may guide future experimental research towards the realization of anisotropic condensate states in coupled 2D devices.

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Sound waves and exural mode dynamics in 2-dimensional crystals

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Starting from a Hamiltonian with anharmonic coupling linear in in-plane acoustic displacements and quadratic in out-of-plane (exural) modes, we have derived coupled equations of motion for in-plane displacements correlations and exural mode density uctuations. We use linear response theory and time-dependent thermal Green's func- tions techniques. As external perturbations we allow for stresses and thermal heat sources. The displacements correlations are described by a Dyson equation where the exural density distribution enters as an additional perturbation, the exural density distribution satis_es a kinetic equation where the in-plane lattice displacements act as a perturbation. In the hydrodynamic limit this system of coupled equations is at the basis of a uni_ed description of elastic and thermal phenomena, such as isothermal versus adiabatic sound motion and thermal conductivity versus second sound. The theory is formulated in view of application to graphene, 2D h-BN and 2H-transition metal dichalcogenides and oxides.

Nonlinear light mixing by graphene plasmons

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Graphene is known to possess strong optical nonlinearity. Its nonlinear response can be further enhanced by graphene plasmons. We report a novel nonlinear electro-absorption effect observed in nanostructured graphene due to excitation of graphene plasmons. We experimentally detect and theoretically explain enhanced nonlinear mixing of near-infrared and mid-infrared light in arrays of graphene nanoribbons. Strong compression of light by graphene plasmons implies that the effect is non-local in nature and orders of magnitude larger than the conventional local graphene nonlinearity. The effect can be used in variety of applications including nonlinear light modulators, light multiplexors, light logic, and sensing devices.

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Theoretical investigation of graphene-phosphorene nanocomposites

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Intralayer deformation in van der Waals (vdW) heterostructures is generally assumed to be small due to the weak nature of the interactions between the layers. In the present work, we investigate the case of "bulk" (periodically-repeated out-of-plane) graphene-phosphorene vdW-heterostructures within the Density Functional Theory framework. We find that such intralayer deformation is important in the case of such graphene-phosphorene vdW-heterostructures, where the armchair lattice parameter of phosphorene contracts by ≈ 4% when compared to its free-standing counterpart. This leads to important changes in the electronic band structure when compared to the isolated layers, with the direct electronic optical transition of phosphorene becoming indirect in such vdW-heterostructure. It also indicates strong substrate effects in general in phosphorene -neglected up to now to the best of our knowledge- and paves the way to substrate-controlled stress-tronic in this material. In addition, we investigate the stability of such vdW-heterostructures as function of the rotation angle between the layers and stacking composition. Finally, we present several models and tools that could reveal useful in the future to analyze and predict the properties of vdW-heterostructures within the Density Functional Theory framework.

Novel spintronic device concept based on the observation of magnetic edge state in graphene nanoribbons

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Graphene nanoribbons with zigzag edge orientation (zGNRs) have an interaction induced gap and a magnetic insulating ground state with antiferromagnetic (AF) spin orientation between the two edges [1]. However, the experimental observation of this magnetism remained elusive due to the lack of the edge orientation control of the investigated GNRs. In this work we have performed electronic structure and magnetic ordering calculations on GNRs by applying the mean-field theory for the Hubbard model and compared them to tunneling spectroscopy measurements on GNRs with precisely zigzag edge orientations. Our calculations reveal that ribbons with zigzag edges have spin polarized edges with both antiferromagnetic (AF) and ferromagnetic (FM) coupling between opposite edges. The ferromagnetic ground state is enabled by the finite doping and both AF and FM states were found to be stable at room temperature. Furthermore, we have found a strong correlation between the electronic and magnetic properties of zigzag GNRs, AF ribbons displaying semiconducting, while FM ribbons showing metallic behavior in excellent agreement with our experimental findings [2].

This result can be exploited for a novel magnetically mediated switching mechanism in GNR based field-effect transistors (FET). In contrast to the conventional FET, where a gate electrode is employed to tune the Fermi level of the system in and out of a static bandgap, here the applied gate voltage can dynamically open and close an interaction gap, with only a minor shift of the Fermi level. The interplay of the band structure and edge spin configuration in zGNRs enables such transistors to carry spin polarized current without employing an external magnetic field [3]. Controlling both charge and spin signal within the simplest FET device configuration could open up new routes in data processing with graphene.

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Hydrogen-Induced Structural Transition In Single Layer ReS_2

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By performing density functional theory-based calculations, we investigate[1] how structural, electronic and mechanical properties of single layer ReS_2 can be tuned upon hydrogenation of its surfaces. It is found that a stable, fully hydrogenated structure can be obtained by formation of strong S-H bonds. The optimized atomic structure of ReS_2H_2 is considerably different than that of the monolayer ReS_2 which has a distorted-1T phase. By performing phonon dispersion calculations, we also predict that the Re_2-dimerized 1T structure (called $\mathbf{1T}^{Re2}$) of the ReS_2H_2 is dynamically stable. Unlike the bare ReS_2 the $\mathbf{1T}^{Re2}$-ReS_2H_2 structure which is formed by breaking the Re_4 clusters into separated Re_2 dimers, is an indirect-gap semiconductor. Furthermore, mechanical properties of the $\mathbf{1T}^{Re2}$ phase in terms of elastic constants, in-plane stiffness (C) and Poisson ratio (ν) are investigated. It is found that full hydrogenation not only enhances the fexibility of the single layer ReS_2 crystal but also increases anisotropy of the elastic constants.

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Interplay of magnetization between graphene and magnetoelectric multiferroics

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Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show [1] that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. Depending on the relative orientation of graphene and $BaMnO_3$, a quasi-half-metal or a magnetic semiconductor can be obtained. A remarkably large proximity induced spin splitting of the Dirac cones (~300 meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.

Going further, we investigate spin dynamics at finite temperature using a Monte Carlo approach with exchange coupling parameters fitted from first principles. We find that graphene strongly affects the magnetic properties of the substrate, well beyond the interface layer, and induces a softening of the Mn magnetization.

Spin Orbit Coupling calculations reveal that the influence of graphene on the substrate is even more radical and is able to change the direction of the easy axis with respect to the bare $BaMnO_3$ surface. We predict a Rashba splitting of the electronic bands near the K point, and the presence of a quantum anomalous Hall effect.

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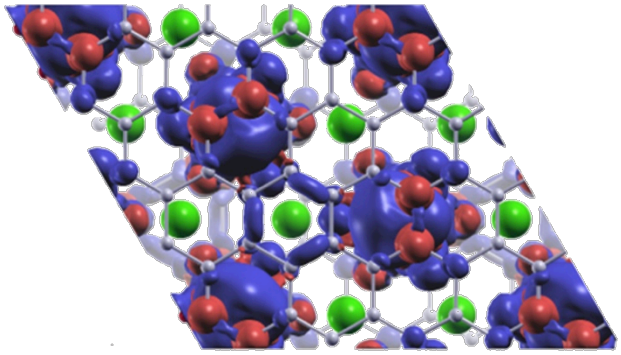

Figure 2 Spin density ($r_\uparrow - r_\downarrow$) of the graphene-$BaMnO_3$ interface (top view). Blue and red color indicate positive and negative sign of spin isodensities. Spin polarization is induced in the pristine C network from the underlying Mn atoms [from Ref. 1].

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