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On behalf of the Organising Committee we take great pleasure in welcoming you for the 1st edition of the Graphene and 2DM Online Conference (GO2020): Fundamental Research Insights.

Graphene and 2D Materials have a huge potential to impact established industrial sectors, building new emerging industries and niche segments and creating economic value. The one-day Graphene and 2DM Online conference (GO2020) will present the most recent advances in fundamental research in electronics, energy storage, biohealth, composites, coatings or sensors.

11 high profile talks from worldwide most influential academia experts in the Graphene and 2DM sector will present speeches in this international event on how advanced materials will change the future of technology and impact positively our daily life.

GO2020 will be a one-day online event that means to gather the key players of the Graphene and 2DM Community and related sectors. This event is launched following the success of previous Grapheneconf editions and considering that all major scientific and technological conferences are being cancelled or postponed worldwide until the end of 2020.

We are indebted to the following Company for their help and financial support: AMO GmbH (Germany)

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

Hope to see you again online in the next edition of the "Graphene & 2DM" Online Conference.

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Biocompatible 2D Material-based Inks: from Printed Electronics to Biomedical Applications

Cinzia Casiraghi

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Solution processing of 2D materials [1] allows simple and low-cost techniques, such as ink-jet printing, to be used for fabrication of heterostructure-based devices of arbitrary complexity. In my group we have developed a simple approach to achieve highly concentrated, defect-free, printable and water-based 2D crystal formulations, designed to provide optimal film formation for multi-stack fabrication [2]. This talk will discuss the progress in printed electronics achieved with these inks: examples of all-inkjet printed heterostructures, such as large area arrays of photosensors on plastic [2], programmable logic memory devices [2], capacitors [3] and transistors on paper [3,4] will be given. Furthermore, we will show that inkjet printing can be easily combined with high quality 2D materials, allowing simple and quick fabrication of complex circuits on paper, such as high-gain inverters, logic gates, and current mirrors [5].

Finally, I will show that our formulation approach also allows to easily tune the charge and surface properties of graphene, by allowing to produce amphoteric, cationic and anionic graphene dispersions *on-demand* in one-pot [6-8]. In particular, cationic graphene dispersions have exceptional intracellular uptake profile as well as stability in the biological medium, making this type of graphene very attractive to use in biomedical applications [7].

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Mass Production of 2D Materials by Exfoliation and Their Applications

Hui-Ming Cheng^{1,2}

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Graphene and two-dimensional (2D) materials have attracted significant interest. So far, only graphene can be produced in ton level, while other 2D materials cannot, which is a key limiting factor for their commercial applications.

First, I will briefly introduce the invention of a green oxidation process to produce graphene oxide with high quality and efficiency in large quantity by oxygen radicals[1]. Then, I will report our recent achievements in mass production of various 2D materials, including hexagonal born nitride (h-BN), transition metal dichalcogenides (TMDCs), black phosphorene, layered complicated oxides, and others, by a new powerful technology which is called interMediate Assisted Grinding Exfoliation (the iMAGE technology) [2]. This method is among the most powerful and efficient methods to produce 2D materials with the highest yield, quality, and production rate. This method can also be used to produce 2D MoS2 flakes from cheap and abundant MoS2 minerals. Furthermore, I will introduce the mass production of functionalized 2D materials by mechanochemical exfoliation [3]. In the end, I will discuss the use of such massively produced 2D materials for energy storage and conversion, functional composites, sensors, and thermal management materials [4-6].

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Short CV:

Dr. Hui-Ming Cheng is a professor and the founding director of Advanced Carbon Research Division of Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, and the Low-Dimensional Material and Device Laboratory of the Tsinghua-Berkeley Shenzhen Institute, Tsinghua University. He focuses on carbon nanotubes, graphene, other 2D materials, and energy storage and conversion materials. He is the founding Editor-in-Chief of Energy Storage Materials and Associate Editor of Science China Materials, and a member of Chinese Academy of Sciences.

Magic Angle Bilayer Graphene - Superconductors, Orbital Magnets, Correlated States and beyond

Dmitri K. Efetov *ICFO, Spain* Dmitri.Efetov@icfo.eu

When twisted close to a magic relative orientation angle near 1 degree, bilayer graphene has flat moire superlattice minibands that have emerged as a rich and highly tunable source of strong correlation physics, notably the appearance of superconductivity close to interaction-induced insulating states. Here we report on the fabrication of bilayer graphene devices with exceptionally uniform twist angles. We show that the reduction in twist angle disorder reveals insulating states at all integer occupancies of the four-fold spin/valley degenerate flat conduction and valence bands, i.e. at moire band filling factors nu = 0, +(-) 1, +(-) 2, +(-) 3, and reveals new superconductivity regions below critical temperatures as high as 3 K close to - 2 filling. In addition we find novel orbital magnetic states with non-zero Chern numbers. Our study shows that symmetry-broken states, interaction driven insulators, and superconducting domes are common across the entire moire flat bands, including near charge neutrality. We further will discuss recent experiments including screened interactions, fragile topology and the first applications of this amazing new materials platform.

Electronic Devices based on 2D Materials – Opportunities and Open Challenges

Max Christian Lemme

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Graphene and two-dimensional (2D) materials have been researched intensely over the past 15 years, and there is continued substantial investment in 2D material research and development. However, although physicists, chemists, material scientists and engineers continue to report new highlights on a daily basis, there are no end-customer microelectronics products on the market today. The main reason is that the process technology to manufacture 2D electronics is not sufficiently mature, which limits the possibility of realizing the promise of outstanding performance in electronics, optoelectronics or sensing. In this talk, I will introduce several applications, where 2D materials clearly could make a difference, such as photodetectors ^{1–3} and sensors ^{4–7}. I will further discuss major bottlenecks towards integration of graphene and 2D materials into semiconductor processing lines ⁸.

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Targeting the Mass Production of CVD Graphene

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For graphene industry, mass production of high quality graphene itself is the starting point and finally determines its future. Since 2008, we have been focusing our emphasis on the chemical vapor deposition (CVD) growth of graphene materials. Our work follows two different lines, CVD growth of graphene on metals including Cu, Ni and Cu-Ni alloys, and direct growth on insulators including traditional glass and glass fibers. All the efforts are targeting commercial level mass production together with equipment design and manufacturing. Listed in the following are the current status of our CVD graphene research: (1) 4-6 inch single crystal graphene wafers on Cu(111) and Cu90Ni10(111)/sapphire, commercial batch production available in 10,000 wafers/year; (2) A3-size graphene films with mm single crystalline domains by static growth, commercially available in 10,000 m2/year; 3) A3-size superclean graphene films with CO2 post-etching technique, commercially available in 10,000 m2/year; 4) roll-to-roll graphene films with 20-micrometer single crystalline domains by dynamic growth technique, commercially available in 20,000 m2/year; 5) 30 x 30 cm2 super graphene glass, commercially available in 5000 m2/year; 6) graphene-coated glass fibers and fabrics by direct growth technique with a capacity of 5000 m2/year. All the CVD systems are homebuilt with scaling-up capacity for commercialization. The talk will give a brief overview of our over 10year efforts from fundamentals to mass productions.

Ion permeation through atomically thin crystals

Marcelo Lozada-Hidalgo

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The basal plane of graphene is impermeable to all molecules and atoms – even for helium, the smallest of gases – at ambient conditions¹. In fact, it was believed that graphene would be impermeable even to protons, nuclei of hydrogen atoms. Unexpectedly, experiments demonstrated that graphene is highly permeable to thermal protons² and that deuterons (nuclei of hydrogen's heavier isotope deuterium) permeate ten times slower than protons³. Graphene is a membrane with subatomic selectivity. This exceptional selectivity suggests that 2D crystals could enable separation of permeants that would be difficult or impossible to achieve with conventional materials. This talk will discuss the progress in using the crystal lattice of 2D materials as sieves and the various unexpected phenomena we have found along the way^{4,5,6,7}.

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FIGURES



Figure 1: a. Artistic impression of proton transport through hexagonal boron nitride. **b**, Electron micrograph of a suspended graphene device. Membrane intentionally damaged to enhance visibility. **c**, Optical image of a CVD graphene proton transport membrane.

Atom-to-atom designed graphene-like structures

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Feynman's original idea of using one quantum system that can be manipulated at will to simulate the behavior of another more complex one has flourished during the last decades in the field of cold atoms. More recently, this concept started to be developed in nanophotonics and in condensed matter. In this talk, I will discuss a few recent experiments, in which 2D electron lattices were engineered on the nanoscale. The first is the Lieb lattice [1,2], and the second is a Sierpinski gasket [3], which has dimension D = 1.58. The realization of fractal lattices opens up the path to electronics in fractional dimensions. Then, I will show how to realize topological states of matter using the same procedure. We investigate the robustness of the zero modes in a breathing Kagome lattice, which is the first experimental realization of a designed *electronic* higher-order topological insulator [4], and the fate of the edge modes in a Kekule structure, upon varying the sample termination [5]. Finally, I will discuss how to realize *p*-orbital Dirac cones and flat bands in designed honeycomb lattices [6].

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FIGURES



Figure 1: Kekule lattices with different ratio of weak and strong bonds and different termination. The existence or not of topological states depends on both, the sample termination and the position of strong bonds [5].

Spin-phonon relaxation from a universal ab-initio density-matrix approach

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Abstract

Designing new quantum materials with long-lived electron spin states urgently requires a general theoretical formalism and computational technique to reliably predict intrinsic spin relaxation times. We present a new, accurate and universal first-principles methodology based on Lindbladian dynamics of density matrices to calculate spin-phonon relaxation time of solids with arbitrary spin mixing and crystal symmetry [1]. This method describes contributions of Elliott-Yafet (EY) and D'yakonov-Perel' (DP) mechanisms to spin relaxation for systems with and without inversion symmetry on an equal footing. We show that intrinsic spin and momentum relaxation time both decrease with increasing temperature; however, for the DP mechanism, spin relaxation time varies inversely with extrinsic scattering time. We predict large anisotropy of spin lifetime in transition metal dichalcogenides. The excellent agreement with experiments for a broad range of materials underscores the predictive capability of our method for properties critical to quantum information science [2-5].

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FIGURES



Figure 1: Spin-phonon relaxation in two-dimensional materials

Emerging Properties in Two-dimensional Strongly Disordered & Amorphous Membranes

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Abstract

After fifteen years of pursuing the fabrication or single crystal growth of monolayer materials, it turns out that for plenty of fundamental and practical reasons, more disordered forms such as reduced graphene oxides, polycrystalline or even totally amorphous forms of ultrathin atomic membranes present superior properties for coating applications and composites. It is particularly remarkable that *scalable disordered atomic membranes* can be now produced in fab environment, but simultaneously it is extremely urgent to establish the upper device performances of devices built from polycrystalline 2D materials, reduced oxide graphene, or the recently achieved *wafer-scale amorphous forms of sp² carbon and boron-nitride membranes* reported in Singapore [1] and Korea [2].

Here I will discuss the variety of physical properties of such disordered or completely amorphous forms of two-dimensional based materials and devices in the context of industrial applications including gas sensing, thermal, electronic and spintronic applications. In absence of usual approximations of periodicity and long range order, the supremacy of so-called order N methodologies [3,4] provide unique enabling tools to access electronic and spin transport in highly structurally complex material models. Anderson localization regimes and universal spin diffusion length will be presented [5] as well as morphology-induced thermal properties in strongly disordered reduced graphene oxides. Finally, thermal and dielectric properties of ultrathin amorphous two-dimensional membranes will be discussed in the light of recent breakthrough experiments [1,2].

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FIGURE

Figure 1: CVD growth of amorphous ultrathin hBN membranes with ultralow dielectric constants (from [2])



Defects in 2D Metal Dichalcogenides: Doping, Alloys, Vacancies and Their Effects in Magnetism, Electronics, Catalysis, Optical Emission and Bio-Applications

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Semiconducting two-dimensional transition metal dichalcogenides (TMDs) such as MoS2, MoSe2, WSe2, and WS2 hold great promise for many novel applications. Recent years have therefore witnessed tremendous efforts on large scale manufacturing of these 2D crystals. A long-standing puzzle in the field is the effect of different types of defects in their electronic, magnetic, catalytic and optical properties.

In this presentation an overview of different defects in transmission metal di-chalcogenides (TMDs) will be presented [1,2]. We will define the dimensionalities and different atomic structures of defects. and discuss how these defects could be imaged with novel optical-driven techniques. We will emphasize doping and alloying in monolayers of MoS2, WS2, and WSe2 and describe their implications in magnetism, as well as in electronic transport [3]. We will also describe the catalytic effects of edges, vacancies and local strain observed in MoxW(1-x)S2 monolayers by correlating the hydrogen evolution reaction (HER) with aberration corrected scanning transmission electron microscopy (AC-HRSTEM) [4]. Our findings demonstrates that it is now possible to use chalcogenide layers for the fabrication of more effective catalytic substrates, however, defect control is required to tailor their performance. By studying photoluminescence spectra, atomic structure imaging, and band structure calculations, we also demonstrate that the most dominating synthetic defect-sulfur monovacancies in TMDs, is responsible for a new low temperature excitonic transition peak in photoluminescence 300 meV away from the neutral exciton emission [5]. We further show that these neutral excitons bind to sulfur mono-vacancies at low temperature, and the recombination of bound excitons provides a unique spectroscopic signature of sulfur mono-vacancies [5]. However, at room temperature, this unique spectroscopic signature completely disappears due to thermal dissociation of bound excitons [5]. One-dimensional hetero-interfaces in TMDs will be shown by AC-HRSTEM in conjunction with their non-linear optical emission, constituting a new way to image 1D defects [6]. Finally, the electronic effects of C-H defects within TMDs will be discussed, as p-type doping could be controlled by the presence of C within TMDs [7].

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Quantum Interference Engineering of Nanoporous Graphene for Carbon Nanocircuitry

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Bottom-up prepared carbon nanostructures appear as promising platforms for future carbon-based nanoelectronics due to their atomically precise and versatile structure.[1] An important breakthrough is the recent preparation of nanoporous graphene (NPG) as an ordered covalent array of graphene nanoribbons (GNRs, **Figure 1a**).[2] Within NPG, the GNRs may be thought of as 1D electronic nanochannels through which electrons preferentially move, highlighting NPG's potential for carbon nanocircuitry. However, the π -conjugated bonds bridging the GNRs give rise to electronic crosstalk between the individual 1D channels, leading to spatially dispersing electronic currents (**Figure 1b**).[3] In this talk, we propose a chemical design of the bridges resulting in destructive quantum interference (QI), which blocks the crosstalk between GNRs in NPG, electronically isolating them. Our multiscale calculations reveal that injected currents can remain confined within a single, 0.7 nm wide, GNR channel for distances as long as 100 nm (**Figure 1c**).[4] The concepts developed in this work thus provide an important ingredient for the quantum design of future carbon nanocircuitry. In addition, our latest results demonstrating an external control of these characteristics will also be presented.

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FIGURES



Figure 1: (a) Scanning tunneling microscopy image of the fabricated NPG. Inset: high-resolution image of the 2D material; (b) Electrical injection simulation in a large-scale model of the fabricated NPG and (c) in our proposed QI-engineered NPG.

Understanding the excitonic physics of organic-inorganic 2D perovskites for efficient and low-cost photovoltaics

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Hybrid (organic-inorganic) halide perovskites (HaPs) have recently emerging as a low-cost semiconductors for optoelectronics, notably yielding single-junction solar cells with efficiencies larger than 22%. Two-dimensional (2D) perovskites (2D-HaPs) are a sub-class of HaPs offering a pathway for improving the efficiency and durability of HaP optoelectronic devices, and for developing devices with new functionalities exploiting the unique physics of these materials. However, there still limited knowledge of both the fundamental physics and the growth of both 2D-HaPs crystals and thin films used for integration in devices. In particular, there is no general understanding of the interplay between, on the one hand, the photo-excited states and electronic properties of 2D-HaPs and, on the other hand, their soft and dynamic lattice structure. Here, using optical spectroscopy and magnetoabsorption, coupled with structural probes, we report the dependence of the formation, dynamics, and recombination of exciton states on the structural and compositional details of hybrid 2D perovskites [1]. Our work reveals the changes in the exciton properties due to the tuning of the thickness of the 2D perovskites and the size of the organic molecules in the lattice (Fig. 1a). The exciton characteristics are explained by an advanced model which includes guantum and dielectric confinement. Moreover, we demonstrate the existence of unique electronic states located at the edge surfaces of the 2D perovskite layers (Fig. 1b), which promote the dissociation of the strongly bound excitons and possibly result from local distortions of the lattice at the edges [2]. By understanding the details of thin film formation and by controlling the phase purity and orientation of the 2D perovskite crystals in films we fabricated single junction solar cells with >17% power conversion efficiencies with state-of-the-art stability. Finally, we will discuss the hetero-coupling between 2D perovskites and transition metal dichalcogenides, which yield photoluminescence enhancement by more than one order of magnitude as compared to their constituent [3].

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FIGURES



Figure 1: (a) Scaling of the exciton binding energy with the perovskite layer thickness. *n* represents the thickness of the perovskite layers in terms of number of octahedra Pbl₆ units in the out-of-plane direction, where the perovskite real thickness is about n times 0.65 nm. (b) Observation of active edge-surface states in certain hybrid 2D perovskite due to local distortions at the edge of the perovskite layers. The top colour pictures are maps of the photoluminescence (PL) detected at two wavelength. The bottom images sketch the location of edge-surfaces in 2D perovskite layers.

N-doping in 3D graphene foams by chemical vapour deposition

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The possibility to realize three dimensional (3D) graphene based architectures, able to strongly increase the high specific surface areas of this challenging material, while maintaining strong mechanical strengths and fast mass and electron transport kinetics, make them very promising in fields like sensing or catalysis [1]. In this contest, dopants like N can be introduced to induce a charge polarization in the carbon lattice, modifying its electronic properties and surface wettability, or to create anchoring sites for chemical reactions often used in organic chemistry to functionalized surfaces, enabling specific reactions and catalysis processes [2,3]. In this work we realize N-doped 3D graphene foams (GF) by chemical vapor deposition on Ni foams used as templates. We used CH₄ and H₂ as gaseous precursors and NH₃ as N-doping source. The synthesis process is widely investigated in order to study the doping process and optimize the N type bonding mechanism. We found that the state in which N rearranges into the graphene lattice strongly depends on the stage of the Chemical Vapour Deposition (CVD) synthesis in which the NH3 is introduced in the reaction chamber. Moreover, if the N doping level is very high, it can affect the lateral growth of the graphene clusters, thus leading to micrometric triangular graphene domains. Morphological characterizations as a function of the CVD process conditions are modelled and their scenario is validated by means of ab-initio calibrated kinetic Monte Carlo simulations. The obtained data are of fundamental importance for a successful application of N-doped GF structures in sensing or catalysis field.

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Figure 1: Scanning electron microscopy image of a sample of N-doped graphene grown by CVD on a nickel foam template

MXenes: the largest family of 2D materials

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Two-dimensional (2D) materials have attracted huge attention in nanotechnology thanks to the enhanced low-dimensional quantum effects resulting in outstanding electronic, optical, and magnetic properties. Among these 2D systems, the emerging family of 2D transition metal carbides and nitrides, known as MXenes, stands out because of the wide chemical diversity allowing for materials property tuning. In contrast to graphite-like layered materials which can be mechanically exfoliated to obtain 2D flakes, MXenes are obtained from the chemical treatment of the three-dimensional MAX phases, represented in **Figure 1** [1,2]. MAX phases are layered ceramics with the general formula $M_{n+1}AX_{n}$, where M represents an early transition metal, A an element from groups 13 to 16, X either a carbon or a nitrogen atom, and n varies from 1 to 3 [3]. Since the discovery of the first MXene, Ti₃C₂T_z, at Drexel University in 2011, more than 30 MXenes have been synthesized, and the stability and properties of dozens more have been investigated using ab initio calculations [4]. The exploration of new MAX phases and derivative MXenes is of great interest to further control materials properties and highlight potential applications, such as catalysis, energy storage, and related electrochemical applications. In this talk, the different classes of MAX phases will be introduced and their potential exfoliation into their 2D counterparts, MXenes, will be discussed (Figure 2) [5]. Additionally, their respective structural, electronic, and elastic properties predicted by ab initio calculations and characterized by various experimental techniques will be discussed.

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FIGURES



Figure 1: Schematic representation of the synthesis process of 2D MXenes, obtained from the selective etching of the AI planes from the parent 3D MAX phases when immersed in HF solution. Adapted from [2].

Figure 2: Computed static exfoliation energy as a function of the bond length for a series of ~90 MAX phases. Data from [6] are also presented (empty circle). Adapted from [4].

Electronic interactions at the graphene interface: the effect of substrate and the media

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Graphene possesses a unique combination of electronic and chemical properties, which makes it particularly suitable for developing electrochemical devices for biomedical applications. Due to its aspect ratio, i.e. large surface exposure for a minimal thickness, graphene is widely used in a number of biological sensing devices, where it is in direct contact with an aqueous electrolyte containing ions and molecules of different nature. Previous works concerning bidimensional (2D) materials-based sensors reveal extremely large dispersions regarding graphene's sensitivity to specific analytes. Such differences are not well understood and may be attributed to intrinsic (eq. related to the graphene quality) and/or extrinsic (eg. the nature of the substrate or the presence of absorbed charges) factors. Thus, understanding the interaction of this 2D material with the aqueous medium and the way charges in the solution may screen those in graphene, is crucial. In this work, we explore how the graphene/electrolyte interface is affected by a combination of factors: substrate, medium (eg. pH, ionic strength) and altered surface chemistry (absorbed charge), providing a more profound understanding of the physicochemical interfacial phenomena. To this end, spectroscopic techniques such as Raman and Electrochemical Impedance were used. We demonstrate that Raman enables addressing charge carriers in graphene supported on conductive or insulating substrates; as well as being an indirect measurement of the adsorbed charge in graphene [1]. Complementary, from impedance spectroscopy we obtain information about the capacitance dependence with the parameters of study: substrate nature, pH, ionic concentration and applied voltage [2]. Additionally, theoretical simulations help in understanding the effect of involved phenomena as the type of the adsorbed charge and the graphene/substrate coupling. Our results have unveiled an intriguing effect of the graphene's close environment on the carrier modulation of graphene, which have revealed the need for uncovering a strategy to place a controlled adsorbed charge on top of graphene, precious information for numerous applications involving graphene-liquid interfaces.

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FIGURES



Figure 1: Left) Schematic lateral view of the graphene electrode device for in situ Raman characterization. Right) Fermi Level modulation (i.e. LO phonon energy) with the ionic strength at different pH.

Dirac fields in curved graphene

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ABSTRACT

From the perspective of high energy physics, graphene can provide us a real framework to study what is believed to be (as close as possible) a quantum field in a curved space-time. The peculiar structure of a graphene sheet determines in fact a natural description of its properties in terms of relativistic Dirac pseudoparticles. The charge carriers' behaviour at Dirac points in curved graphene can be thus obtained exploiting a Dirac spectrum description for particles living in a curved bidimensional background, in the large wavelength approximation [1].

The study of particular curved configurations, together with the quantization of some physical quantities due to the particular geometry of the manifold, can lead to characteristic observable effects. In particular, some optical responses of the graphene sheet can be obtained in peculiar ranges of energy including the visible light energy spectrum [2].

A more generic, geometrical top-down approach to realize the physics of graphene charge carriers can be obtained exploiting the holographic principle, where the 1+2 dimensional theory for graphene is realized as the boundary theory of a four-dimensional gravity model in Anti de Sitter (AdS) spacetime. The result is achieved through suitable boundary conditions for the D=4 fields, and an effective model for spin-1/2 fields on a curved background is obtained [3]. The unconventional symmetry of the boundary model allows to introduce suitable internal degrees of freedom, which can provide an application of the model to the description of general graphene-like 2D materials at the Dirac points K,K'. In particular, the two valleys correspond to the two independent sectors of the boundary model, connected by a parity transformation. The fermion masses entering the corresponding Dirac equations are related to the torsion parameters of the substrate in the three-dimensional model: the parity-even and odd components of the corresponding masses are identified with Semenoff and Haldane-type mass contributions, respectively [3].

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Fig.1: Optical conductivity for graphene nanoscroll



Fig.2: Holographic correspondence

GRAPHENE AND 2DM ONLINE CONFERENCE (GO2020)

FIGURES

Charge-to-Spin Conversion in Low-Symmetry Topological Materials

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In this work, we theoretically show that the reduced symmetry of strong spin-orbit coupling materials such as MoTe2 or WTe2 enables new forms of intrinsic spin Hall effect that produce large and robust in-plane spin polarizations in coexistence with the traditional out-of-plane component. Through quantum transport calculations on realistic devices in the diffusive regime, we show that spin-charge interconversion can reach efficiencies of 80%, while also possessing long spin diffusion lengths (~100 nm). Such combination is largely superior to what is typically found in conventional SHE materials. These findings vividly emphasize how crystal symmetry governs the intrinsic SHE, and how it can be exploited to broaden the range and efficiency of spintronic functionalities. We also propose specific experimental guidelines for the confirmation of the effect.



Figure 1: Nonlocal resistance (solid lines) as a function of channel length, L, for spins polarized along x, y and z. Error bars result from averaging over 150 disorder configurations (channel width is 50 nm). Dashed lines are fits using diffusive theory. Left inset: Diagram of the nonlocal spin valve. Black (red) regions denote the device (leads), with leads 2 and 3 being ferromagnetic. Current I0 flows from lead 2 to 1 and the nonlocal voltage is measured between leads 3 and 4. Right inset: Energy-dependence of the spin relaxation lengths for all spin components. The dot-dashed line marks the conduction band minimum of MoTe2

Development of *ab-initio* method to multiwave-length dependent Raman spectroscopy of 2D-nanomaterials

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Abstract

We developed how to analyse non-resonant Raman spectra by using the Placzek approximation based on semi-classical approximation of electronic and vibrational transition energies [1]. Upon calculated frequency-dependent dielectric tensors, we can compute polarized Raman intensities by averaging over all in- and out-plane polarizations, allowing us to capture Raman resonance effects in first-order Raman scattering. Our *first-principle* investigation covered a broad family of nanocarbons from well-known cases, e.g. graphene, fullerene, and graphene nanoribbons till systems with unique architecture, like fully flattened single-walled carbon nanotubes and graphitic prismatic edge dispersion of the D peak, attributed to the curvature which acts as activating defect as confirmed in recent experiments [2,3]. Given its robustness, the application of our approach can be extended to reproduce the Raman characterisation of other nanomaterials beyond graphene, like phosphorus allotropes encapsulated in single-walled carbon nanotubes [4].

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Figure 1: (a) Atomic Force Microscopy height image of 3 flattened (FCNT) and 3 cylindrical (CNT). (b) Corresponding Raman spectra normalized over the G peak recorded at 2.4 eV. (c) Calculated Raman spectra of a zig-zag (70,0) fully FCNT at different excitation energies. (d) Eigendisplacements of the strongest vibrations contributing to the Raman D peak with its non-zero Raman tensor components. (e) Colour mapping representation of dispersive character of the D peak.

Lightwave Valley Polarization in Graphene

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Abstract: We investigate a Valleytronic device based on graphene with charge separation at different sublattices (and correspondingly at nonequivalent valleys K and K') as high as 60 percent. We characterize the maximality condition of valley polarization and investigate the parameters and conditions upon which we can coherently control the carriers and store data via valley degree of freedom. The valley polarization is controlled by the amplitude as well as the carrier-envelope phase of the pulse – one cycle optical field - and the curvature of the electron trajectory in the reciprocal space. We believe the results of our study will step forward the valleytronics and shed light on ultrafast data storage and processing with utmost reliability and robustness.

The possibility of incorporating a valley degree of freedom to store and carry information has drawn numerous attention and led to substantial electronic applications labeled as valleytronics. The valley pseudospin has the potential to serve as a robust quantum signal processor and data storage with a petahertz bandwidth. Despite some attempts, the generation and detection of VP in pristine graphene has been elusive due to the presence of inversion symmetry. In this letter, we report VP with efficiency as high as 60 percent by utilizing a single-cycle elliptically polarized pulse with controllable polarity, amplitude, and carrier-envelope phase (ϕ_{CEP}). Such a noticeable VP in monolayer graphene is attributed to the nonperturbative dynamics of electrons in the strong electric field of the laser pulse, the global topology of the honeycomb band structure, and the nonequivalent Berry phase of $\pm \pi$ at the K and K' valleys [1,2]. In fact, the incident electric field of the ultrafast laser breaks the inversion symmetry giving rise to a nontrivial Berry curvature and produces the valley-contrasting population in the reciprocal space.



Figure 1: (a) Illustrate the parametric waveform of the electric field, F, and the vector potential, A, for different polarization states of the pulse. Valley polarization of gapless graphene is plotted versus field amplitude (b), ellipticity (c) and carrier-envelope phase (d).

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Plasma-etched functionalized graphene as a metal-free electrode catalyst in solid acid fuel cells

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Abstract

Graphene has demonstrated considerable potential to replace costly precious metal catalysts in a broad range of technological applications[1, 2]. As such, extensive research is being conducted on investigating the substitution capability of graphene, particularly with respect to the fuel cell industry[3, 4]. In this work, graphene was subjected to O_2 or N_2 plasma treatment to create catalytically active sites through the introduction of functional surface groups and defect site generation. Density functional theory (DFT) calculations were used to evaluate the effect of plasma treatment on the activity of the graphene sheets in the oxygen reduction reaction (ORR) coupled with experimental results. ORR activities were adequately enhanced by plasma treatment. DFT calculations further identified that zigzag carbon atoms could be the most active site for the ORR in O₂ and N₂ plasma-etched graphene. In addition, the armchair carbon atom adjacent to the heteroatom is another primary active site for N₂ plasma-etched graphene. The C=O functional aroups in conjunction with the armchair carbon also showed high ORR activity. The O_2 and N_2 plasma-treated graphene was successfully used as an electrode catalyst in a solid acid fuel cell (SAFC). These results provide important basic information about the value of using plasma-etched graphene in SAFCs and will aid future efforts in the development of catalytically active and stable non-precious metal materials for use in fuel cell cathodes.

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FIGURES

Figure 1: Simple schematic drawing of electrochemical cell (Graphene|CsH₂PO₄|Pt/C/CsH₂PO₄)



Suitable substrates for the synthesis of stable aluminene allotropes

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Following the example of graphene, recent studies discovered a number of atomically thin monoelemental materials. Many of them were synthesized, while some of them still await their experimental realization [1,2]. Motivated by the huge application potential, inherited from its bulk counterpart, the present study concerns the conditions under which the aluminium monolayer, aluminene, could be synthesized in the laboratory for the first time [3]. We start by considering four different allotropic modifications: planar, buckled, triangular and puckered. The study shows that planar and triangular allotropes can be stabilized by strain engineering imposed upon the monolayer. Ab initio simulations show that these allotropes have appropriate cohesive energies and stable lattice dynamics. We discover that Cu(111) and graphene can act as suitable substrates for the synthesis of aluminene. Substrate-monolayer interaction causes the necessary in-plane strain to stabilize the phonon dynamics. The studied aluminene allotropes are stable with respect to thermal effects at room temperature. STM images are simulated to facilitate future experimental characterization of aluminene. Aluminene preserves the good thermal properties (specific heat) of aluminium, further advancing its application as an ultra-thin thermal insulator or heatsink. The study will stimulate experimental studies focused on both nanomaterial synthesis and applications of atomically-thin aluminium layers. At the end further insights into the monolayer-substrate relationship are given.

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FIGURES



Figure 1: Top-down view of a single-layer aluminene model placed on Cu(111) surface substrate. On the right the predicted STM imaging is shown revealing bright spots where the AI atoms could be found with respect to the bottom Cu atoms.

Inkjet printable water-based inks made by electrochemically exfoliated graphene

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Abstract:

The field of printed electronics has developed rapidly, driven by printing techniques offering low-cost and simple methods for devices fabrication, whilst demonstrating compatibility with most substrates including those that are soft and flexible [1]. Inkjet printing of graphene inks are very attractive for applications in flexible and foldable electronics, such as wearable electronics and the Internet of Things. However, the ink preparation is still very time consuming as high concentrations can be achieved only with prolonged sonication (>24 h) or with expensive setups [2, 3]. In this work, we demonstrate a water-based inkjet printable ink made from electrochemically exfoliated graphene. The printable ink production is achieved in less than 5 h, leading to a stable (for over a month) formulation with concentrations up to 2.25 mg mL⁻¹ [4]. The formulated ink consists of over 75% single and fewlayers graphene with and average lateral size of 740 nm. Such ink formulation allows stable jetting, rapid ink drying (<10 sec) as well as ensuring wetting of untreated substrates such as paper and glass. Thermal annealing of the printed films allows to achieve high C/O ratio which translates into one of the highest electrical conductivity (i.e. \sim 3.91 x 10⁴ S m⁻¹) reported so far for solution-processed inkjet printable graphene, without the use of any harsh chemical processing.

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FIGURES



Figure 1: Comparison of the electrical conductivity measured on our inkjet printed electrochemically exfoliated graphene after annealing at 300 °C for 1 h with literature based on different types of inkjet printable graphene formulations.

Solvent interactions with two-dimensional materials: A computational investigation of the dispersion of graphene monolayers in commonly used solvents

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Maintaining stable dispersions of two-dimensional (2D) materials is a prerequisite for several applications, including surface coatings, printed circuits and some electronic devices. The dispersions are typically produced by the liquid phase exfoliation (LPE) of layered materials. The stability of the solution, i.e., the ability of a solvent to maintain an adequate concentration of suspended flakes over time, is strongly dependent on the chosen solvent [1]. To identify an optimal solvent for a particular 2D material, it is important to determine the role of (i) the initial exfoliation (ii) the free energy of solvation and (iii) the reaggregation rate, the latter two of which will depend strongly on the nature of the solvent – solute interface.

Here, we use density functional theory (DFT) and molecular dynamics (MD) to investigate the stabilization mechanism. We show that solvent molecules interact via a van der Waals (vdW) interaction with the monolayers, with negligible charge transferred between the two [2]. We find that distinct solvation shells are formed around the 2D layer (Figure 1). The first solvation shell is formed irrespective of the nature of solvent (i.e., whether polar or non polar) due to vdW interactions. This first shell then interacts with rest of the solvent via a combination of both electrostatic and dispersion forces. We show that the formation of these solvation shells is always favourable by calculating the enthalpic and entropic contributions to the free energy of interaction. However, energetic considerations such as these cannot explain the experimental solvent-dependence. Instead, kinetic effects can dominate. We find that interfacial solvent molecules with high diffusion coefficients parallel to the graphene layer result in the lowest experimental concentration of graphene in solution. This can be explained by the enhanced ease of reaggregation in the high diffusion regime (Figure 2). Solvents with smaller diffusion coefficients correspond to higher experimental graphene concentrations. In the low diffusion limit however, this relationship breaks down. We suggest that here the concentration of graphene in solution depends primarily on the separation efficiency of the initial LPE step.

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FIGURES





Figure 1: Position (top panel) and angle (bottom) distribution function for N-Methyl-2-Pyrrolidone (NMP) molecules as a function of distance from a graphene monolayer. The insert shows how the co-adsorption of NMP at two different angles results in the double-peak structure of the first solvation shell. Figure 2: Re-aggregation model: The solvent molecules must diffuse out between two reaggregating graphene layers. The parallel diffusion coefficient of the first solvation shell will determine the reaggregation efficiency.

Optical studies of the growth kinetics of individual carbon nanotubes

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Abstract

Carbon nanotubes (CNTs) due to their unique properties are promising materials for electronic and optical applications. However, several unsolved problems stand on the way toward their practical usage, especially the direct synthesis of CNTs with desired chirality and structure. To address this question, our team developed optical methods to image individual CNTs in real growth conditions (at ambient pressure, on a substrate) and relate their growth kinetics with their chirality. More precisely, we grew horizontally-aligned carbon nanotubes on quartz substrate by chemical vapour deposition (CVD)1 varying the temperature and precursor pressure during the synthesis. Such a substrate-aligned growth allows us to collect in situ optical images of nanotubes by a unique optical setup2. This imaging technique provides crucial information about the nanotube growth kinetics such as their growth rate, lifetime and nucleation time with high temporal resolution (down to 10 ms). Further Raman analysis of grown CNTs3 completes our set of data with information about the nanotube chirality and defectiveness thus allowing us to correlate nanotube structure and growth kinetics. The Raman analysis of CNTs on quartz substrate is known to be complicated by radial deformation and axial strain but our study revealed that a careful analysis of these information-rich secondary Raman features (beside the classical RBM frequency and Gband shape) can be used to precisely assign the CNT chirality. This allowed us to precise the relation relating the RBM frequency and the CNT diameter for CNTs grown on quartz.

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Boundary modes using impurities: graphene and the Kane-Mele topological insulator

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We provide a new direct and non-numerical technique to describe the formation of edge states in the Kane-Mele model [1]: a topological insulator created by adding spin-orbit interactions to graphene. This technique is based on the T-matrix formalism. We start with an infinite system and model the boundary using a line-like infinite-amplitude potential. We also mention an analytical application of our method to obtain, within a lattice model, the wave functions of the edge states in zigzag- and bearded-edge graphene.

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FIGURES



Figure 1: Spectral function obtained with our method for the Kane-Mele model, with (a) a weak impurity potential and (b) a strong impurity potential. The states created by the impurity can be seen in blue, while the bulk states are in red.

Optical Tuning of Hole and Electron Transport in Ambipolar WSe₂ Interfaced with a Bicomponent Photochromic Layer: From High-Mobility Transistors to Flexible Multilevel Memories

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Abstract

The interfacing of two-dimensional materials (2DMs) with photochromic molecules provides an efficient solution to reversibly modulate their outstanding electronic properties and offers a versatile platform for the development of multifunctional field-effect transistors (FETs). Our work mainly focuses on 2DM-based optically switchable multilevel high-mobility FETs obtained by interfacing such 2DM with photochromic diarylethene (DAE) molecules acting as light-sensitive components (Figure 1). The efficient and reversible photochemical isomerization of the DAEs between the open and the closed isomer, featuring different energy levels, makes it possible to generate photoswitchable charge trapping levels, resulting in the tuning of charge transport through the 2DMs by alternating illumination with UV and visible light. We have demonstrate the feasibility and general applicability of our approach to optically control the transport of electrons (n-type dominant WSe₂), or holes (p-type dominant black phosphorus),^[1] or both charge carriers (ambipolar WSe₂),^[2] depending on the nature of the target 2DM. Noteworthy, the high output current modulation efficiency in ambipolar WSe₂ (97% for holes and 52% for electrons) ensures 128 distinct current levels, corresponding to a data storage capacity of 7 bit. The device is also implemented on a flexible and transparent polyethylene terephthalate substrate, rendering the 2DMs/DAEs hybrid structures promising candidates for flexible multilevel nonvolatile memories.^[2]

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FIGURES



Figure 1: Dynamic output current-time curve under periodic UV irradiation. Insert is the schematic illustration of the FET device architecture based on WSe₂/DAE blend with the energy level diagram.

Ultra-broad spectral photoresponse in FePS₃ air-stable devices

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Abstract

The family of transition metal phosphorus trichalcogenides, with general formula MPX₃ (with M a transition metal, P phosphorus and X = S or Se chalcogens), is gaining relevance as they offer competitive advantages when compared to other semiconducting and/or magnetic two-dimensional materials [1]. The photoresponse of FePS₃ has recently been addressed in the context of photodetection applications limited only to the ultraviolet spectral range [2]. Here, we push forward the state of the art, presenting a detailed spectral distribution of the electrical photoresponse of FePS₃ nanosheets, finding that FePS₃ is a narrow gap p-type semiconductor with a high enough conductivity to enable the electrical detection of optical excitations in a broad wavelength range. In addition, we observe a significant stability of FePS₃ nanosheets when exposed to air and/or light, higher than for other magnetic materials, which facilitates device preparation, characterization and, eventually, application. With views to the future, this work manifests the relevance of FePS₃ not only for ultrabroad photodetection but as a key material for investigations on magneto-optics and opto-spintronics at the 2D limit among a wide spectral range.

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FIGURES



Figure 1: (a) Optical image of a FePS₃ device onto a SiO₂/Si substrate with pre-patterned Ti/Au contacts (1-3). (b) *I-V* plot at different applied gate voltages ($V_g = -10, 0 \ 10 \ V$). (c) Photocurrent versus time at different optical excitation energies. (d) Our experimental Tauc plot (blue and grey dots) and absorbance measurements reported by Brec, et al. (red dots) [3]. (e) Rise time of the FePS₃ photodetector as a function of the incident photon energy. The inset shows the trend of the photocurrent with time as a function of energy.

Electrophoretic coating of LiFePO₄/Graphene oxide on Carbon Fibers as High-Performance Cathode Electrodes for Structural Batteries in Aeronautics

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Structural battery composites, typically based on Carbon Fibers (CF), are a class of structural power composites which can be included in the framework of airplanes and cars to reduce weight and provide energy for distributed electronics at the same time.[1] CF can be easily used as anode in Li ion batteries, but need chemical functionalization to be used as cathode. Here, we describe a binder-free method to deposit a composite of lithium iron phosphate (LiFePO₄) and electrochemically exfoliated graphene oxide (EGO) on CF. To this aim, we use Electrophoretic Deposition (EPD) which is a versatile, scalable and cost-effective technique to deposit uniform coatings on electrodes for Lithium Ion Batteries.[2] We performed comparative tests varying the surface tension and chemistry of the solvent using pulsed bias to achieve uniform LiFePO₄/EGO coatings (**Figure 1a**). The optimal conditions allowed to achieve a high LiFePO₄ mass ratio >90 wt%, also featuring good adhesion on the CF and low cracking or degradation upon battery cycling.

Samples were characterized by XRD, Raman and SEM measurements. The electrochemical performance of the coated CF was investigated through cyclic voltammetry and galvanostatic charge/discharge showing excellent rate performance (**Figure 1b**) at different current densities, as tested in Half-Cell vs. Li, outperforming similar state-of-the-art cathode materials. Besides the promising performance of the LiFePO₄/EGO we describe here, the EPD method shall be used for deposition on CF of composite materials made of carbon and metal oxides,[3] paving the way towards facile electrophoresis synthesis of cathode materials for all Li batteries.

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Figure 1. (a) SEM LiFePO₄/EGO Coated CF. Inset: cross-section view (b) Specific capacities (normalized over the total electrode mass) of the LiFePO₄/EGO optimum sample at various C-rates.

Fast response, high responsivity and broadband Graphene/n-Si photodetector

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To surmount the limiting low efficiency in near ultraviolet and infrared regions of Si photodetectors (PDs) [1], and to improve its temporal response, we present a detector based on Graphene/n-Si hetero-junction [2,3]. In this device graphene takes on a multiple role: semi-transparent light window, Schottky junction constituent, photo charges generator and collector. The designed PD multifinger geometry allows to obtain the typical I-V characteristics of a three terminals device (Fig.1) which can be used in photovoltaic (PV) and in photoconductive (PC) mode. The obtained PDs which operate at room temperature, are sensitive in the spectral region from the UV (240 nm) to the IR (2000 nm). Moreover, they have high responsivity up to 10⁷ A/W, a rise time of a few ns, an external quantum efficiency more than 300%, and a linear response for different light sources. The obtained results are among the highest respect others graphene and carbon nanostructures-based devices thanks to the high quality of the graphene deposited on a large area of 8 mm² supported by our device design [4,5] of the interdigitated electrodes, preserving the excellent properties of graphene when switching from a nanoscale to the macroscopic dimensions of commonly used devices.

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FIGURES

graphene/n-Si Photodetector

spectral range: 240 – 2000 nm

Responsivity: 10⁷ A/W

Rise time: 1 ns

Active area: 8 mm²

Figure 1: Source-drain current I_{SD} vs. gate voltage V_G acquired in dark conditions for different values of V_{SD} . Inset: device schematic under illumination in PC mode

Graphene field effect transistors using TiO₂ as the dielectric layer

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It is very important to find a suitable substrate for graphene electronic devices. In this work, we report the electron mobility and electron density of three graphene field effect transistors using a 280 nm titanium dioxide dielectric layer and a graphene channel of area $300 \times 300 \ \mu\text{m}^2$. We achieve electron mobilities up to 1877 cm²/V and the Dirac point appears in small gate voltages, as compared to similar SiO₂ transistors. Also, we obtain the TiO₂ surface roughness through profilometry and confirm that electron mobility is inversely proportional to the channel's surface roughness.

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FIGURES



Figure 1: (a) 3D printed mount for the electronic characterization of the GFET. (b) The circuit's diagram. The sample (c) is inserted in the middle of the mount in (a).



Figure 2: (Left) Comparison of the TiO₂ GFET with respect to a typical SiO₂ GFET [1]. (Right) Effect of roughness on electron (blue circles) and hole (red squares) mobilities of TiO₂ GFETs.

Nanographene oxide and PEGylated reduced nanographene oxide as platforms for anti-cancer drug delivery

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Cancer is the second leading cause of death globally. Currently used pharmacological treatments (chemotherapy) present several drawbacks, including the need for high doses of cytotoxic drugs, systemic administration and consequent long-term and late developing severe side effects. Hence, there is a pressing need for more effective drug delivery strategies. Over the past decades, several therapeutic nanocarriers have been explored to deliver anti-cancer drugs to cancerous tissues. Graphene-based materials (GBM) possess large surface area, holding potential for synergistic biologic and drug release effects [1]. In this study, we explored nanographene oxide and PEGylated reduced nanographene oxide as platforms for drug delivery using 5-fluorouracil (5-FU), a widely used drug with anti-cancer activity [2]. Nano-sized graphene oxide (GOn) was produced through the modified Hummer's method [3] followed by ultrasonication using a custom-built industrial grade system. Through this method, we assure the achievement of reproducible large-scale batches of nano-sized GBM. Afterwards, following a single-step procedure, GOn was thermally reduced and noncovalently functionalized with poly(ethylene) glycol bis(amine) (PEG-NH₂) to obtain stable aqueous dispersions (rGOn-PEG) [4]. Oxidation degree, reduction and PEGlyation of GOn were characterized by XPS, FTIR and UV-vis spectroscopy, as well as thermal analysis by TGA. Particle size was determined by transmission electron microscopy (TEM). Surface charge was measured using a zetasizer. GOn and rGOn-PEG (0.125 mg/mL) were sonicated for 30 min and mixed with 5-FU dispersions at a drug concentration varying between 0.25-5 mg/mL, in water. Aliquots were collected from 0 min to 72h, centrifuged (13000 rpm), and the difference in free 5-FU quantified by measuring its absorbance (265 nm). GBMs and drug absorbance spectra (200-850 nm) were obtained using a UV-Vis spectrophotometer. GOn and rGOn-PEG were obtained with mean lateral dimensions of 287 nm and 521 nm, respectively, as determined by TEM. XPS analysis revealed that the O at.% was of 31.95% and 15.87% for GOn or rGOn-PEG, respectively. GOn reduction was further confirmed by a redshift in the characteristic absorbance peak and increased rGOn-PEG absorbance in the nearinfrared range of UV-vis spectra, in comparison to unmodified GOn. GOn and rGOn-PEG dispersions showed colloidal stability with zeta potential values around -25.6±0.8 mV and -10.2±0.3 mV (pH=7.4), respectively. 5-FU was successfully loaded by simple molecular physisorption on GOn and rGOn-PEG. Maximum drug loading efficiency was achieved almost immediately after mixing GBMs with 5-FU, regardless of concentrations tested. Drug loading capacities of 5.8±0.8 mg 5-FU/mg GOn and 3.6±1.2 mg 5-FU/mg rGOn-PEG were achieved. This can be explained by favorable interaction between GOn oxygen-containing groups and hydrophilic 5-FU, and possibly by PEG hinderance of drug adsorption. This study shows the successful production and single-step functionalization of nanosized GBM and the potential using GOn and rGOn-PEG as platforms for anti-cancer drug delivery.

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ACKNOWLEDGMENTS

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Electron Optics in Phosphorene pn Junctions: Negative Reflection & Anti-Super-Klein Tunneling

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Ballistic electrons in phosphorene pn junctions show optical-like phenomena. Phosphorene is modeled by a tight-binding Hamiltonian that describes its electronic structure at low energies, where the electrons behave in the armchair direction as massive Dirac fermions and in the orthogonal zigzag direction as Schrödinger electrons. Applying the continuum approximation, we derive the electron optics laws in phosphorene pn junctions, which show very particular and unusual properties [1]. Due to the anisotropy of the electronic structure, these laws depend strongly on the orientation of the junction with respect to the sublattice. Negative and anomalous reflection are observed for tilted junctions (Figure 1), while the typical specular reflection is found only, if the junction is parallel to the zigzag or armchair edges. Moreover, omni-directional total reflection, called anti-super-Klein tunneling, is observed if the junction is parallel to the armchair edge (Figure 2). Applying the nonequilibrium Green's function method on the tight-binding model, we calculate numerically the current flow. The good agreement of both approaches confirms the atypical transport properties, which can be used in nano-devices to collimate and filter the electron flow, or to switch its direction.

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FIGURES



Figure 1: Electron optics in phosphorene pn junctions. Negative reflection is found for tilted junctions.



Figure 2: Omni-directional total reflection, called anti-super-Klein tunneling, is observed if the junction

FeOOH/Cyanographene hybrid material for efficient operation in organic electrolytes as supercapacitor electrode Smita Talande

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Abstract

Supercapacitors (SCs) are considered as a promising clean energy storage device. However, to meet the continuously rising energy demand for portable power, it is crucial to enhance the energy density of present SCs, without sacrificing their power and high life-cycle. Toward this goal, integration of pseudocapacitive materials (such as iron oxides, FeOx) has been pursued. High-performance FeOxbased electrodes are mostly prepared by employing hydrothermal, chemical vapor, atomic layer or electro-deposition methods, and even with the combination of these methods which require current collectors other than the commercial AI thin foils. Therefore, a significant amount of inactive mass is added to the device and the fabrication is incompatible with the currently used roll-to-roll pastedeposition processes. Importantly, they operate in low-voltage aqueous electrolytes, limiting their energy. Hence, we developed FeOx-based material with high affinity for organic electrolytes owing to hybridization with a covalently functionalized graphene derivative (cyanographene, G-CN) used as compatibilizer and charge carrier support for the FeOOH nanoparticles. After a facile, cost-effective and up-scalable 15 min microwave-assisted synthesis, the hybrid was casted as paste on AI foil for the assembly of symmetric SCs. Therefore, exploiting the properties of G-CN to purposefully modify the features of FeOOH, a combined high energy and power density was achieved (with respect to total mass of the electrodes, i.e. including current collectors), surpassing previous FeOx-based SCs.

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Imprinting chirality and doping in graphene nanopores

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ABSTRACT

Functionalizing and imprinting chirality on 2D nanoporous membranes are key factors to drive specific host-guest interactions for selective sensing and sieving. Although a variety of pore structures can be obtained with Van der Waals supramolecular networks [1], stable membranes require stronger, covalent networks. Recent advances in this direction, such as the on-surface synthesis of nanoporous graphene (NPG) [2,3], demonstrate the feasibility of tailoring nanopores with the same atomic precision covalent 2D membranes.

Here we use pyrimidine functionalized bisanthracene precursors that undergo each of the reaction steps required for the realization of doped, chiral nanopores in the same graphene matrix. We have tracked each reaction step with STM demonstrating that chirality is imprinted from precursors to each of the intermediate products, up to the formation of pores in coupled graphene nanoribbons. Our combined tunnelling spectroscopy and ab-initio study indicates that the role of the N-dopants is to shift the conduction and valence bands rigidly without modifying the band gap, an effect that is hindered by the Fermi level pinning on the metal support [4], and to introduce localized states that can act as specific anchoring centres for chiral host-guest interactions. Our results pave the way to find out feasible on-surface routes to synthesise functionalized and chiral NPGs with longer range order.

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Figure 1: Schematic representation of the chemical path to synthesize nitrogen-doped NPG with axial chirality, and STM topography image of one of the two enantiomers that coexist on the surface. The image is obtained at constant height, with a CO-functionalized tip.

Effective Reduction of Oxygen Debris in Graphene Oxide

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Abstract (Arial 11)

Graphene oxide (GO) raised substantial interest in the last two decades thanks to its unique properties beyond those of pristine graphene, including electronic energy band-gap, hydrophilic behavior and numerous anchoring sites required for functionalization[1]. In addition, GO was found to be a cheap mass-production source for the formation of the pristine graphene. However, the presence of numerous clusters containing oxygen functional groups (called oxygen debris[2]) on the GO surface hinders the GO integration in electronic devices.

Here, we present a simple method aimed to reduce the density of oxygen debris weakly bonded to the surface. The method consists of minimal treatments, like sonication and/or water rinsing processes. Whereas this simple method removed epoxy and hydroxyl oxygen groups weakly attached to the graphene matrix, the double C=O bonds are almost not affected by the applied treatment, as demonstrated by X-ray photoelectron spectroscopy and Fourier transform infrared spectroscopy. Scanning tunneling microscopy and high-resolution transmission electron microscopy measures designated non-uniform distribution of the oxidation sites, appearing as clusters concentrated preferentially on GO defected regions, albeit separated by pristine graphene areas. The results should have an impact in the implementation of GO in electronic devices deposited on different substrates.

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Figure 1: Characterization of the as-purchased GO multilayer samples: (a) A STM image; (b) Fourier transform of image in (a), showing two distinct regions: An inner part at low frequency, corresponding to a distorted region as framed by a green line in (b); An outer-ring at a higher frequency, related to the "graphenic" region marked by blue-line in (a). (c) Inverse Fourier transform image considering only the higher frequencies in (b)



Figure 2: (a) STM topography image of single layer and (b) STS curve from image (a). (c) High-Resolution Core-Level C1s XPS spectra of graphene oxide in a "graphenic" region, all images are after sonication and rinsing (iii).

Ni₂C formation at the graphene/Ni(111) interface: a first-principles investigation

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The peculiar graphene properties are very sensitive to its coupling with the substrate. In case of graphene (Gr) grown on Ni(111) surface, this is strongly affected by the formation of an intercalated carbide (Ni₂C) layer, which, remarkably, occurs only under rotated graphene (RG) and not under epitaxial graphene (EG) domains [1,2]. We performed first principles simulations based on density functional theory to explain the preferential surface segregation of the Ni-dissolved C atoms under rotated graphene domains [3]. Furthermore, a complete description of the electronic properties of Gr with and without carbide, in rotated and epitaxial domains is obtained. The atomic projected density of states confirms that carbide formation decouples Gr from the substrate and restores its semi-metallic nature. Finally, we obtained the specific C1s core level shifts that are the fingerprints of different Gr/Ni₂C/Ni(111) configurations in good agreement with the experimental results.

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FIGURES



Figure 1: The structure of Ni_2C at Ni(111) under epitaxial graphene (EG, left panel) and rotated graphene (RG, right panel). C atoms of graphene are represented by small transparent red spheres and C atoms of carbide as larger orange spheres. Ni atoms of carbide are represented by big light blue spheres, and Ni atoms of Ni(111) by blue spheres. The "clock reconstruction" of carbide is emphasized with green and dark blue squares. The Ni(111) lattice, not clearly visible under carbide, is denoted by black network in the upper part of the left panel. The unit cell depicted with dashed black lines has been carefully identified to accommodate the three different lattices (Ni(111) substrate, carbide layer, graphene overlayer) both in case of epitaxial and rotated graphene.

Unlocking the Potential of Carbon Incorporated Silver-Silver Molybdate Nanowire with Light

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We present a novel form of Ag₂MoO₄-based hybrid nanowire (NW) with a few remarkable attributes. Firstly, the NW is embedded and decorated with Ag NPs. Secondly, carbon atoms are intentionally incorporated within the matrix of the NW. Thirdly the hybrid nanowires are created *via* a facile process. Namely, focused laser micropatterning of Ag NPs on GO film as seeding sites and subsequent formation of the hybrid NWs by placing the patterned GO films on heated Mo foil on a hotplate. This unique process resulted in the production of hybrid Ag/Ag₂MoO₄ NWs that emit unique red fluorescence emission. And finally remarkable photodoping effect is observed from a single strand of optically tuned carbon-doped silver nanoparticles embedded silver molybdate nanowire. We demonstrate applications of these hybrid NWs as micro-display and time limiting, logic components for secure transmission of messages.

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FIGURE

Figure 1: Schematic of the (a) FLB setup, (b) top- and (c) side-view of how the sample and metal source are arranged during the heating process. (d-e) FM of the samples (d) before and (e) after growth of Ag/Ag₂MoO₄ NWs under UV excitation. Inset are the corresponding BF images. (f) FLB patterned micro-art of a *Cyprinus carpio*. Inset of (f) shows a multi-colour display obtained using different materials. SEM images of Ag NPs patterned GO samples taken at (g) 0h, (h) 1h, (i) 2h and (j) 3h of growth in the presence of Mo foil. Below the SEM images are models illustrating the growth process. (k) I_{sd}-V_{sd} of single Ag/Ag₂MoO₄ NW before (Day0), one day (Day1) and two days (Day2) after photodoping with 325 nm focused laser beam. (l) I_{sd}-V_{sd} of Day 1 sample with back gate, V_{bg}.

Electronic properties of low-angle twisted bilayer graphene

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Abstract

Twisted bilayer graphene (tBG) at and around specific magic angles [1] exhibiting correlated insulating phases and superconductivity has boosted the new field of "twistronics" [2] where strong electronelectron interactions play a dominant role in the electronic properties of the system. Below a threshold twist angle $\theta_c \sim 1^\circ$, this superlattice undergoes self-organized lattice reconstruction [3], forming a periodic domain and thus modifying strongly its electronic structure, compared to those osberved above such threshold angle. Although low-angle tBG has been intensively investigated using effecttive electronic approaches (see an example in [4]), an in-depth investigation using more accurate calculations is still highly desirable. In this work, we developed and performed atomistic calculations using the Green's function techniques to solve tight-binding models, where the lattice reconstruction obtained by simulations as in [5] is taken into account. Indeed, it was shown that the lattice reconstruction presents very significant effects on the electronic structure of low-angle (around and below θ_c) tBG systems. Especially, the second magic angle around $\theta \approx 0.5^\circ$ predicted in [1] is no longer observed (see Fig.1), which is a direct consequence of the mentioned lattice reconstruction. In addition, the local electronic properties and the helical network in these tBG systems were systemmatically investigated. Our work thus presents valuable contributions, that could be helpful for further development of the field "twistronics", e.g., as it helped to interpret the experimental data [6].

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FIGURES

Fig.1: Electronic bandstructure of twisted bilayer graphene around the expected first (left) and second (right) magic angles reported in [1]. The lattice reconstruction obtained as in [5] was taken into acount.

Textile Sensor based on Graphene

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In textile electronics, it is possible to put electronic devices in everyday life objects, such as clothes, home textiles or other textiles objects. However, to develop this technology it is required advances in materials and manufacturing processes, particularly combine flexibility, electrical properties of semiconductors and metals with solution and low temperature processing [1]. Graphene is a twodimensional material, with incredible properties such as: flexibility, transparency, high and electrical conductivity [2]. Therefore, graphene is a strong candidate material for textile electronics, either as electrode or sensor. A conductive textile coated with graphene exhibited conductivity of 8·10⁻³ Ω cm⁻¹ ¹ and sheet resistance lower than 1 Ω sq⁻¹, while maintaining its mechanical properties [3, 4]. Graphene also has a great sensitivity capability, capable of biomolecules and gases detection [5]. In this work we present the development of textile embedded sensor of humidity and temperature based on Few-Layer Graphene (FLG). The coating of textiles is done through solution. The solution is prepared through graphene's exfoliation by blend shearing and it was used Raman spectroscopy to verify the quality of graphene solution. This solution was deposited directly on top of the clean textile samples, through solvent evaporation at controlled temperature. Observation at Scanning Electron Microscope (SEM) was, performed to make morphological analysis. As it can be seen in Fig. 1, the FLG solution does not alters the textile fibers, and adheres strongly to the fiber, making textile conductive. Temperature and humidity tests revealed a dependence with electrical conductivity of the samples. Finally, the samples were submitted to relative humidity and temperature tests, in a controlled environment, provided by a climatic chamber. It is observed a strong relation between both, humidity and temperature, with the electrical behaviour of the graphene coated textile samples. These results indicate that resistive sensors based on graphene embedded textiles can be used for environmental and biological monitoring applications.

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FIGURES



Figure 1: Textile sample: a) before and b) after FLG deposition, SEM image.

Composite super-moiré lattices in double aligned graphene heterostructures

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Van der Waals heterostructures, as vertical stacks assembled by different 2D crystals, have been widely used to produce combinations with predetermined functionalities. Apart from the selection and the sequence of 2D crystals, controlling the twist angle between stacking layers opened the use of another degree of freedom, especially for two crystals with similar lattice mismatch, which forms moire pattern. Unlike the singly aligned heterostructures with one moire pattern, we reported a doubly aligned structure in which fully encapsulated graphene simultaneously aligned to the top and bottom hBNs.[1] In this case, two periodic potentials due to the moire pattern are applied on graphene simultaneously (which can be proved by two secondary Dirac points in transport measurement and two sets of hexagonal patterns in Fourier transformation of AFM image as shown below and their differential will create another set of supermoires, among which the one with largest period can be independent of the difference in the lattice constants between two crystals and break through the restrictions of this lattice mismatch to achieve the period much larger than 14nm. This would open up the prospect for the design of graphene band reconstruction at arbitrary low Fermi energies.

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FIGURES





Figure 1: Rxx as a function of carrier concentration *n* with two moire periods 15.3nm (blue),14.0nm (green). The moiré and super-moiré peaks marked by arrows and labelled with their periods in the unit of nanometres. Largest supermoire with the period 36.3nm, marked by red.

Figure 2: Fourier transform of the AFM image showing two sets of distinct hexagonal patterns (red and green dashed hexagons).

Large anisotropic single crystal epitaxial graphene flakes isolated from SiC wafers

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Beyond fundamental studies on mechanically exfoliated HOPG, best electronic devices are based on high quality graphene obtained either by CVD on Cu foils or epitaxial graphene (EG) on SiC [1]. In this work, we report some preliminary results on the development of electrical devices based on large anisotropic single crystal EG flakes obtained on the C-face of SiC by high temperature sublimation [2]. The as-grown isolated EG flakes can be detached and transferred to e.g. SiO₂ substrate by PMMAassisted electrochemical delamination technique, which is a non-destructive, reproducible and lowcost exfoliation method that has been adapted to EG on SiC [3]. For the fabrication of graphene electrical contacts simple alignment and patterning by e-beam lithography, thin film evaporation and resist lift off process was employed. As-deposited EG materials consist in hundreds-um-long, tens-ofµm-wide SLG to FLG EG islands, covering typical regularly step-bunched SiC (Fig. 1 (a, b)). The transferred materials on SiO₂ somehow reproduce that SiC substrate terrace topography (Fig. 1(c)). Examples of Raman spectra of transferred EG are shown in (Fig. 1 (d). The electrical characteristics have been tested via 4-probe method on three different devices. The linear I-V relationship reveals the presence of ohmic contacts displaying resistances ranging from $1.2k\Omega$ to $2.3k\Omega$ (Fig. 1 (f). Yet, these values could be easily improved by applying dedicated treatments prior e.g. to metal deposition, such as plasma treatments [4] of the contact areas or post deposition treatments such as rapid thermal annealing [5]. Both structural and electronic characterization indicate that high crystalline quality of EG is basically preserved upon electrochemical transfer as well as device fabrication.

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Figures 1: (a) AFM image of as-grown EG on SiC; (b) optical image of as-grown EG on SiC; (c) AFM image of transferred EG on SiO₂ (Z scale=20nm); (d) exemplary Raman spectra after transfer; (e) optical image of a large anisotropic EG flake interfaced by 4 probes electrical device; (f) optical image and electrical characteristics a SLG/BLG electronic device.

Ultrafast CVD growth graphene monolayer and single-crystal in cold-wall reactor

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Abstract

The method of high-quality graphene synthesis with a full cycle lasting less than 3 minutes, which is the fastest graphene synthesis cycle to date, is demonstrated in this work. The possibility of synthesizing graphene monolayers and single crystals up to 50 micrometres in size (see Figure 1) is demonstrated as well. To assess the quality of graphene, the most important criteria were selected: sheet resistance, charge mobility in a field effect transistor, Raman spectrum, film uniformity and graphene grain size. The key parameters for the synthesis of graphene are: the temperature of the copper foil, the concentration of the precursor and the synthesis time, as well as the rate of heating and cooling of the copper foil. The effect of these synthesis parameters on the quality of CVD-graphene is presented in this work. Graphene was synthesized by chemical vapor deposition in a cold-wall commercial reactor made by Rusgraphene LLC. The copper foil was heated by the resistive method, and methane was used as a precursor.

A distinctive feature of this equipment is the ability to quickly heat the foil in less than 1 minute and abrupt cooling of the foil. This makes it possible to more accurately control the synthesis of graphene on copper foil, namely, to heat the substrate in a short time and interrupt the synthesis at the moment when the graphene nuclei have grown sufficiently, but have not yet formed a single layer.

FIGURES

Figure 1: Optical images graphene single crystal. (All scale bar is 50 micrometres)

Direct observation of large strain through van der Waals gaps on epitaxial Bi₂Te₃/graphite: pseudomorphic relaxation and the role of Bi₂ layers on the Bi_xTe_y topological insulator series

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Layered materials can usually grow without strain on top of distinct substrates if the only interaction between them is due to van der Waals forces [1]. In such scenario it would be expected that the heterointerface made up of weak bounds would not affect the overlayed material significantly for several large lattice-mismatched systems [1]. Here we have studied the first stages of the heteroepitaxial growth of layered bismuth telluride topological insulator on top of highly oriented pyrolitic graphite (HOPG) by molecular beam epitaxy. Atomic Force Microscopy (AFM) images show hexagonal/triangular flat islands with exposed HOPG areas for the low coverage regime (Figure 1a), and the lattice parameter of these Bi₂Te₃ structures were measured by X-ray diffraction (XRD) (Figure 1b). The existence of pseudomorphic strain at the initial Bi_2Te_3 layers was retrieved by both X-ray diffraction and Raman spectroscopy. We have found out evidence that Bi₂Te₃ layers near the interface are subject to an in-plane compressive strain, leading to a pseudomorphic out-of-plane lattice expansion. Furthermore, the presence of Bi₂Te₃ islands locally distorts the topmost layer of HOPG, resulting in tensile strain which is measured by Raman spectroscopy. The observed relaxation of 0.1 -0.2 % for each van der Waals gap is used to calculate elastic constants of Bi₂ bilayers (Figure 1c), which are crucial building blocks to the formation of other Bi_xTe_y topological insulator compounds. Finally, the impact of such strain in Bi₂Te₃ electronic structure was investigated by DFT calculations. The results show that band structure of this strained material remains unchanged at the center of the Brillouin zone, confirming the robustness of surface states, but it is consistently affected at the M and K zone edges (Figure 1d).

REFERENCES

FIGURES

Figure 1: (a) Typical hexagonal Bi₂Te₃ island on HOPG. **(b)** Experimental in-plane lattice parameter as a function of island height (blue dots). **(c)** Comparison of in-plane lattice parameter for the Bi_xTe_y series for measured values (white/dashed bars). **(d)** Calculated band structure of Bi₂Te₃.

Investigation of donor/acceptor relation for non-covalent Graphene doping using *N*-Heteropolycycles

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In recent years, non-covalent functionalization of graphene with organic molecules has attracted considerable attention due to the possibility of controlled chemical doping. Graphene shows strong π - π interactions with aromatic molecules allowing the deposition of a range of organic materials from solution with scope for molecular self-assembly^[1]. However, a number of aspects have not been sufficiently addressed, for example, it is unclear in which way the periphery around the aromatic core and potentially pre-organization of the molecules prior to deposition has an impact on supramolecular arrangement and packing density on the surface. In addition, it is particularly difficult to quantitatively relate the doping strength to the donor/acceptor properties of the molecules, as molecular packing (governed by the overall structure of the molecule) has to be decoupled from electronic properties (governed by the aromatic core).

In our study we use different classes of *N*-Heteropolycycles for the non-covalent functionalization of CVD graphene with the aim to fundamentally shine light on chemical doping and surface modification. This class of organic molecules is especially suitable, as the structure can be systematically varied. In particular, the donor/acceptor strength can be varied via the substitution pattern of the core and thus tuned independently from the molecular periphery. We focus on a series of derivatives of tri-isopropylsilyl-Tetraazapentacene^[2] (TIPS-TAPs), Tetraazaperopyrene^[3] (TAPPs) and N-Heterotriangulenes^[4] (NHTAs) to investigate the impact of different molecular structures on the electronic and surface properties of graphene to understand how to precisely tune graphene to the different needs in electronic applications, without altering its lattice structure. Raman spectroscopy (in combination with AFM/KPFM) is a particularly versatile characterization technique, as both doping and packing density of the molecule can be evaluated simultaneously. Additionally surface energy values can be extracted by contact angle measurements.

Figure 1: Deposition of different *N*-Heteropolycycles (**a**: NHTAs, **b**:TIPS-TAPs, **c**: TAPPs) leading to changes in graphene Raman intensity ratio I2D/IG (= Fermi level) depending on the donor/acceptor strength of the molecules, represented by their HOMO/LUMO energies.

Our studies show that the observed changes in electronic structure of graphene are primarily affected by the electronic structure of the molecules themselves, as long as the used substituents are comparable in their steric effects. For acceptor-type molecules, (e.g. TAPPs and TIPS-TAPs) a correlation between LUMO energy of the molecules and Fermi level shift in graphene is observed independent of how much molecule is deposited. For donor-type molecules (e.g.) NHTAs a similar correlation involving the HOMO energy can be seen. The Raman data is supported by changes in the work function. Surface energy values could only be measured for the TAPPs, since the other molecules are partially removed through solvents involved in contact angle measurements.

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 GRAPHENE AND 2DM ONLINE CONFERENCE (GO2020)

Adsorption of metal ions and bactericidal actions using mixed zeolites and graphene oxide-based membranes

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Adsorption by composite membranes is considered an effective and economical wastewater treatment methodology to raise the emerging problem of the clean water shortage. Recently, graphene oxide (GO) and reduced-graphene oxide (r-GO) have been considered as potential candidates for use as a barrier layer of the separation membranes due to their high surface area, chemical stability, ultrathin 2D structure and controllable surface chemistry [1]. Additionally, GO and r-GO have attracted intensive interest because of their ability to contrast the membranes fouling and/or biofouling [2] thus reducing the use of chemical treatments in water disinfection. In this work, a novel design strategy is proposed to remove metal ions from water by a nanocomposite membrane based on reduced graphene oxide (r-GO) and zeolites. The aim is to directly prepare a r-GO layer on a highly microporous mat in order combine the strong selectivity, ion exchange properties and chemical stability of zeolites materials. Graphene oxide from natural graphite flakes (Sigma-Aldrich) according with modified Hummers method and the nanocomposite membranes were synthesized in the MackGraphe Research Center laboratories. Zeolite 3A and 13X were selected for their highly hydrophilic character, high thermal stability and because they were readily available, at low cost and with a high degree of purity and crystallinity. Zeolites "milky solutions" were prepared using an ultrasonic processor (UP400S, Hielscher), diluting 50 mg of zeolites powders in 100 ml of deionized water. All materials were characterized by SEM, AFM, FT-IR, XRD, TG/DTA and WCA. The ultra-thin nano-channelled membrane r-GO/CHNs (Copper Hydroxide Nanostrands) and the nano-composite membranes r-GO/ZEO3A (zeolite 3A) and r-GO/ZEO13X (zeolite 13X) were synthetized by an innovative one-step deposition method on a nylon substrate and then employed to remove from water common cations, particularly Na⁺, NH₄⁺, K⁺, Ca²⁺, Mg²⁺ (always ubiquitous in natural water and wastewater effluents). Adsorption tests highlighted a strong selectivity to Mg²⁺ thus attesting that functional groups exhibited strong metal-ligand interaction ion in aqueous solutions. Further, their antibacterial activity was tested against bacterial strains representative for Gram-positive (S. aureus Sa2 and E. faecalis ATCC 29212) and Gram-negative (E. coli APN1, P. aeruginosa PaPh32 and AC12a) species. In conclusion, this method for fabrication of the composite r-GO/zeolite and r-GO/CHNs membranes may provide many new opportunities for the development of novel antimicrobial membranes, environmentally compatible, efficient in water purification technologies for waste water and industrial waste.

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Boron phosphide based 2D heterostructures

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Abstract

With fascinating physical properties of the van der Waals (vdW) heterostructures are emerging as promising materials for future possible optoelectronic devices. Motivated by the recent studies on vdW heterostructures, we investigate the electronic and optical properties of boron phosphide based 2D heterostructures that we especially focused on the monolayer boron phosphide (MBOP)/monolayer blue phosphorus (MBP) and monolayer gallium nitride (MGaN)/monolayer boron phosphide (MBOP) in the framework of density functional theory (DFT). We analyze the variation of the energy band gap, the characteristics of the energy band diagrams, charge redistribution by stacking and the electrostatic potential along the perpendicular direction. The dynamical stability of these structures is ensured by the phonon spectra. We conclude that the heterostructures have remarkable optical absorption over the UV range together with being transparent to the visible spectrum, and may be a prominent material for future optoelectronic devices.

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FIGURES

Figure 1: MBOP/MBP heterostructures [1]

Figure 2: MGaN/MBOP heterostructures [2]

Exploration of a 2D Material Monte Carlo Simulator: Parallelization Strategy and Noise Characterization of MoS₂

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ABSTRACT

Two dimensional (2D) metal dichalcogenides are under an intensive research which is mainly motivated by their inherent bandgap and their feasible applications beyond gapless graphene [1]. The dichalcogenides possess fascinating properties such as an atomic-scale thickness and a direct bandgap, promising novel optical and electronic properties [2]. An exhaustive study of electronic transport of these materials is essential to assess their application by advanced physically-based models as an ensemble Monte Carlo (MC) technique which present well-recognised benefits to model the stochastic and quantum-mechanical transport processes at nanoscale.

In this work, an in-house ensemble MC simulator has been developed and widely tested for the study of different 2D materials such as graphene, silicene, molybdenum disulfide (MoS_2) and other transition metal dichalcogenides [3, 4, 5, 6]. We have focused on exploiting the advantages that this tool offers to characterize the microscopic noise sources in MoS_2 due to charge fluctuations. The random stochastic processes of the Monte Carlo method allows us to analyse different fluctuation magnitudes in depth such as the diffusion coefficient, or evaluate the influence of a scattering on the fundamental thermal noise source, which represents a novel approach for the study of noise in these materials.

A parallelization strategy under Message Passage Interface (MPI) has also been employed to upgrade our purely sequential MC simulator, which is essential for diminishing the heavy computational burden of the simulations performed. The motion of simulated particles in the ensemble MC technique depends on their previous history probabilistically govern by Boltzmann Transport Equation using classical free flights interrupted by quantum-mechanical scattering events. This combination of classical and quantum-mechanical probabilities require well balanced approaches to distribute particles to CPU cores in order to achieve balance computer performance [7]. A deep analysis all the particularities of the physical model and the balanced parallelisation approaches has been therefore developed.

The results for analysis of the high-frequency behaviour and the diffusive properties of the electronic transport will be presented for MoS_2 and a decrease in the CPU times of simulations of the 2D materials will be explored.

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Topological Aharonov-Bohm Interferometers Defined By Inhomogeneous Electric Field In Silicene

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We study topologically protected currents as a source of Aharonov-Bohm oscillations in clean systems in silicene [1]. Chiral channels [2,3] in the system are formed by flips of the electric potential perpendicular to the structure [4,5]. In our calculations we define four terminal system in quantum ring shape (Fig. 1(a)), where two different configurations of resistance measurement are proposed: with current probes plugged to two nearest leads (e.g. $4\rightarrow 1$) and (ii) in straight line (e.g. $3\rightarrow 1$) as presented in Fig. 1(b) and 1(c), respectively. The current direction is determined by the valley state at Fermi level defined for each input lead. The K and K' valley in channels propagate current in different directions (see Fig. 1(d)), hence the direct cross-transport of the electron (e.g. $1\rightarrow 3$) is forbidden due to the lack of backscattering. We show that oscillations of resistance measurement in external magnetic field (Fig. 1(e)) are related to the current confinement at quarters of the ring. The period of these oscillations agree with Aharonov-Bohm interference at n/4 (n=1,2,3,4) of the area of the circle.

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FIGURES

Figure 1: (a) Scheme of the four-terminal system with (d) current direction marked by black (white) arrow for (K') K valley. Conductance measurement configurations (b) R' and (c) R in external magnetic field (e) in units of von Klitzing constant R_K

Using Cationic Pyrene Derivatives to Produce Aqueous Graphene Dispersions with Exceptional Stability and Biocompatibility

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Liquid-phase exfoliation (LPE) is a simple, mass-scalable and cost-effective method to produce solution processed graphene [1,2]. A stabiliser must be used to effectively disperse defects-free graphene in water, the solvent, which is abundant, cheap and environmentally friendly and essential for biological applications [3]. Pyrene derivatives, e.g. 1-pyrenesulfonic acid or 1-pyrenecarboxylic acid, have shown high efficiency for exfoliating graphite, compared to other types of stabilisers such as surfactants or polymers [4-6]. However, most of studies shown successful exfoliation with anionic pyrene derivatives. Only few studies have reported the use of cationic pyrene derivatives, and often with low concentration and/or limited dispersion stability [7.8]. Amphoteric pyrene-derivatives were also reported, however with limited stability at neutral pH [9]. In this work we produced and tested various cationic pyrene derivatives as stabilisers for LPE in water. Cationic pyrene derivatives were designed and synthesised with different functional groups and varying carbon linker chain length between the pyrene core and the charged group to get insights on the exfoliation mechanism and to understand how to design the pyrene derivative to achieve efficient exfoliation [10]. Some of the cationic pyrene derivatives were used to produce the graphene dispersions with excellent biocompatibility, cell internalisation capacity, and colloidal stability even in the biological environment, showing great potential of for biomedical applications[10].

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FIGURES

Figure 1: (a) Graphene dispersions prepared with the cationic pyrene derivatives (diluted by factor of 10), (b) structure of cationic pyrene derivatives, and (c) cellular uptake of the graphene nanosheets estimated using confocal microscopy.

Graphene on Silicon Nanoscale

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The possibility of low-temperature synthesis of graphene on the surface of porous silicon (PS) is associated with the excess surface energies of nc-PS nanocrystallites ; the boundary interface nanocrystallites nc-PS / c-Si monocrystal matrix; the dangling bonds of silicon atoms of nanocrystallites skeleton nc-PS. This opens up new prospects for the development of methods for the low-temperature synthesis of graphene without metal catalysts for the decomposition of carbon precursors, including using the ALD method.

Keywords: porous silicon, energy, nanocrystal, dangling bonds, interface, skeleton, low-temperature synthesis, graphene.

The actuallity of developing low-temperature synthesis of graphene is associated with the development of flexible electronics based on organic polymers, which are planned to be done in the next 5 years [1]. Currently existing low-temperature (300–500 ° C) LPCVD- [2], PECVD- [3], REALD- [4] methods for the synthesis of graphene are either imperfect to obtain a stable and uniform large area of graphene, LPCVD [5], or possess the same drawbacks as the high-temperature CVD method for the synthesis of graphene on metal catalysts, high cost and energy consumption, PECVD, or complicated for large-scale application, REALD.

Recently, the possibility of low temperature <400 ° C synthesis of multilayer graphene [6] and few layer graphene, carbon graphene nanocomposite [7] on the surface of porous silicon PS has been shown. The high energy activity of PS is associated with the catalytic activity of nanosized silicon nc-PS for low-temperature decomposition of a carbon precursor [6], and also with previously known quantum-size effects such as a decrease in the melting temperature of a crystal with a decrease in size [8], a change in the energy gap of nanocrystals [9], and energy saturation dangling bonds of Si atoms of nanocrystallites of the skeleton nc-PSi [10]; the appearance of elastic deformation forces at the nanocrystal / c-Si matrix interface due to mismatch defects [11]. The possibility of synthesizing graphene on the PS surface without the use of metal catalysts can open up a new perspective for the integration of silicon and graphene electronics without metal interconnects [6], and the development of flexible electronics based on organic polymers using the ALD method [12].

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Figure 1: Raman spectra of samples a) PS <C> 350 ° C, b) PS <C> 500 ° C, c) PS <C> 1050 °C

Gate-tunable graphene-based Hall sensors on flexible substrates with increased sensitivity

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Hall sensors are widely used in application fields like consumer electronics and automotive for position precision and switching applications. Key parameters of Hall sensors are the current related (Si), the voltage related (Sv) sensitivities and the magnetic resolution (Bmin). Graphene, because of its very high mobility μ and low charge carrier concentration n (Sv $\approx \mu$ and Si $\approx 1/n$) as well as its mechanical flexibility, appears to be an ideal material for Hall sensors. Previously, graphene based Hall sensors outperforming all other technologies on flexible substrate were demonstrated. However, the sensitivity of flexible graphene Hall sensors is not yet outperforming rigid Hall sensors based on conventional semiconductors, at least if the graphene Hall sensor is fabricated with a scalable approach. [1,2]

In this work, we demonstrate a novel concept for operating graphene-based Hall sensors using an alternating current modulated gate voltage, which provides two important advantages compared to Hall sensors under static operation: 1) The sensor sensitivity can be doubled by utilizing both n- and p-type conductance. 2) A static magnetic field can be read out at frequencies in the kHz range, where the 1/f noise is lower compared to the static case. Sensitivity up to 0.55 V/VT and Bmin down to 290 nT/ \sqrt{Hz} at 2 kHz gate frequency were found for Hall sensors fabricated on flexible foil. This significantly outperforms state-of-the-art flexible Hall sensors and is comparable to the values obtained by the best rigid III/V semiconductor Hall sensors.

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FIGURES

Figure 1: a) Microscope image of the top gated graphene Hall sensor on flexible substrate. b) Hall voltage under DC (black) and AC (red) operation

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Anatase TiO₂ Nanosheets with Enhanced Catalytic Properties

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Titanium oxide (TiO_2) is an inorganic compound that belongs to the wide group of *d*-metal oxides. This material has been widely studied over the past few decades in several applications, ranging from photocatalysis, electronics and healthcare [1]. In particular, the anatase phase of TiO₂ has been shown to possess the highest catalytic activity [2]. However, two-dimensional (2D) TiO₂ anatase has been shown to have even better catalytic performance due to its higher surface to volume ratio, specific exposed facets and a large fraction of unsaturated surface atoms, compared to bulk TiO₂ [3]. However, the synthesis of 2D TiO₂ is still very challenging because the bulk crystal is not layered, hence TiO₂ nanosheets cannot be directly produced by liquid-phase exfoliation.

One of the most used strategies for the synthesis of 2D TiO₂ anatase is based on hydrothermal route, employing a structure-directing agent such as hydrofluoric acid (HF) [4]. In this work we used a fluorine-free strategy to synthesize TiO₂ anatase nanosheets with average lateral size of 30-40 nm and thickness of 3-4 nm, and with exposed high energy facets, namely the (001), (100) and (010), as shown by Transmission Electron Microscopy. The as-prepared material has been tested for oxygen evolution reaction (OER) and compared to the commercial TiO₂ P25 nanoparticles and other materials reported in literature, showing enhanced OER properties with onset-overpotential and Tafel slope of 1.58 V and 75 mV dec⁻¹, respectively in alkaline conditions (1M KOH) [5].

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