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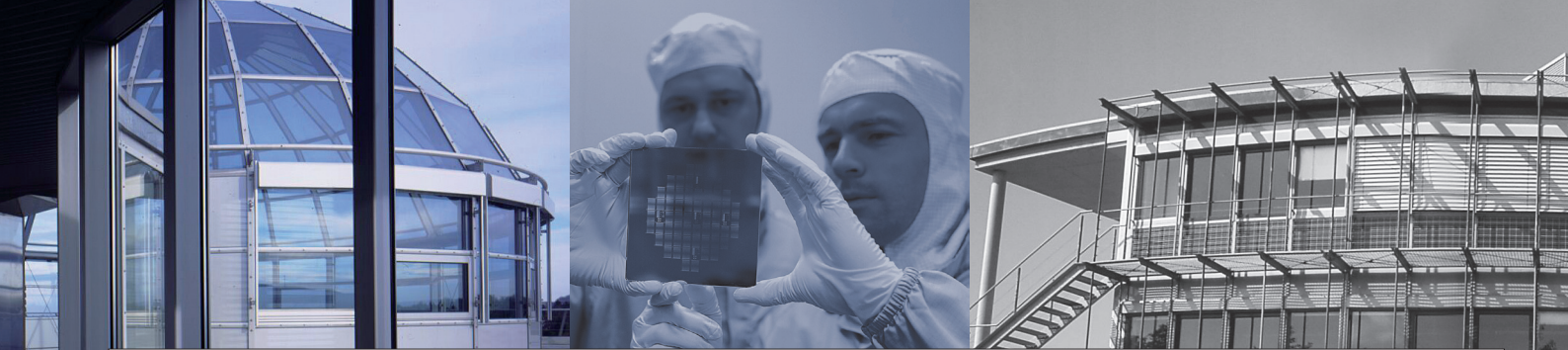
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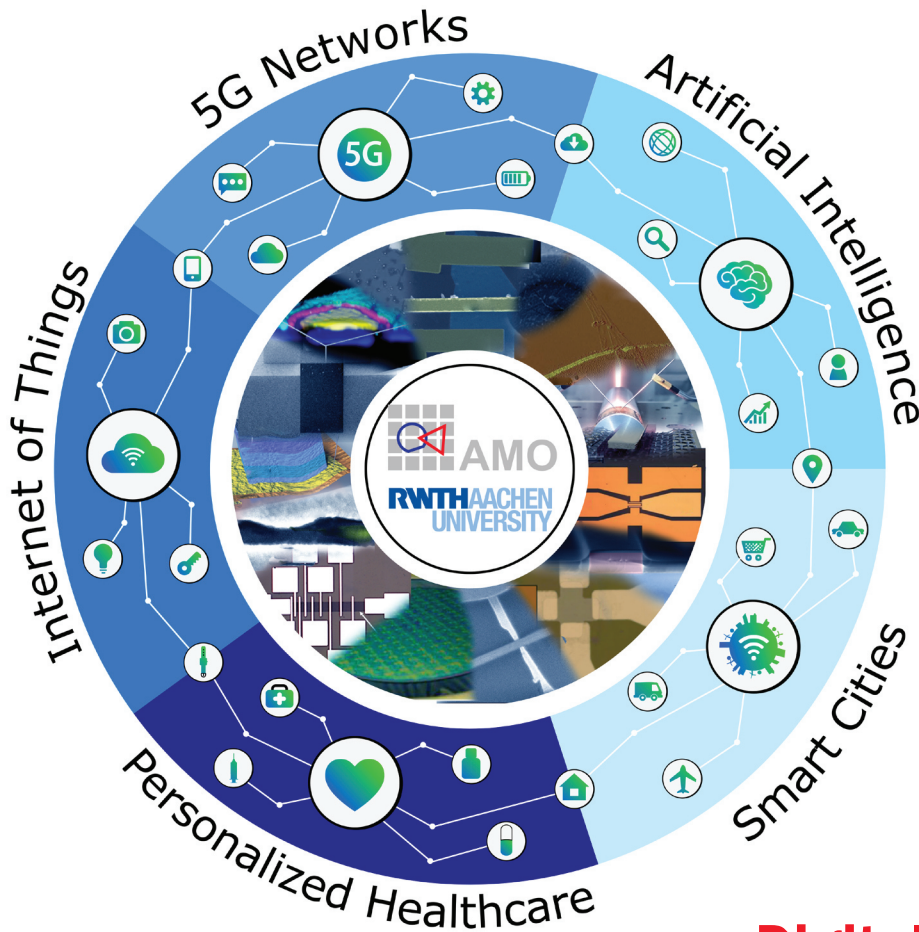
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F OREWORD

On behalf of the Organising Committee we take great pleasure in welcoming you for the 2nd edition of the "Graphene and 2DM" Online Conference (GO2021): Fundamental Research Insights (April 20-21, 2021).

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 two-day GO2021 Online conference will present the most recent advances in fundamental research in chemistry, electronics, topological materials, energy storage, biohealth, composites, coatings or sensors.

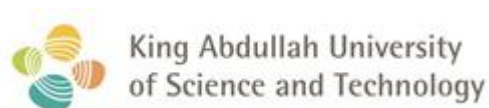
26 high profile most influential academia worldwide experts in the Graphene and 2DM sector will present speeches in this international event on how advanced materials will change the future of technology and impact positively our daily life.

GO2021 will be a two-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 the first edition in 2020 and considering that all major scientific and technological conferences are being cancelled or postponed worldwide until the second semester of 2021.

We are indebted to AMO GmbH (Germany) for their help and financial support. We also would like to thank all the speakers and participants that join us this year.

Hope to see you again online or in-person in the next edition of the "Graphene & 2DM" Conference: Fundamental Research Insights..

GO2021 Organising Committee



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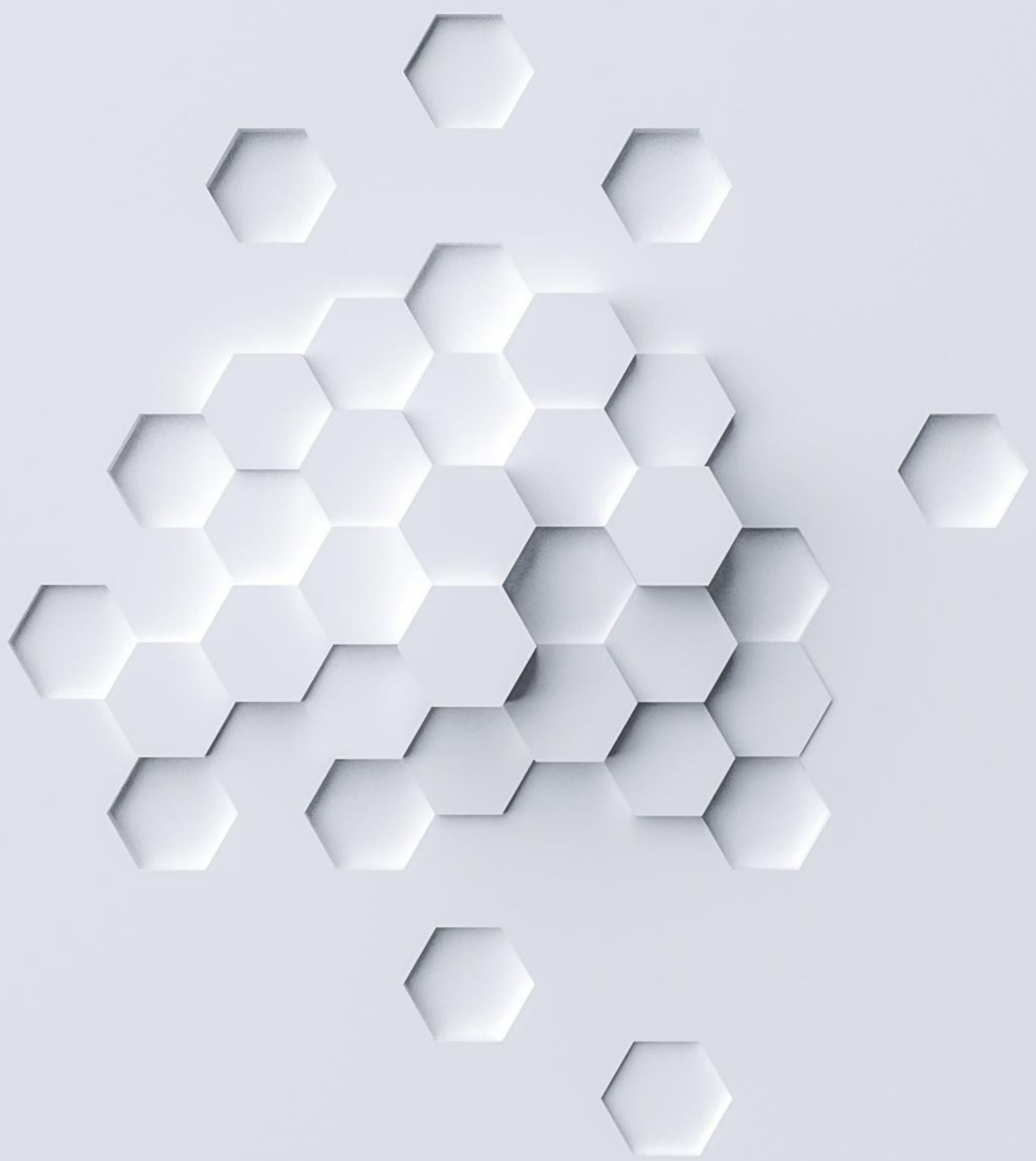
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Liquid phase exfoliation, degradation and functionalisation of layered materials

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Abstract

Liquid exfoliation has become an important production technique to give access to large quantities of two-dimensional nanosheets in colloidal dispersion. Importantly, this is a highly versatile technique that can be applied to numerous layered materials beyond graphene. In this talk, our recent advances in the liquid exfoliation, optical characterisation and degradation of a range of 2D-materials will be summarised. Materials under study include group VI TMDs, PdSe₂, PtSe₂,[1] MPS₃ (M: Ni, Mn, Fe),[2] InSe, RuCl₃, CrTe₃ and porous organic sheet stacks (2D polymers).[3] All materials can be exfoliated and size-selected in a similar way yielding nanosheet dispersions with well-defined changes in their lateral dimensions and thickness. Inherently, lateral nanosheet size and layer number are linked, in agreement with a recently developed model of energy equipartition of tearing and delamination events.[4]

The availability of a broad range of size-selected nanosheets allows us to study degradation in various environments through optical spectroscopy systematically. For materials beyond graphene, BN and transition metal dichalcogenides (TMDs), we find evidence for degradation in optical absorbance and extinction spectroscopy that allow us to track degradation kinetics. In the case of group VI-TMDs, we use photoluminescence measurements as function of time and temperature in dispersion to selectively track monolayers. Depending on the surfactant used as stabilizers, monolayers of WS₂ react in ambient conditions in a photo-induced, as well as thermal degradation pathway with activation energies of ~25-30 kJ/mol and ~50 kJ/mol, respectively.[5] This confirms the recently observed difference in nanosheet reactivity depending on the surfactant coverage.[6] Finally, we present our attempts to passivate reactive defects through functionalisation.

REFERENCES

- [1] *2D Mater* **2020**, 7, 045027.
- [2] *Chem. Mater.* **2019**, 31, 9127-9139.
- [3] *Angew. Ch. Int. Ed.* **2020**, 59, 5683-5695.
- [4] *ACS Nano* **2019**, 13, 7050-7061.
- [5] Karger, L.; Synnatschke, K.; Settele, S.; Hofstetter, Y.; Vaynzof, Y.; Backes, C., *submitted to Adv. Mater.* 2021.
- [6] *Angew. Ch. Int. Ed.* **2020**, 59, 13785-13792.

Two-Dimensional Charge-Density-Wave Quantum Materials

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The charge density wave (CDW) phase is a quantum state consisting of a periodic modulation of the electronic charge density accompanied by a periodic distortion of the atomic lattice in quasi-one-dimensional (1D) or quasi-two-dimensional (2D) metallic crystals. Several layered transition metal dichalcogenides (TMDs) exhibit unusually high transition temperatures to different CDW symmetry-reducing phases, opening possibility for practical device applications. One of the most promising materials, 1T-TaS₂, has the CDW transition between the nearly-commensurate (NC-CDW) and the incommensurate (IC-CDW) phases at 350 K. The transition from the IC-CDW phase to the normal metal phase is observed at even higher temperature. In this keynote talk, I will review our recent experimental results on controlling the CDW phase transitions in quasi-2D materials with an applied electric field, and discuss possible device applications of quasi-2D CDW materials.

We have demonstrated the room-temperature voltage-controlled oscillators and logic circuits, which operate on the basis of the NC-to-IC CDW transition in the quasi-2D 1T-TaS₂ channels, triggered by the applied voltage [1-2]. We found that the quasi-2D 1T-TaS₂ CDW devices reveal exceptional hardness against X-ray and proton radiations [3-4]. We explained this property of the CDW devices by the high carrier concentration in all their phase states, two-terminal design, and the quasi-2D channel geometry. The low-frequency electronic noise spectroscopy has been used as an effective tool for monitoring the CDW phase transitions, particularly the switching from the IC-CDW phase to the normal metal phase in the quasi-2D 1T-TaS₂ channels [5]. The noise spectral density exhibits sharp increases at the phase transition points, which correspond to the step-like changes in resistivity. The noise spectroscopy was instrumental in revealing the “hidden phase transitions” in vertical 1T-TaS₂ devices [6].

The data on the “narrow-band noise” in quasi-2D CDW devices [7] and the switching speed of the CDW phases will also be presented [8]. Despite the similarities of the “narrow-band noise” in quasi-1D and quasi-2D CDW materials, we argue that the nature of the current oscillations in quasi-2D 1T-TaS₂ is different from the “narrow-band” noise. Analysis of the biasing conditions and electrical current indicates that the observed oscillations are related to the current instabilities due to the voltage-induced transitions between the NC-CDW and IC-CDW phases [7]. By combining the results of our experiments with a numerical analysis of the transient heat diffusion in the quasi-2D 1T-TaS₂ devices on Si/SiO₂ substrates, we clearly reveal the thermal origins of the CDW phase switching in such devices [8]. In spite of this thermal character, our numerical modelling suggests that a suitable reduction of the size of these CDW devices should allow their operation at GHz frequencies.

The work at the University of California, Riverside (UCR) was supported, in part, by the U.S. Department of Energy, Office of Basic Energy Sciences, under the contract No. DE-SC0021020 “Physical Mechanisms and Electric-Bias Control of Phase Transitions in Quasi-2D Charge-Density-Wave Quantum Materials”.

REFERENCES

- [1] G. Liu, *et al.*, Nature Nanotechnology, 11 (2016) 845.
- [2] A. G. Khitun, *et al.*, IEEE Electron Device Letters, 39 (2018) 1449.
- [3] G. Liu, *et al.*, IEEE Electron Device Letters, 38 (2017) 1724.
- [4] A. K. Geremew, *et al.*, Nanoscale, 11 (2019) 8380.
- [5] A. K. Geremew, *et al.*, ACS Nano, 13 (2019) 7231.
- [6] R. Salgado, *et al.*, Appl. Phys. Express, 12 (2019) 037001.
- [7] A. K. Geremew, *et al.*, Appl. Phys. Lett., 116 (2020) 163101.
- [8] A. Mohammadzadeh, *et al.*, Appl. Phys. Lett., 118 (2021) 093102.

2D-Electrolytes

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Abstract

I will discuss a new class of materials called 2D-electrolytes that share properties of 2D-materials and electrolytes and undergo morphological transitions triggered by environmental changes.

REFERENCE

2D-electrolytes: theory, modelling, synthesis, and characterization, M. C. F. Costa et al., *Advanced Materials*, in press. DOI:10.1002/adma.202100442

FIGURES



Electrical and electrochemical applications of liquid exfoliated nanosheets

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Abstract

Liquid phase exfoliation (LPE), is a simple and versatile method to exfoliate layered crystals like graphite, BN and MoS₂ to give 2-dimensional nanosheets such as graphene in large quantities. These dispersions can be straightforwardly processed, allowing the production of composites or the printing of nanosheet networks. In this talk, I will discuss our latest results on exfoliation of new layered materials, for example SnP₃, which displays superlative lithium storage. I will also describe the printing of size-selected nanosheet networks using aerosol jet printing as well as their electrical properties. By combining networks of different nanosheet types, it is possible to form heterostructures for device applications. For example, when mixed with a polymer conductive nanosheets can yield extremely sensitive strain sensors. Alternatively, using graphene electrodes and high permittivity BiOCl nanosheets as dielectric, it is possible to print capacitors with dielectric constants >50. However, for many applications, graphene networks are too resistive to be useful. I will demonstrate metallic nano-platelets (Figure 1) which yield networks with conductivities approaching 10⁷ S/m, display state of the art EMI shielding performance and show unusual electrical properties. Finally, I will demonstrate that a number of non-layered materials can be converted to nanosheets using LPE (Figure 2). Such quasi-2D materials demonstrate outstanding performance in a number of applications, for example Li ion battery electrodes.

FIGURES

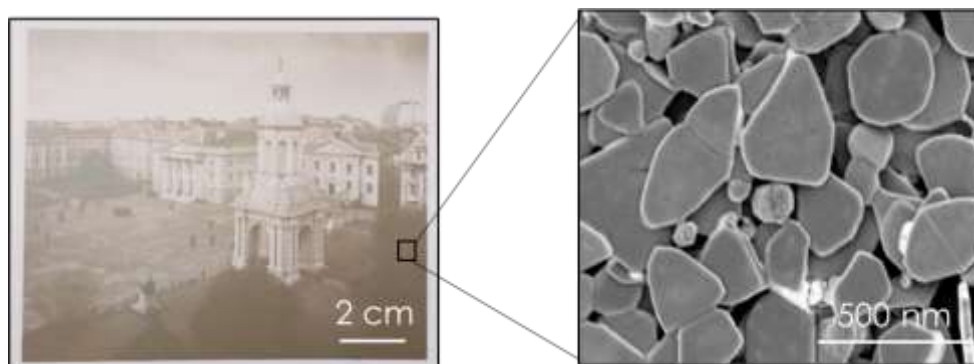


Figure 1: Printed network of metallic nano-platelets.



Figure 2: Liquid phase exfoliation of the mineral, fool's gold (pyrite).

Moiré superlattice networks in twistrionics bilayers of transition metal dichalcogenides

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We apply a multiscale modelling approach to study moiré superlattice in twisted homo- and heterobilayers of transition metal dichalcogenides (TMD), taking into account the interlayer hybridisation of the electronic orbital and lattice reconstruction due to stacking-dependent adhesion. First of all, we develop DFT-parametrized interpolation formulae for interlayer adhesion energies of MoSe₂, WSe₂, MoS₂, and WS₂ with both parallel and antiparallel orientation of their unit cells and arbitrary offset of the honeycomb lattices in the adjacent layers [1,2]. Then, we combine those interpolation formulae with elasticity theory and analyze the bilayer lattice relaxation into mesoscale domain structures. We find that 3R and 2H stacking domains develop for, respectively, bilayers with parallel (P) and antiparallel (AP) orientation of the monolayer unit cells, separated by a network of dislocations, for twist angles $\theta < \theta_P \sim 2.5^\circ$ and $\theta < \theta_{AP} \sim 1^\circ$. Such lattice reconstruction has been verified by STEM imaging [2]. We also show that the triangular domain structures of P-oriented homobilayers would manifest itself in local tunnelling characteristics of marginally twisted bilayers [1,2]: these domains feature the layer asymmetry of band-edge wave functions and also the ferroelectric interlayer polarisation. For AP bilayer, we show that the deformation of the lattices around domain walls (which resemble twist dislocations oriented along the planes of in bulk 2H crystals) generate piezo-electric charges [1], reaching local density up to $\pm 0.5 \times 10^{12} \text{e/cm}^2$ at the junctions of the honeycomb domain wall network, whereas the 3R stacking domains in P-bilayers feature weak ferroelectric (interlayer) charge transfer [3,4]. Finally, we use DFT modelling of bandstructure of bilayers with various stacking configurations and interlayer distances to develop and parametrise $\mathbf{k} \cdot \mathbf{p}$ theory Hamiltonians in the relevant parts of the Brillouin zone, and, then, establish the electronic structure of the bilayer across the moire supercell, taking into account the ferroelectric and piezoelectric charge transfers [5].

REFERENCES

- [1] V. V. Enaldiev, V. Zólyomi, C. Yelgel, S. J. Magorrian, and V. I. Fal'ko, Phys. Rev. Lett. 124, 206101 (2020).
- [2] A. Weston, Y. Zou, V. Enaldiev, A. Summerfield, N. Clark, V. Zolyomi, A. Graham, C. Yelgel, S. Magorrian, M. Zhou, J. Zultak, D. Hopkinson, A. Barinov, T. Bointon, A. Kretinin, N.R. Wilson, P.H. Beton, V.I. Fal'ko, S.J. Haigh, R. Gorbachev, Nature Nanotechnology 15, 592 (2020)
- [3] V. Enaldiev, F. Ferreira, S. Magorrian, V. Fal'ko, 2D Mater 8, 025030 (2020)
- [4] F. Ferreira, V. Enaldiev, V. Fal'ko, S. Magorrian - arXiv:2103.06093
- [5] F. Ferreira, S. Magorrian, V. Enaldiev, D. Ruiz-Tijerina, V. Fal'ko - arXiv:2103.06320

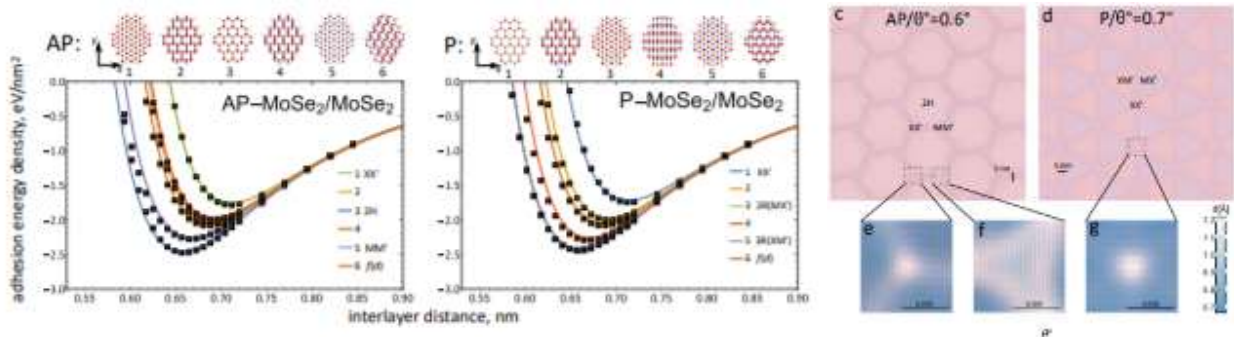


Figure: (Left) Interlayer distance dependence of adhesion energy for various stacking configurations of P- and AP-bilayers. (Right) Domain wall network in twisted bilayers due to the growth of 3R (for P) 2H (for AP) domains.

Bilayer Graphene as a Model Hydrodynamic Semiconductor

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Hydrodynamic electronic transport occurs when carrier-carrier collisions constitute the dominant scattering mechanism. This regime has attracted intense recent interest with its discovery in two dimensional materials, for which interactions are intrinsically strong and disorder plays a minimal role. Here we show that bilayer graphene is a model hydrodynamic semiconductor, in which carrier-carrier collisions play a dominant role over a wide range of temperature and carrier density. Remarkably, a simple model captures the complex interplay between carrier-carrier scattering and conventional dissipative scattering. This model, depicted in Figure 1 below, consists of a universal Coulomb drag contribution that dominates at charge neutrality and decays with increasing density, and a non-universal dissipative contribution corresponding to collective motion of the electron-hole plasma. We compare this model to electrical transport measurements of ultraclean bilayer graphene encapsulated within hBN, with dual gates providing independent control over carrier density and bandgap. At charge neutrality, these samples show electron-hole limited conductivity over a wide temperature range (Fig. 2a). A single set of fit parameters provides quantitative agreement with experiments at all densities, temperatures, and gaps measured, allowing for separate extraction of the electron-hole and dissipative contributions (Fig. 2b). Our work provides an intuitive understanding for electron-hole limited transport in a semiconductor across a wide range of parameters and provides a unique link between semiconductor physics and the emerging field of viscous electronics.

REFERENCES

- [1] C. Tan, D. Y. H. Ho, L. Wang, J. I. A. Li, I. Yudhistira, D. A. Rhodes, T. Taniguchi, K. Watanabe, K. Shepard, P. L. McEuen, C. R. Dean, S. Adam, J. Hone, submitted.

FIGURES

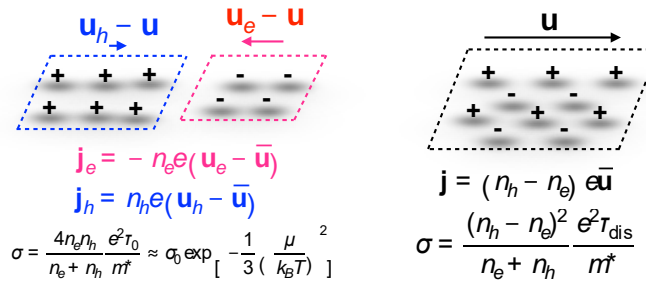


Figure 1: Schematic of Coulomb drag and center-of-mass contributions to hydrodynamic conductivity.

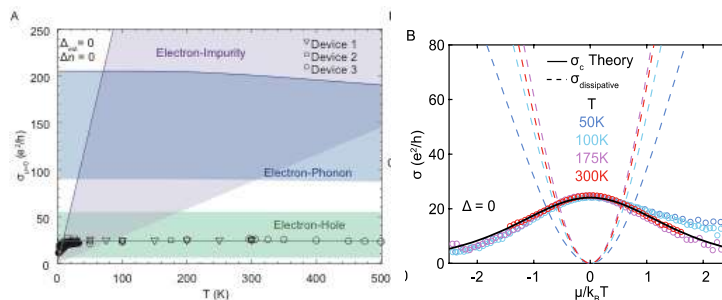


Figure 2: (A) Measured conductivity of bilayer graphene at charge neutrality, with predicted contributions from impurity, phonon, and electron-hole scattering. (B) Extraction of the universal Coulomb drag and non-universal dissipative terms.

BN materials for 2D devices: learnings from optical properties

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With the rise of 2D materials, BN layers and crystals have become a strategic material for the fabrication of van der Waals heterostructures. Stacked with any other 2D material either as a substrate or as capping layer or as dielectric layer, it can reveal the best of their physical properties [1, 2]. Up to now, the prototype devices are mostly assembled via mechanical exfoliation and transfer of atomic layers. But active researches are developing worldwide to fabricate the large-surface crystals required for device industrialisation. In this context, optical diagnostics are highly desired to qualify hBN materials for their integration into 2D devices.

In this talk, the recently acquired basic knowledge on the luminescence properties of free excitons in hBN measured by cathodoluminescence [3] and the vibrational properties by Raman spectroscopy [4,5] are exploited for this purpose. The reference data are taken from the high quality crystals grown at high pressure and high temperature (HPHT) mostly used in devices [6]. They are compared with those of hBN materials obtained either using a chemical process followed by high pressure annealing [7] or a direct synthesis at atmospheric pressure (APHT) with boron isotope control. The APHT crystals have been shown recently to be a credible alternative to HPHT ones for high-performance graphene devices [8].

REFERENCES

- [1] C. R. Dean et al., *Nature Nanotech*, 5 (2010) 722.
- [2] F. Cadiz et al, *PRX* 7 (2017) 021026
- [3] L. Schué et al., *Phys. Rev. Lett.* 122 (2019) 067401
- [4] L. Schué et al., *2D Mat.* 4 (2017) 015028
- [5] I. Stenger et al., *2D Mat.* 4 (2017) 031003
- [6] T. Taniguchi, K. Watanabe, *J. Cryst. Growth* 303 (2007) 525
- [7] Y. Li et al, *Nanotechnology* **30**, 035604 (2019)
- [8] J. Sonntag et al., *2D Materials* 7 (2020) 031009

Lattice dynamics in low-angle twisted bilayer graphene

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Twisted bilayer graphene is created by slightly rotating the two crystal networks in bilayer graphene with respect to each other. [1-4] For small twist angles, the material undergoes a self-organized lattice reconstruction, leading to the formation of a periodically repeated domain. The resulting superlattice modulates the vibrational [1,3] and electronic structures [4] within the material, leading to changes in the behavior of electron-phonon coupling and to the observation of strong correlations and superconductivity.

In this talk, I will report on the phonon spectra of twisted bilayer graphene (tBLG) that were computational analyzed for a series of 692 twisting angle values in the $[0, \pi/6]$ range. The evolution of the phonon bandstructure as a function of twist angle is examined using a band unfolding scheme where the large number of phonon modes computed at the Γ point for the large moiré tBLG supercells are unfolded onto the Brillouin Zone (BZ) of one of the two constituent layers. In addition to changes to the low-frequency breathing and shear modes, a series of well-defined side-bands around high-symmetry points of the extended BZ emerge due to the twist angle-dependent structural relaxation. I will also review how these results have been confirmed experimentally in collaboration with the group of Ado Jorio: Observations of the crystallographic structure with visible light are made possible by the nano-Raman technique, which reveals the localization of lattice dynamics, with the presence of strain solitons and topological points causing detectable spectral variations.

REFERENCES

- [1] Sheremetyeva, N., Lamparski, M., Daniels, C., Van Troeye, B. & Meunier, V., "Machine-learning models for Raman spectra analysis of twisted bilayer graphene," *Carbon N. Y.* (2020). DOI: 10.1016/j.carbon.2020.06.077
- [2] Gadelha, A. C., Ohlberg, D. A. A., Rabelo, C., Neto, E. G. S., Vasconcelos, T. L., Campos, J. L., Lemos, J. S., Ornelas, V., Miranda, D., Nadas, R., Santana, F. C., Watanabe, K., Taniguchi, T., van Troeye, B., Lamparski, M., Meunier, V., Nguyen, V.-H., Paszko, D., Charlier, J.-C., Campos, L. C., Caçado, L. G., Medeiros-Ribeiro, G. & Jorio, A., "Localization of lattice dynamics in low-angle twisted bilayer graphene," *Nature* **590**, 405–409 (2021). DOI: 10.1038/s41586-021-03252-5
- [3] Lamparski, M., Van Troeye, B. & Meunier, V., "Soliton signature in the phonon spectrum of twisted bilayer graphene," *2D Mater.* (2020). DOI: 10.1088/2053-1583/ab7874
- [4] Nguyen, V. H., Paszko, D., Lamparski, M., Troeye, B. Van, Meunier, V. & Charlier, J.-C., "Electronic localization in small-angle twisted bilayer graphene," ArXiv, cond-mat.mes-hall/2102.05376 (2021).

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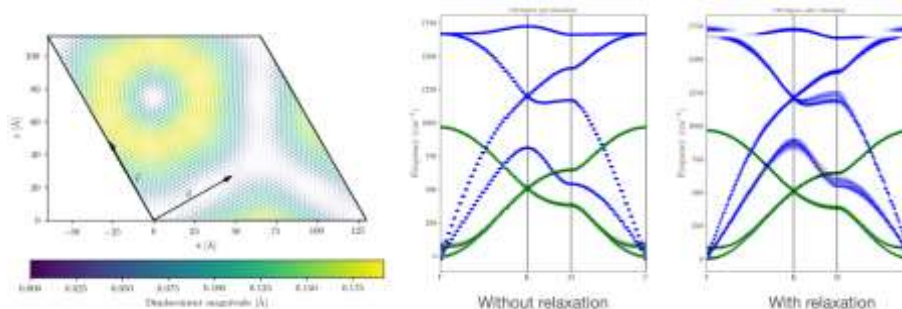


Figure 1: Crystal field due to reconstruction in moiré pattern (top) and unfolded phonon bandstructure with and without full atomic reconstruction. Adapted and reproduced from Ref. [3].

Stable-fragile-delicate: new notions in topological band theory

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Topological quantum matter is a very active research direction in condensed matter physics. Over the past two decades, many topological materials have been identified in a tight interplay between theory and experiments. In this process, the theoretical framework, in particular topological band theory, has been continuously refined. In this talk I will give an overview of our current understanding of topological classifications of electronic bands, with a focus on two-dimensional materials. In particular, I will discuss the differentiation between atomic insulators, so-called delicate topology [1] and fragile topology. As a concrete example, I will discuss how graphene, when decorated with adatoms, can host fragile topological flat bands [2]. I will contrast these bands with the ones arising in moiré heterostructures.

REFERENCES

1. Nelson, A., Neupert, T., Bzdušek, T., and Alexandradinata, A., [arXiv:2009.01863](https://arxiv.org/abs/2009.01863)
2. Skurativska, A., Tsirkin, S.S., Natterer, F.D., Neupert, T., and Fischer, M.H., [arXiv:2101.08273](https://arxiv.org/abs/2101.08273)

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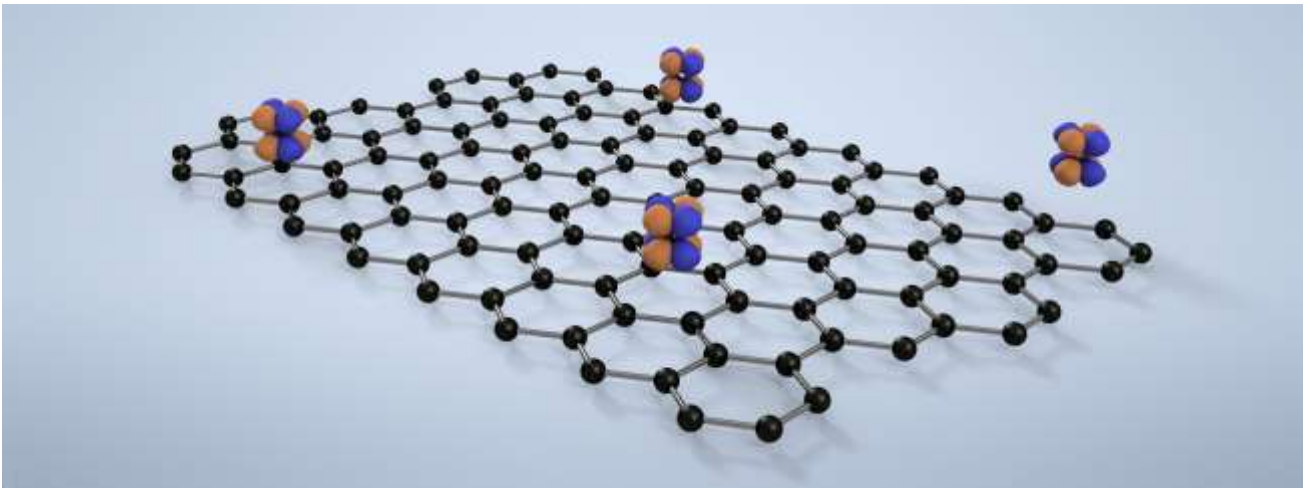


Figure 1: Schematic of graphene decorated with adatoms giving rise to a fragile topological flat band with d-orbital character.

Molecular functionalization of 2D materials: high-performance opto-electronic devices

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Two dimensional materials exhibit exceptional physical and chemical properties which can be further enhanced and enriched via the controlled functionalization with molecules and (supra)molecular assemblies thereof yielding hybrid systems with ad hoc characteristics for applications in (opto)electronics, sensing and energy. Molecules can be designed and synthesized in order to physisorb or chemisorb onto 2D materials in a controlled fashion.

In my lecture I will review our recent findings on the functionalization of 2D materials to engineer hybrid systems via:

- physisorption of molecular switches onto the two surfaces of scotch tape and CVD 2D ambipolar semiconductors, following a Janus approach, as a route to confer two distinct and additional properties to WSe_2 , rendering the 2D material-based transistors capable to respond to three different independent stimuli.
- chemisorption of doubly-thiolated molecules onto solution-processed semiconducting transition metal dichalcogenides as a way to simultaneously heal sulfur vacancies in metal disulfides (MS_2) and covalently bridge adjacent flakes, thereby promoting percolation pathways for the charge transport, leading to an increase by one order-of-magnitude in field-effect mobility, I_{ON} / I_{OFF} ratio, and switching times of liquid-gated transistors.

Our modular strategies relying on the combination of 2D material with molecules offer a simple route to generate multifunctional 2D materials-based coatings, foams and nanocomposites with pre-programmed properties to address key global challenges in electronics, sensing and energy applications.

FIGURES



Figure 1: 1,4-benzenedithiol molecules simultaneously healing sulfur vacancies in solution-processed MoS_2 and covalently bridging adjacent flakes, to create percolation pathways for the charge transport in transistors.

2D Bismuth for Flexible Thermoelectric and Photoelectric Electronics

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Abstract

Bismuth(Bi) is a post transition metal with a high carrier mobility $\sim 20\,000\text{ cm}^2\text{ V}^{-1}\text{ s}^{-1}$ [1] and low thermal conductivity $\sim 10\text{ W m}^{-1}\text{ K}^{-1}$ [2]. Bismuthene, 2D Bi, is similar to black phosphorus with tunable bandgap[3, 4] and expected isotropic properties. It is of great interests and importance to exploit its potential in thermoelectric devices, photodetectors, transistors and other nanoelectronics.

Although there have been studies on 2D Bi and its transistor devices[5], thermoelectric and photodetectors on hard substrates[6], there is a lack of experimental demonstration on the large-area uniform 2D Bi and its devices especially on flexible substrates[7]. Herein, we prepared 2D Bi with precise thickness control on Si and flexible polyimide substrates by physical vapor deposition, and integrated solid-state devices to probe thermoelectric and photoelectric response. 2D bismuth exhibited superior mechanical flexibility, and descent electrical properties that can be controlled via thickness and interface engineering. E-beam evaporated 2D bismuth could yield Seebeck coefficient and electrical conductivity comparable to molecular epitaxy counterparts, and an 50% enhanced performance on polyimide than Si. Our results suggest 2D bismuth with photoelectric and thermoelectric effects holds great promise for flexible multifunctional devices.

REFERENCES

- [1] D. L. Partin, J. Heremans, D. T. Morelli, C. M. Thrush, C. H. Olk, and T. A. Perry, *Physical Review B*, 6(1988), 3818-3824
- [2] H. K. Lyo and D. G. Cahill, *Physical Review B*, 14(2006), 144301
- [3] H. Huang et al., 23(2018), 235201
- [4] H. Zhao et al., *J. Semicond.*, 8(2020), 081001
- [5] W. Zhong et al., *Nanotechnology*, 47(2020), 475202
- [6] J. D. Yao, J. M. Shao, and G. W. Yang, *Scientific Reports*, 5(2015), 12320
- [7] Q. Q. Zhou et al., *Acs Applied Electronic Materials*, 5(2020), 1254-1262

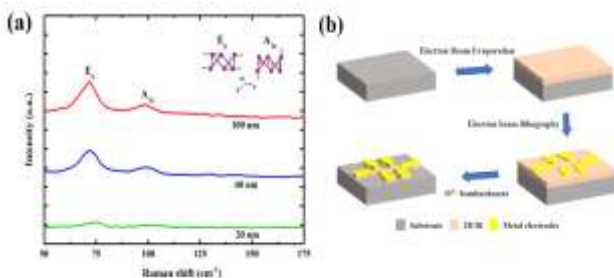


Figure 1: Raman spectra of 2d Bi in different thicknesses. (a) A_{1g} and E_g characteristic peaks corresponding to two vibration modes. (b) FET fabrication with lithography, deposition and etching processes.

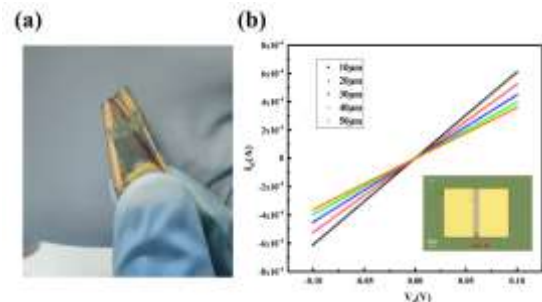


Figure 2: Field effect transistors of 2D Bi on polyimide. (a) Mechanical flexibility and light transmittance of the device. (b) I_d - V_d curve with different channel widths.

Novel graphene, BP and perovskite-based 2D devices

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Abstract

In this talk, I will introduce several novel 2D devices based on graphene and beyond graphene. The first part is related to graphene devices. Tunable graphene LED [1] and graphene artificial throat [2] has been demonstrated. The second part is related to 2D perovskite devices. Record low operation current 2D perovskite-RRAM has been demonstrated [3]. Great stability has also been demonstrated via hBN-2D perovskite stacking [4]. The third part is related to BP devices. Reconfigurable BP-SnSe synapse has been demonstrated [5]. Moreover, the reconfigurable BP p-n junctions have been demonstrated with ideality factor close to 1 [6].

REFERENCES

- [1] X. Wang+, H. Tian+, et al., Nature Communications, 6 (2015) 7767.
- [2] L. Tao+, H. Tian+, et al., Nature Communications, 8 (2017) 14579.
- [3] H. Tian*, et al., ACS Nano, 11 (2017) 12247.
- [4] L. Zhao+, H. Tian+*, et al., Joule, 2, (2018) 2133.
- [5] H. Tian, et al., ACS Nano, 11 (2017) 7156.
- [6] H. Tian*, et al., IEEE Transactions on Electron Devices, 65 (2018) 5118 .

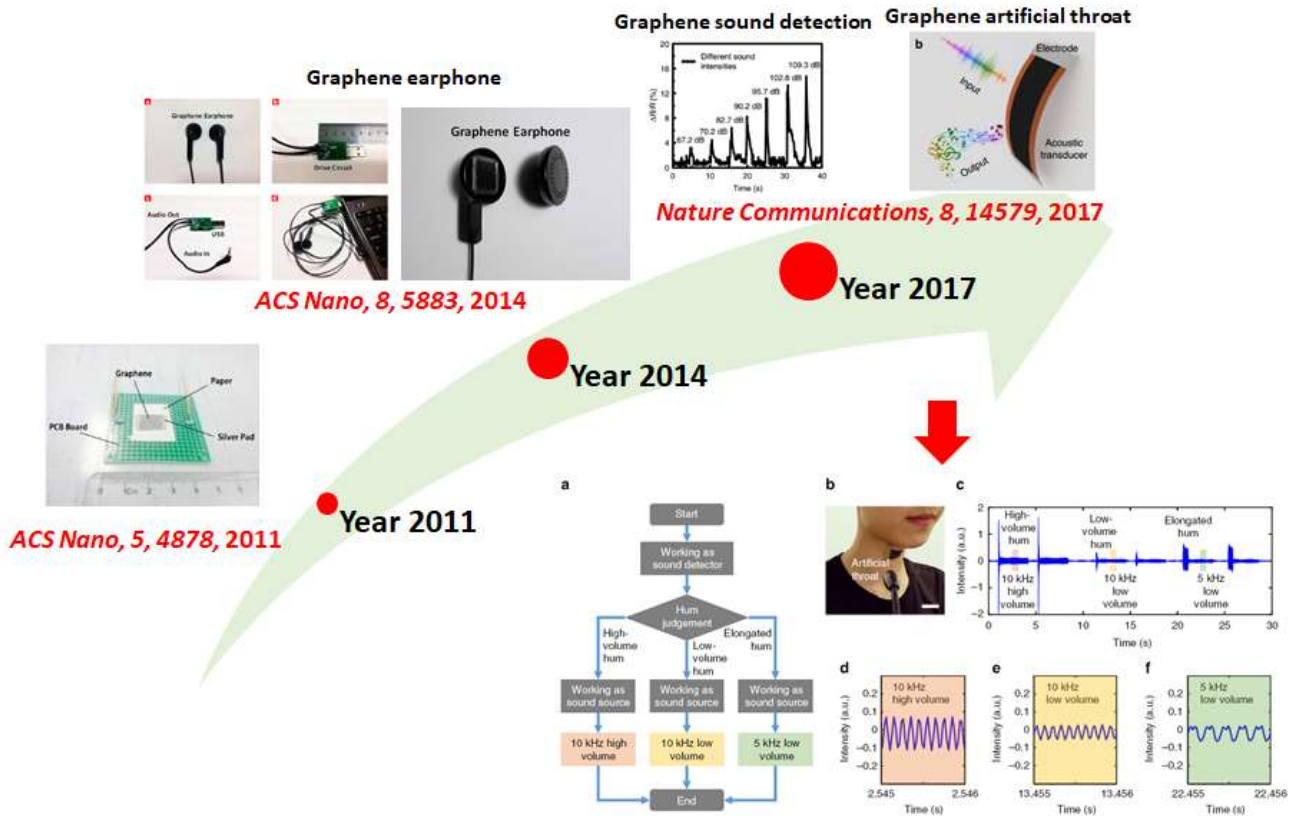


Figure: the development of graphene-based acoustic devices in my group.

Interface coupling and band topology in van der Waals materials

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Abstract

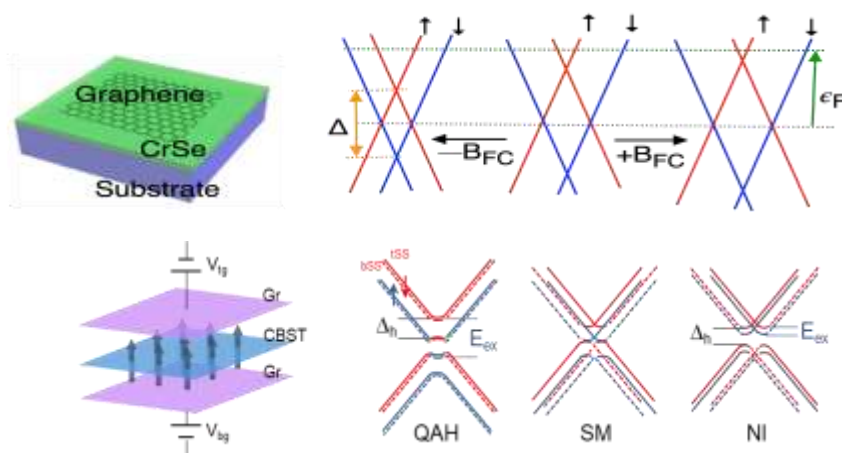
Van der Waals materials like graphene, transition metal dichalcogenides and topological insulators have been extensively investigated over the past decades due to their fascinating physical properties. The investigation of these materials and their heterostructures has spurred significant advances and new dimensions in modern materials research and nanotechnology. Among them, graphene-based heterostructures exhibit rich physics with exotic properties, which are promising for future electronic and spintronic devices. Spin splitting in graphene is required to develop graphene-based multifunctional spintronic devices with low dissipation and long-distance spin transport. Magnetic proximity effects are a promising route to realize exchange splitting in the material. By coupling graphene to an antiferromagnet, magnetism can be induced into graphene and a large exchange splitting energy around 134 meV can be obtained [1]. Besides antiferromagnets, graphene coupled to other 2D materials like transition metal dichalcogenides can enhance its spin-orbit coupling and result in a topological phase transition. Similarly, in a topological insulator, magnetism can be induced by magnetic doping and lead to the quantum anomalous Hall effect. By controlling the exchange energy of a magnetic-doped topological insulator *via* a perpendicular electric field, a reversible switching between topological and trivial insulating phases can be achieved. Additionally, strong electronic correlation can be induced in monolayer graphene by means of nanoscale strain engineering, leading to giant pseudo-magnetic fields (PMFs), flat bands and spontaneous symmetry breaking in graphene with periodic wrinkles [2]. Valley-Hall transistors built on such strained graphene are shown to demonstrate quantum valley Hall and quantum anomalous Hall effects with a range of Chern numbers in the absence of external magnetic fields. The topological phases and the underlying physics in all the aforementioned systems will be discussed.

REFERENCES

1. Yingying Wu, Gen Yin, Lei Pan, Alexander J. Grutter, Qunjun Pan, Albert Lee, Dustin A. Gilbert, Julie A. Borchers, William Ratcliff II, Ang Li, Xiao-dong Han & Kang L. Wang, Nature Electronics, 3, 604-611 (2020).
2. Chen-Chih Hsu, Marcus L. Teague, Jiaqing Wang & Nai-Chang Yeh, Science Advances, 6, aat9488 (2020).

FIGURES

Figure 1: (top) Large exchange splitting in a graphene/CrSe heterostructure. (bottom) Controlling the topological phase transition in a Cr-(Bi,Sb)₂Te₃ magnetic-doped topological insulator.



Spin, Charge, and Phonon Coupling Effects in a 2D Magnet

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The coupling between spin, charge, and lattice degrees of freedom plays an important role in a wide range of fundamental phenomena. 2D magnets is an emerging platform for studying these coupling effects. In this talk, I will present such an example in a van der Waals zigzag antiferromagnetic insulator NiPS₃. We observe an exciton photoluminescence with a narrow linewidth of ~ 350 μeV with near unity linear polarization. In addition, the optical reflection exhibits strong linear dichroism (LD) over a broad spectral range. The optical anisotropy axes of LD and of photoluminescence are locked to the zigzag direction. Their temperature dependence is also reminiscent of the in-plane magnetic susceptibility anisotropy. Our results suggest that LD and photoluminescence probes the symmetry breaking magnetic order parameter of 2D magnetic materials. Furthermore, we observe over ten exciton- A_{1g} phonon bound states on the high energy side of the exciton resonance, which we interpret as signs of a strong modulation of the ligand-to-metal charge transfer energy by electron-lattice interactions. Our work establishes NiPS₃ as a 2D platform for exploring magneto-exciton physics with strong correlations.

Gate-defined Josephson junctions in magic-angle twisted bilayer graphene

Folkert de Vries

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Magic-angle twisted bilayer graphene has emerged as a uniquely versatile experimental platform that combines metallic, superconducting, magnetic and insulating phases in a single crystal [1,2]. In particular the ability to tune the superconducting state with a gate voltage opened up intriguing prospects for novel device functionality. We present the first demonstration of a device based on the interplay between two distinct phases in adjustable regions of a single magic-angle twisted bilayer graphene crystal [3,4]. We electrostatically define the superconducting and insulating regions of a Josephson junction and observe tunable DC and AC Josephson effects (see Figure 1). We show that superconductivity is induced in different electronic bands and describe the junction behaviour in terms of these bands, taking in consideration interface effects as well. Shapiro steps, a hallmark of the AC Josephson effect and therefore the formation of a Josephson junction, are observed. This work is an initial step towards devices where separate gate-defined correlated states are connected in single-crystal nanostructures. We envision applications in superconducting electronics and quantum information technology as well as in studies exploring the nature of the superconducting state in magic-angle twisted bilayer graphene.

REFERENCES

- [1] Cao, Y. et al., Nature 556 (2018) 43–50
- [2] Lu, X. et al., Nature 574 (2019) 653–657
- [3] de Vries, F. K. et al. Nature Nanotechnology, in print.
- [4] Rodan-Legrain, D. et al. Nature Nanotechnology, in print.

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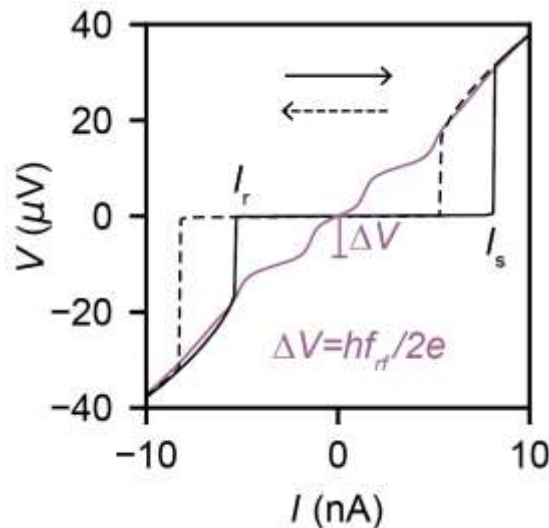


Figure 1: Current (I) versus voltage (V) linetraces showing the AC (magenta) and DC (black) Josephson effects. The solid and dashed arrows indicate the sweep direction of the current.

Electrical and thermal generation of spin currents by magnetic graphene

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In graphene-based van der Waals heterostructures, the superior spin and charge transport properties of graphene are enriched via the proximity to other 2D materials. By the proximity effects, one can induce spin-orbit and magnetic exchange interactions in the graphene which provide strong coupling between charge and spin currents [1-3]. In particular, our recent investigation of spin transport in graphene in the proximity of a 2D interlayer antiferromagnet CrSBr has shown strong spin polarization of conductivity in graphene ($\sim 14\%$). The spin-dependent conductivity arises from a large induced exchange interaction that also results in the observation of spin-dependent Seebeck effect in graphene. This is the first-time experimental realization of the active role of magnetic graphene in the electrical and thermal generation of spin currents, addressing the most technologically relevant aspects of the induced magnetism. The spin-dependent conductivity and Seebeck coefficient, together with the long-distance spin transport introduce magnetic graphene as an ultimate building block for ultra-compact magnetic memory and sensory devices and can provide substantial advances in 2D spintronic/caloritronic technology [3].

REFERENCES

- [1] Ghiasi, T.S., et al., *Nano letters* 17.12 (2017): 7528-7532.
- [2] Ghiasi, T.S., et al., *Nano letters* 19.9 (2019): 5959-5966.
- [3] accepted in *Nature Nano*. arXiv:2007.15597 (2021).

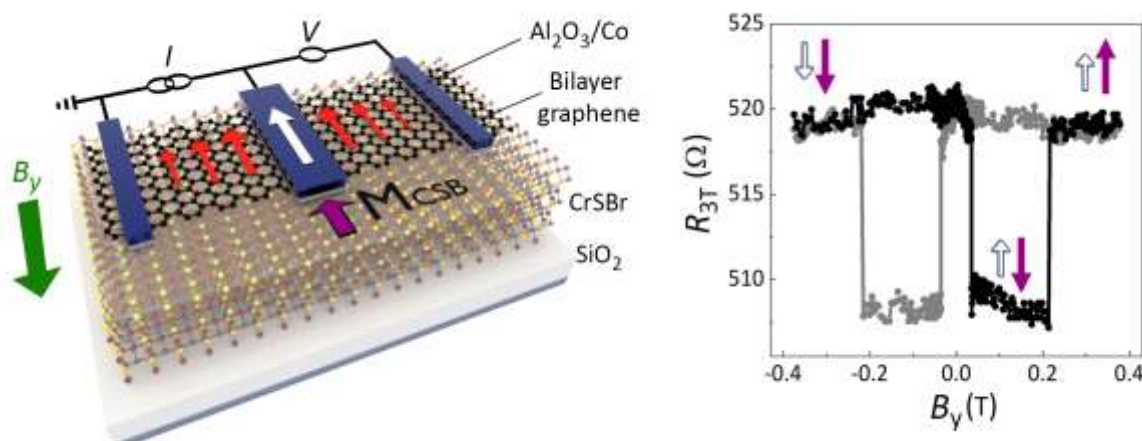


Figure 1: Schematic picture of the studied device with a bilayer graphene/CrSBr van der Waals heterostructure. The resistance measured in the three-terminal geometry ($R_{3T}=V/I$) with Al₂O₃/Co electrodes versus the external magnetic field (B_y) shows a considerable change, depending on the relative orientation of the Co magnetization (white arrow) and that of CrSBr (M_{CSB} , purple arrow). The induced magnetization in graphene by M_{CSB} , allows for higher conductivity of the spin up electrons (red arrows) in the graphene channel.

Pseudospintronics - Graphene transistor based on tunable topological properties of Dirac fermions

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Arguably the biggest challenge with graphene-based electronic switching is the lack of a band-gap. Unfortunately, forcing a band-gap through differential doping or vertical fields increases the effective mass and kills mobility. In contrast, the topology of spins/pseudospins in Dirac cone materials offers truly novel opportunities in electron dynamics, beyond just their impact on mobility, especially since off current tends to pose the main challenge in switching. We argue that the transmission of electrons across PN junctions can actually be gate-modulated significantly^[1-5] due to added constraints imposed by their winding (Chern) number – winding of pseudospins in bulk monolayer/bilayer graphene, spins in topological insulators and Weyl semi-metals, magnetization in skyrmionic materials. Experiments have successfully demonstrated key components along this path, including the control of trajectory through negative index (Veselago) behavior^[2], control of their transmission by gate modulation of conductance (Klein tunneling)^[3], magnetoconductance minima in Corbino discs (anti-Klein tunneling)^[4], current saturation in bulk graphene, and angle-dependent transmission (Malus' law) across bulk graphene PN junctions^[5]. Based on these data, we explain the opportunities for Dirac fermionic switches and the material challenges along the way.

REFERENCES

- [1] "Spin control with a topological semi-metal", AW Ghosh, Physics 13, 28 (2020)
- [2] "Electron optics with p-n junctions in ballistic graphene", Science 353, 1522 (2016)
- [3] "Graphene Transistor Based on Tunable Dirac-Fermion-Optics", PNAS 116, 6575 (2019)
- [4] "Manifestation of Chiral tunneling in tilted graphene pn junction", R. N. Sajjad, S. Sutar, J. Lee and A. W. Ghosh, Phys. Rev. B 86, 155412 (2012).
- [5] "Manipulating Chiral transmission by Gate Geometry: Switching in Graphene with transmission gaps", ACS Nano, vol. 7 :11 , pp. 9808-9813, 2013

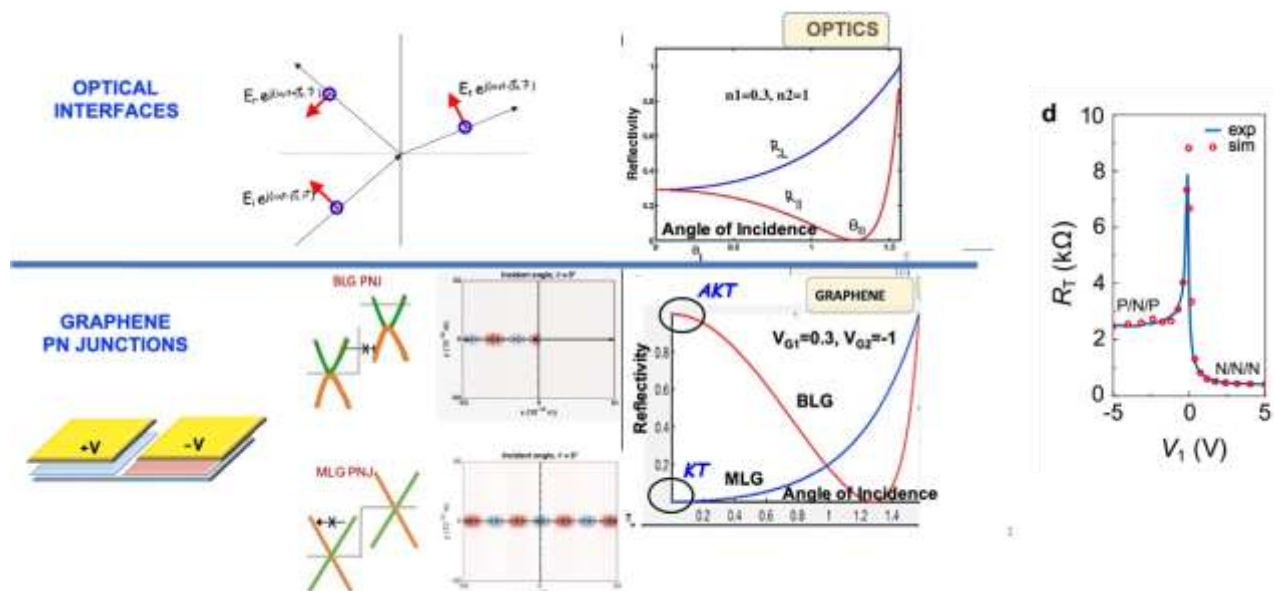


Figure 1: (Top Left) Optical Reflectivity at material interfaces at normal incidence depends on refractive index ratio at the interface. (Bottom Left) Electron reflectivity at graphene PN junctions depends only on topology of pseudospins around the Fermi circle, and is zero (Klein tunneling) for odd layer and unity (Anti-Klein tunneling) for even layers. The pinned value at normal incidence allows us to collimate electrons with a split gate and realize a *Klein tunnel transistor* with bulk graphene, based on gate-geometry alone. (Right) Experiments showing conductance modulation by gating from NNN to PNP doping in bulk graphene [2].

Polymer Derived Ceramics route and derivatives applied to the synthesis of Boron Nitride

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Due to its intrinsic properties, hexagonal boron nitride (h-BN) is currently an increasingly attractive material, especially for applications related to two-dimensional materials. However, its properties are highly dependent on the synthesis approach used. The polymer-derived ceramics (PDCs) route allows to elaborate h-BN with adapted textural and structural properties.[1]

Here we will demonstrate the value of the PDCs route for the synthesis of h-BN. First, we will see how the PDCs route alone from borazine precursor allows, at relatively low temperature and atmospheric pressure, the growth of h-BN single crystals with sizes of a few microns. Crystallization is improved by adding 5 wt% Li₃N to the preceramic polymer.

Next, we will show that by coupling the PDCs route with gas pressure sintering (GPS), using the same preceramic polymer and 25 wt% Li₃N, the crystal size is increased to hundreds of microns (figure 1). The resulting pure h-BN single crystals can then be exfoliated into h-BN nanosheets.

Finally, the combination of the PDCs route with atomic layer deposition (ALD) has enabled the successful synthesis of functional BN nano-/heterostructures from highly structured sensitive templates, making this ALD process a promising alternative for the fabrication of functional BN nanostructures.

REFERENCES

- [1] B. Matsoso, W. Hao, Y. Li, V. Vuillet-A-Ciles, V. Garnier, P. Steyer, B. Toury, C. Marichy, C. Journet, *Journal Of Physics: Materials*, 3 (2020) 034002

FIGURES

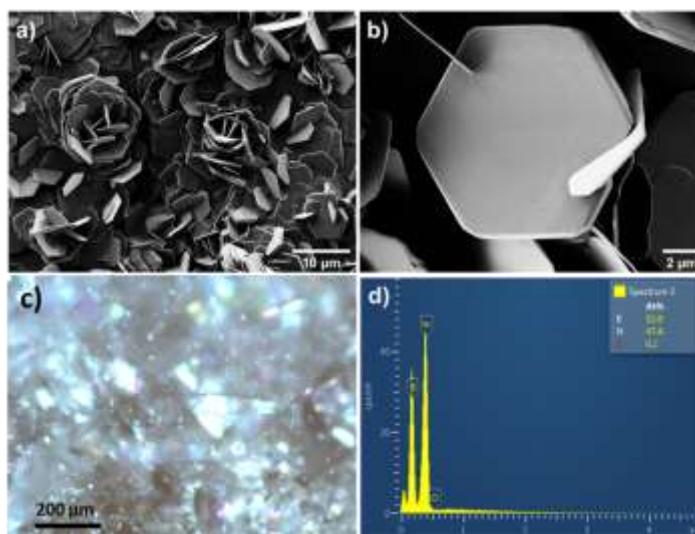


Figure 1: (a), (b) Low resolution SEM micrographs of h-BN sample obtained by the combination of PDCs and GPS. In (a) faceted flower-like crystals are observed and (b) shows the detail of one h-BN crystal. Corresponding (c) optical image and (d) EDS spectrum recorded using SEM.[1]

Engineering graphene Josephson junction for sensitive photon detector

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Abstract

Sensitive microwave detectors are essential in radioastronomy, dark-matter axion searches and superconducting quantum information science. The conventional strategy to obtain higher-sensitivity bolometry is the nanofabrication of ever smaller devices to augment the thermal response. However, it is difficult to obtain efficient photon coupling and to maintain the material properties in a device with a large surface-to-volume ratio owing to surface contamination. Here we present an ultimately thin bolometric sensor based on monolayer graphene. To utilize the minute electronic specific heat and thermal conductivity of graphene, we develop a superconductor–graphene–superconductor Josephson junction bolometer embedded in a microwave resonator with a resonance frequency of 7.9 gigahertz and over 99 per cent coupling efficiency. The dependence of the Josephson switching current on the operating temperature, charge density, input power and frequency shows a noise-equivalent power of 7×10^{-19} watts per square-root hertz, which corresponds to an energy resolution of a single 32-gigahertz photon, reaching the fundamental limit imposed by intrinsic thermal fluctuations at 0.19 kelvin [1]. We will also discuss our experimental demonstration of 1,550-nm infrared single photon detector [2] as well as theoretical modelling for ultra-light dark matter search using graphene-based sensor [3].

REFERENCES

- [1] Gil-Ho Lee et al., *Nature*, 586 (2020) 42–46
- [2] Evan D. Walsh et al., arXiv:2011.02624
- [3] Doojin Kim, Jong-Chul Park, Kin Chung Fong, Gil-Ho Lee., arXiv:2002.07821

Predicting the strain effects in 2D materials: the case of ZrS3 monolayers

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Thermoelectric materials have attracted much attention because they produce electricity without moving parts, which makes them ideal to engineer reliable devices that require minimal maintenance for long periods for applications such as harvesting human body heat and solar generators. We present here the influence of strained deformations on the mechanical and electronic properties of ZrS3 monolayers. Density functional theory (DFT) calculations are employed at the hybrid HSE06 level on the atomistic structures optimised with PBE to evaluate the anisotropic response of the electronic band gap and mobilities, as well as the thermopower, the electrical and thermal conductivities, and the figure of merit. Direct examination of the electronic band structures reveals that the band gap can be increased by up to 17% under uniaxial strain, reaching up to 2.32 eV for ZrS3. We also detect large variations in the electrical conductivity in this material, which is multiplied by 3.40 under a 4% compression for ZrS3. In contrast, our DFT calculations predict much smaller changes in the Seebeck coefficient. In addition, the modelling of mechanical deformation is also used to find the anisotropic behaviour of the Poisson ratios. We also present at which conditions these strain engineering results should be trusted, yielding an enhancement of the figure of merit of nearly two times with respect to the unstrained case

Keywords: Density Functional Theory; 2D materials; nanoscale electronic and thermal transport..

REFERENCES

- [1] F. Saiz and R. Rurali, Nano Express, 2020, 1, 010026.
- [2] F. Saiz, J. Carrete, and R. Rurali, Nanomaterials, 2020, 10, 704.
- [3] F. Saiz, J. Carrete, and R. Rurali, Nanoscale Advances, 2020, 2, 5352.

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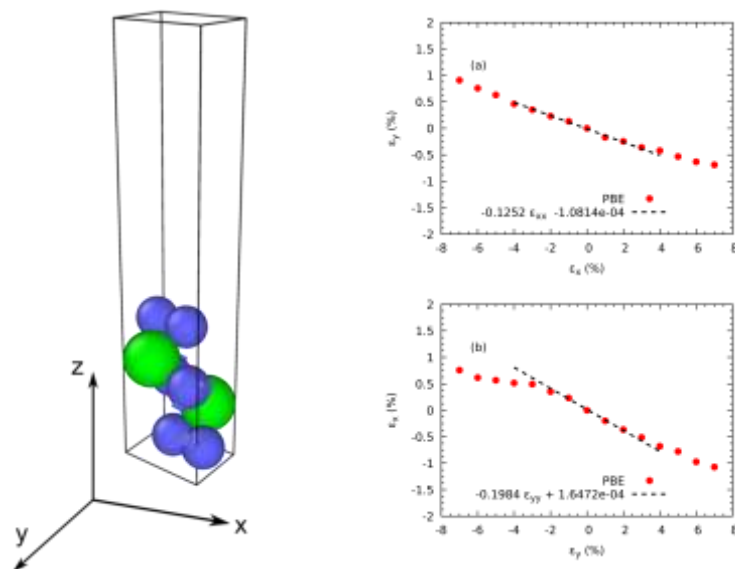


Figure 1: Please make a brief schematic diagram as ‘Graphical Abstract’. Insert those Graphics and Synopsis here. Please make sure that this can clearly illustrate your work.

Engineering wafer-scale epitaxial two-dimensional materials for advanced high-performance nanoelectronics

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Abstract: Atomically thin two-dimensional (2D) metal dichalcogenides (MX_2) have attracted great interest in extending Moore's law beyond silicon due to their unique structural and electronic properties.^[1-5] As one of the most promising substrates for wafer-scale single crystalline 2D MX_2 deposition, the single crystalline c-plane sapphire (0001, $\alpha\text{-Al}_2\text{O}_3$) has been considered as a suitable substrate to achieve this, due to its specific lattice orientation, atomically smooth surface and high quality single crystal nature. MX_2 deposition on this kind of substrates can show a specific orientation preference, which is determined by the crystal symmetry and the surface terraces of the sapphire substrates.^[6-7] However, the single crystalline c-plane sapphire has a complex surface structure, typically composed of a terrace and step structure as a result of the sapphire ingot grinding and polishing processes, which can influence the surface termination of sapphire wafers.^[8] It has been demonstrated that the atomic steps on sapphire have significant effects on the growth behaviour of the MX_2 .^[9] It is poorly understood how inhomogeneous sapphire surface structure influences the epitaxial growth of the 2D materials and device performance. In this work, we observe the inhomogeneous surface terrace structure of sapphire wafers can result in different nucleation rate and then growth of monolayer 2D MX_2 among the terraces. This influences further the electrical properties of the coalesced monolayer and the performance of monolayer MoS_2 transistors. This finding is applicable to other MX_2 materials and brings breakthrough knowledge to understand better how the sapphire surface structure influence the MX_2 epitaxial growth and the performance of related electronic devices.

REFERENCES

- [1] Y. Shi, X. Liang, B. Yuan, V. Chen, H. Li, F. Hui, Z. Yu, F. Yuan, E. Pop, H.-S. P. Wong, M. Lanza, *Nature Electronics*, 1 (2018), 458-465 (2018).
- [2] Y. Shi, C. Pan, V. Chen, N. Raghavan, K. L. Pey, F. Puglisi, E. Pop, H.-S. P. Wong, M. Lanza, *IEDM* (2017), pp.5.4.1.
- [3] Q. Smets, G. Arutchelvan, J. Jussot, D. Verreck, I. Asselberghs, A. N. Mehta, A. Gaur, D. Lin, S. E. Kazzi, B. Groven, M. Caymax, I. Radu, *IEDM* (2019), pp. 23.2.1.
- [4] Q. Smets, D. Verreck, Y. Shi, G. Arutchelvan, B. Groven, X. Wu, S. Sutar, S. Banerjee, A. N. Mehta, D. Lin, I. Asselberghs, I. Radu, *IEDM* (2020), pp.3.1.1.
- [5] I. Asselberghs, Q. Smets, T. Schram, B. Groven, D. Verreck, A. Afzalian, G. Arutchelvan, A. Gaur, D. Cott, T. Maurice, S. Brems, K. Kennes, A. Phommahaxay, E. Dupuy, D. Radisic, J. F. de Marneffe, A. Thiam, W. Li, K. Devriendt, C. Huyghebaert, D. Lin, M. Caymax, P. Morin, I. Radu, *IEDM* (2020), pp. 40.2.1.
- [6] A. Aljarb, Z. Cao, H.-L. Tang, J.-K. Huang, M. Li, W. Hu, L. Cavallo, L.-J. Li, *ACS Nano*, 11 (2017), 9215.
- [7] Y.-C. Lin, B. Jariwala, B. M. Bersch, K. Xu, Y. Nie, B. Wang, S. M. Eichfeld, X. Zhang, T. H. Choudhury, Y. Pan, R. Addou, C. M. Smyth, J. Li, K. Zhang, M. A. Haque, S. Fölsch, R. M. Feenstra, R. M. Wallace, K. Cho, S. K. Fullerton-Shirey, J. M. Redwing, J. A. Robinson, *ACS Nano*, 12 (2018), 965.
- [8] Y. Hayashi, R. G. Banal, M. Funato, Y. Kawakami, *J. Appl. Phys.*, 113 (2013), 183523.
- [9] L. Chen, B. Liu, M. Ge, Y. Ma, A. N. Abbas, C. Zhou, *ACS Nano*, 9 (2015), 8368.

Engineering van der Waals heterostructures for spintronics

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In recent years, spin-based technologies, in which information is carried by spin instead of charge, have become promising for “beyond-CMOS” devices. Graphene and other two dimensional materials have rapidly established themselves as intriguing building blocks for spintronics applications. Owing to graphene intrinsic low spin-orbit interaction, spins can flow snugly through its crystal lattice over long distances resulting in an ideal spin channel but, at the same time, making it difficult to manipulate spins, which is the cornerstone for successfully implementing spin-based devices. In this talk a series of experiments where we study spin transport and relaxation mechanisms in graphene based van der Waals heterostructures will be presented [1,2]. It will be demonstrated how proximity-induced spin-orbit interaction in graphene --imprinted by an adjacent semiconducting transition metal dichalcogenide such as WS_2 -- results in anisotropic spin dynamics. Besides, it will be shown how the enhancement of spin-orbit interaction in graphene can be utilized for room temperature spin-to charge conversion driven by both the spin Hall and the spin galvanic effect on these layered systems [3].

REFERENCES

- [1] L. A. Benítez, J. F. Sierra et al., *Nature Physics* 14, (2018) 303;
- [2] L. A. Benitez, J. F. Sierra et al., *APL Materials*, 7, (2019) 120701
- [3] L. A. Benítez, W Savero Torres, J. F. Sierra et al., *Nature Materials* 19, (2020).

Controlled Growth of High-Quality CVD Graphene

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Graphene has garnered widespread interest and confer remarkable potential for next-generation technological applications, which relies on the controllable and mass-production of high-quality graphene films. Chemical vapor deposition (CVD) is considered the most promising method, and great progress has been achieved over the last decade^[1]. Currently, this field is being pushed to new heights that pursuit structure control (e.g. orientation, layer, stacking order, contamination, doping, etc.) and low-cost production (e.g. increasing the production capacity and growth rate)^[2]. In this talk, I will introduce our recent works on controlled growth of high-quality graphene films via CVD approach. By designing and preparing single-crystal Cu foils, we have opportunities in realizing the epitaxial growth of large-area single-crystal graphene film^[3]. We designed and constructed a pilot-scale CVD system suitable for producing A3-size graphene films, which works well and output high-quality graphene films with high capacity. In another hand, we also explore the possibility on controlling the layer number and stacking order, which is motivated by the emerging twistrionics. Here I will present our state-of-the-art hetero-site nucleation method for growing twisted bilayer graphene (tBLG)^[4]. Gas-flow perturbation and switching of the graphene edge termination play crucial roles in triggering the formation of interlayer twist. The growth mechanism is carefully investigated by using an isotope-labelling technique. The as-obtained tBLGs show high crystalline quality, which is confirmed by the Raman spectra, atomically clear Moiré patterns in TEM image and ultrahigh carrier mobility (over 50,000 cm² V⁻¹ s⁻¹ at room temperature).

REFERENCES

- [1] L. Sun, G. Yuan, L. Gao, J. Yang, M. Chhowalla, M. H. Gharahcheshmeh, K. K. Gleason, Y. S. Choi, B. H. Hong, Z. Liu, *Nat. Rev. Methods Primers* **2021**, 1, 5.
- [2] J. Zhang, L. Sun, K. Jia, X. Liu, T. Cheng, H. Peng, L. Lin, Z. Liu, *ACS Nano* **2020**, 14, 10796.
- [3] Y. Li, L. Sun, H. Liu, Y. Wang, Z. Liu, *Inorg. Chem. Front.* **2020**, 8(1): 182-200.
- [4] L. Sun, Z. Wang, Y. Wang, L. Zhao, Y. Li, B. Chen, S. Huang, S. Zhang, W. Wang, D. Pei, H. Fang, S. Zhong, H. Liu, J. Zhang, L. Tong, Y. Chen, Z. Li, M. H. Rummeli, K. S. Novoselov, H. Peng, L. Lin, Z. Liu, *Nat. Commun.* **2021**, Accepted.

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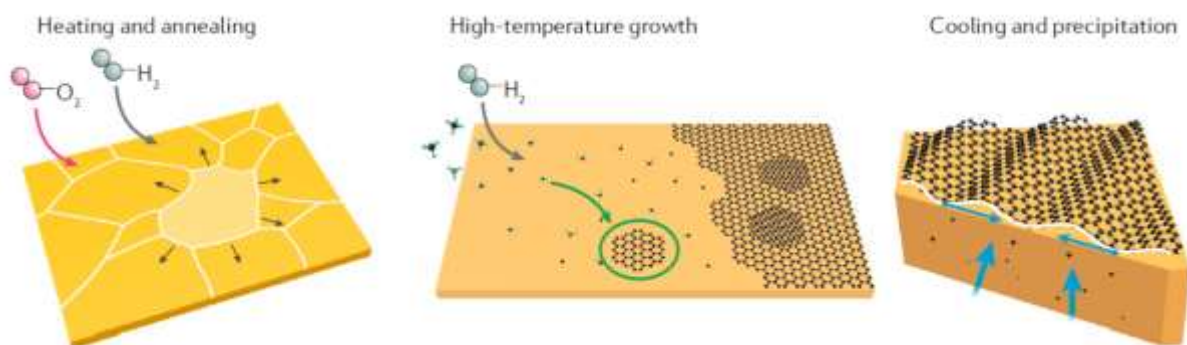


Figure 1: Major steps of growing graphene films on metal substrate.

Wafer-scale graphene: a transfer-free approach

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Graphene has several unique properties which make it an attractive material for sensors, optoelectronics, or as nano/micro-electro-mechanical systems (NEMS/MEMS). To allow integration into semiconductor technology, graphene deposited by chemical vapour deposition (CVD) on a metal catalyst is widely regarded as the most promising method as it results in high-quality material which is required for many of the before-mentioned applications.

A downside of CVD graphene is that it requires the transfer of the graphene from the, typically, Cu, Ni, or Pt catalyst. This transfer step introduces polymer contamination, cracks, wrinkles and can result in adhesion issues with the target substrate, especially for non-flat substrates [1]. While significant progress has been made in CVD graphene and transfer [2], there still does not exist an ideal recyclable growth template and, especially, a repeatable and scalable transfer method.

In this work, we present our wafer-scale transfer-free alternative based on Mo as catalyst which can circumvent the above-mentioned issues involved with transfer [3]. The key to this technology is the pre-patterning of the Mo catalyst layer by photolithography. Upon removal of the catalyst, the few-layer graphene adheres to the substrate at the edges of the pattern. Therefore, lithographic control over the location and size of the graphene is achieved.

By keeping the Mo underneath the graphene through post-processing to realize devices adhesion issues can be prevented. Furthermore, it enables surface and bulk micromachining allowing suspended graphene device formation on wafer-scale, fig. 1 [4]. Limitations of the technology are that the growth is coupled to the target substrate, and that - so far - we have only been able to achieve this for few or multi-layered graphene.

Finally, we have demonstrated that our transfer-free process can also be integrated with CMOS, fig. 2 [5]. We inserted the graphene deposition step directly after the front-end of our in-house CMOS process. Care must be taken to protect the graphene layer during the back-end processing of the two-level interconnects. With this, we have demonstrated an alternative route for graphene device integration on CMOS which avoids many of the challenges related to transfer and can enable the realization of smart (suspended) graphene-based sensors.

REFERENCES

- [1] S. Wagner et al., *Microelectronic Engineering*, vol. 159 (2016), 108-113
- [2] D. Neumaier et al., *Nature Materials*, vol. 18 (2019), 525-529
- [3] S. Vollebregt et al., *Proc. of IEEE MEMS* (2016), 17-20
- [4] J. Romijn et al., *Proc. of IEEE NEMS* (2018), 11-14
- [5] J. Romijn et al., *Proc. of IEEE MEMS* (2019), 260-263

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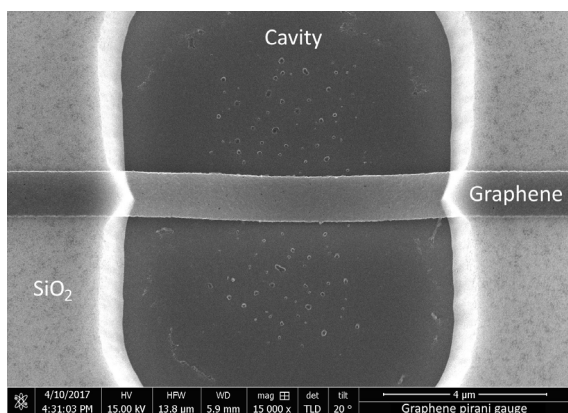


Figure 1: SEM image of a transfer-free suspended multi-layer graphene-based Pirani pressure sensor. The graphene bridge is 1 μm wide, while the SiO₂ is 600 nm thick.

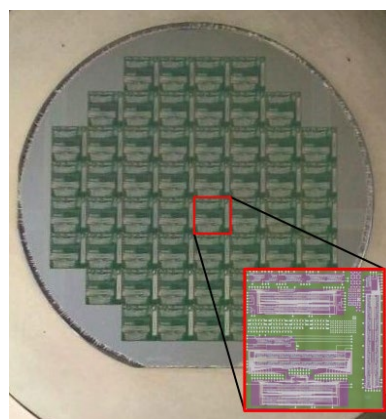


Figure 2: Wafer (10 cm) with digital CMOS circuits and transfer-free graphene integrated alongside. Both the graphene devices and CMOS circuits were found to be working.

Wafer Scale Integration of Graphene

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Abstract

Graphene has great potentials for applications in different fields such as electronics, optoelectronics, and sensors. However, the final functional application still relies on the state-of-the-art platform such as silicon technology process line, due to its maturity for circuit and system realization. Therefore, a path to integrate graphene to such traditional fabrication platform needs to be developed, in order to make the fancy material closer to reality. In this presentation, graphene processing will be introduced from different technology aspects, such as material growth, transfer, interface treatment, doping control, electrical contact optimization. The status and progress at AMO will be introduced. The new project 2D Experimental Pilot Line will be introduced, the target of which is to facilitate graphene foundry service to public in Europe.



ABSTRACTS
ORALS

Valley currents via ballistic edge modes in graphene superlattice near the main Dirac point

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In carefully stacked two-dimensional materials, topological bands generate Hall like conductivity and topologically protected edge states in zero magnetic field. By placing single layer graphene (SLG) on hexagonal boron nitride (h-BN), it might be possible to transform SLG into a topological phase by varying their crystallographic alignment. Recent measurements of nonlocal resistances (Rnl)[1] in a narrow energy range focusing with the secondary Dirac point (SDP) [2] in SLG/h-BN superlattice Hall bars have been interpreted as arising due to the valley Hall effect and quantum valley Hall state. Here we report h-BN/SLG/h-BN Hall bars which have a negligible Rnl of SDPs, but at the main DP Rnl is reaching quantum-limit at 9 K. We investigate valley currents near the main Dirac point [3] and also demonstrate nonlocal measurements over a distance of 15 μm indicating ballistic behaviour in good agreement with recent theoretical works [4] that are trying to shed some light into these intriguing experiments.

REFERENCES

- [1] C.R. Woods, L. Britnell, et al., Nature Physics 10 (2014) 451.
- [2] G.L Yu, R.V. Gorbachev et al. Nature Physics 10 (2014) 525.
- [3] Y. Li, M. A., et al. Communications Physics 3 (2020) 224
- [4] T. Aktor, J. H Garcia, S.roche et al. Physical Review B 103 (2021) 115406.

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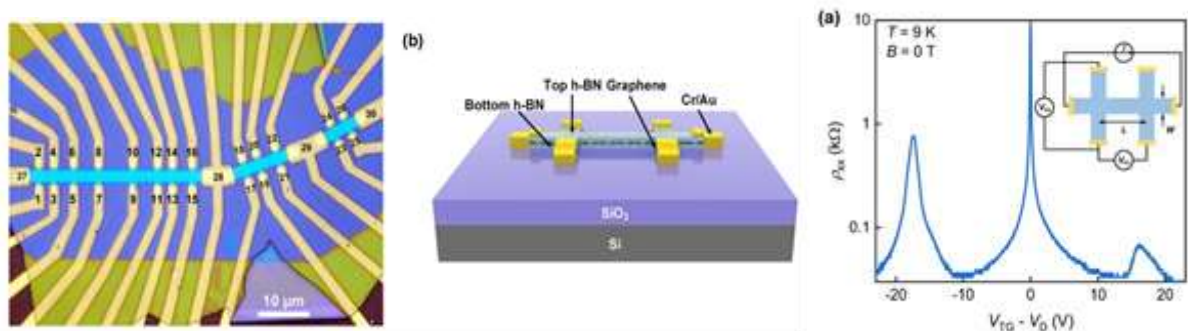


Figure 1: From left to right, h-BN/SLG/h-BN device structure via optical micrograph, schematic illustration of a typical device, Longitudinal resistivity (ρ_{xx}) vs gate voltage ($V_{TG} - V_D$) in zero magnetic field at 9 K. Inset shows schematic illustrations of the local measurement setup, where L is the distance between the current path and voltage probes, and W is the device width.

Optimizing Graphene Photothermoelectric Detectors

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

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

REFERENCES

- [1] A.C. Ferrari et al., *Nanoscale* **7**, 4598 (2015).
- [2] X. Cai et al., *Nat. Nanotechnol.* **9**, 814 (2014).
- [3] S. Schuler et al., *Nano Lett.* **16**, 7107 (2016).
- [4] S. Castilla et al., *Nano Lett.* **19**, 2765 (2019).
- [5] J. Muench et al., *Nano Lett.* **19**, 7632 (2019).
- [6] A. Antidormi, A.W. Cummings, arXiv:2102.11225 (2021)

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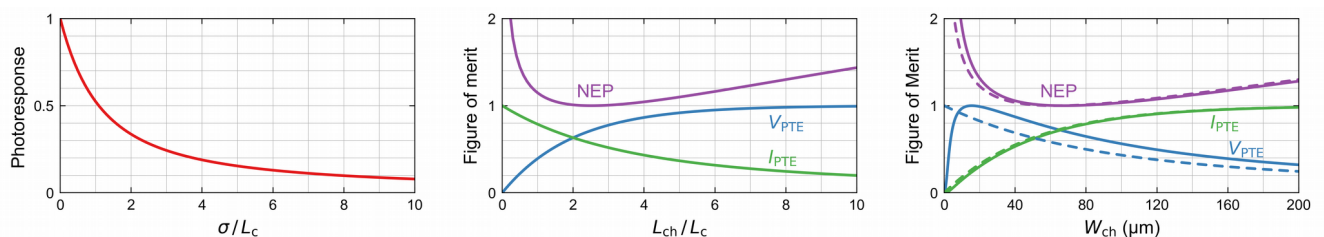


Figure 1: Graphene photodetector performance as a function of light profile size (left), channel length (middle), and channel width (right). NEP is the noise-equivalent power, I_{PTE} is the photocurrent, and V_{PTE} is the photovoltage. I_{PTE} and V_{PTE} are normalized to their maximum values, and NEP to its minimal value.

Differences in magnetic properties of CrI_3 and CrBr_3 monolayers caused by spin-orbit coupling

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After the discovery of magnetism in monolayer CrI_3 , the magnetic properties of different two-dimensional materials from the chromium-trihalide family are intuitively assumed to be similar, yielding magnetic anisotropy from the spin-orbit coupling on halide ligands. Here we reveal[1] significant differences between seemingly similar CrI_3 and CrBr_3 magnetic monolayers (see Figure 1) in their magnetic anisotropy, resulting Curie temperature, hysteresis in an external magnetic field, and evolution of magnetism with strain, all predominantly attributed to a distinctly different interplay of atomic contributions to spin-orbit coupling in two materials.

REFERENCES

- [1] C. Bacaksiz, D. Šabani, R. M. Menezes, and M. V. Milošević, *Physical Review B*, **103** 125418 (2021).

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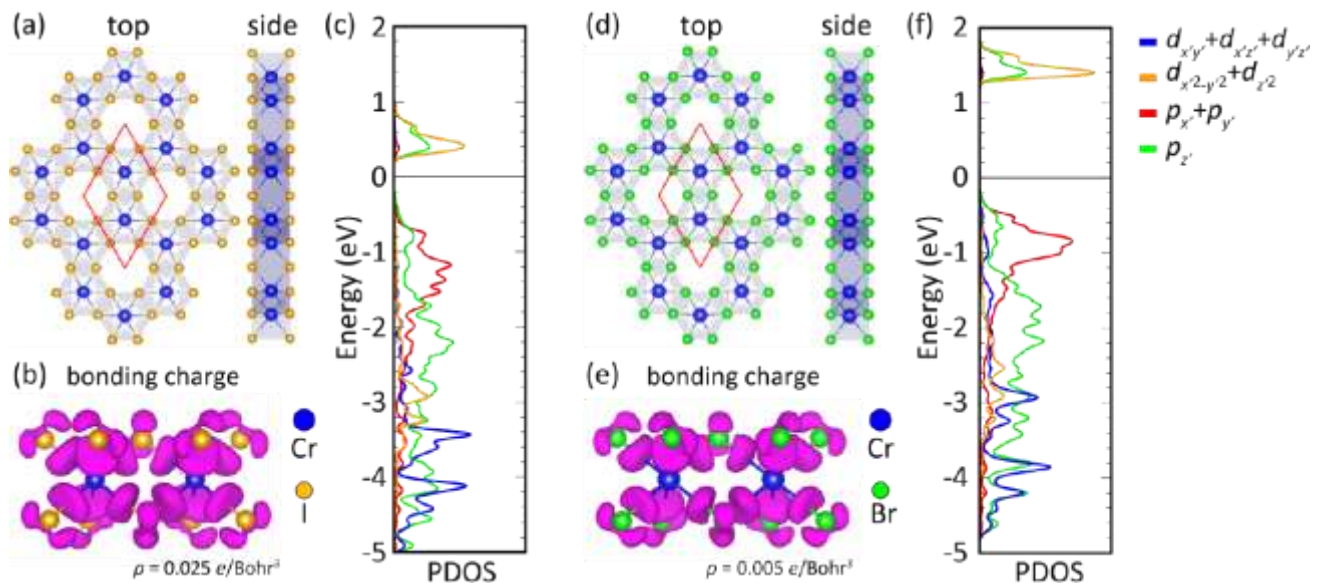


Figure 1: Schematic representation of the structure of monolayer CrI_3 (a) and CrBr_3 (d). Panels (b) and (e) show the difference between the charge distribution after crystallization and the total charge distribution of bare atoms, which then indicates the bonding and antibonding charges in the two materials. Panels (c) and (f) show the density of states of two materials, decomposed according to the atomic orbitals. Subscripts x' , y' , and z' in the orbitals denote the local coordinates of the corresponding atoms.

Experimental observation of giant thermal diffusivity of Dirac fluid

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The transport of heat and charge in solids is typically described in terms of diffusive and ballistic motion of point particles. However, for strongly interacting electrons under certain circumstances a viscous, fluid-like behaviour has been predicted. Only recently, with the advance of ultraclean 2D electron systems such as graphene, it has become feasible to experimentally access this hard-to-reach regime of electron hydrodynamics [1-11]. To date, hydrodynamic viscous transport has been observed via electrical device measurements [2-7] and scanning probe microscopy [8, 9]. An even more elusive manifestation of hydrodynamic behavior exists: the quantum-critical Dirac-fluid regime with enhanced thermal transport. This regime has been accessed at cryogenic temperatures, where it manifested in a violation of the Wiedemann-Franz law [10] and as a contribution to the Drude scattering rate [11].

Here, we present direct experimental signatures of electron hydrodynamics, including the Dirac-fluid regime, at room temperature in standard quality graphene [12]. We directly track the motion of optically excited electronic heat pulses in the temporal domain using a split-gate device via ultrafast thermoelectric microscopy. This novel technique allows us to quantify heat transport on the femtosecond-nanometer scale and at room temperature. We are able to tune in and out of the Dirac-fluid regime of electron motion using carrier temperature and carrier density as control knobs. We observe a thermal diffusivity of the Dirac fluid that is more than two orders of magnitude larger compared to the non-interacting, diffusive regime. The effect persists at room temperature and shows agreement with transport calculations.

Besides the fundamental breakthrough, we believe that the surprisingly large thermal transport, together with the possibility of switching the effect on and off, could lead to important technological applications, such as nanoscale thermal management.

REFERENCES

- [1] M. Polini, A.K. Geim, *Physics Today* **73**, 6 (2020) pp. 28-34
- [2] D.A. Baudurin, et al., *Science* **351** (2016) pp. 1055–1058
- [3] P.J.W. Moll, et al., *Science* **351** (2016) pp. 1061–1064
- [4] R. Krishna Kumar, et al., *Nat. Phys.* **13** (2017) pp. 1182–1185
- [5] B.A. Braem, *Phys. Rev. B.* **98** (2018) pp. 241304
- [6] J. Gooth, et al., *Nat. Commun.* **9** (2018) pp. 4093
- [7] Berdyugin, et al., *Science* **364** (2019) pp. 162–165
- [8] J. A. Sulpizio, et al., *Nature* **576** (2019) pp. 75–79
- [9] M.J.H. Ku, et al., *Nature* **583** (2020), pp. 537-541
- [10] J. Crossno, et al., *Science* **351** (2016) pp. 1058–1061
- [11] P. Gallagher, et al., *Science* **364** (2019) pp. 158–162
- [12] A. Block et al., *arXiv preprint* (2020) arXiv:2008.04189

Disentangling Orbital and Valley Hall Effects in Bilayers of Transition Metal Dichalcogenides

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The orbital Hall effect (OHE) is the orbital angular momentum analogue of the spin Hall effect (SHE) and refers to the appearance of a transverse orbital angular momentum current after applying a longitudinal electrical field [1]. Recently it has been predicted that the 2H monolayers of transition metal dichalcogenides (TMD) exhibit relatively large orbital Hall conductivity within their semiconducting energy gap, where the spin Hall conductivity vanishes [2,3]. However, since the valley Hall effect (VHE) in these systems also generate a transverse flow of orbital angular momentum, it becomes experimentally challenging to differentiate between these two effects in these materials. The VHE requires an inversion symmetry breaking to occur, and this happens in the monolayer TMD but not into the bilayer. Using density functional theory (DFT) calculations, we demonstrated the bilayers of the 2H-MoS₂ exhibits sizable orbital Hall conductivity signals in its insulating state without SHE and VHE. Using low-energy models, we further explored the transport properties of these systems. We topologically characterized the orbital Hall insulating phase in TMD monolayers and bilayers in terms of orbital Chern numbers whose values are related to the edge states in nanoribbons. Our results strongly suggest that bilayers of TMDs are highly suitable platforms for direct observation of the orbital Hall insulating phase in two-dimensional materials.

REFERENCES

- [1] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, *Physical Review Letters*, 95, (2005), 06660.
- [2] Canonico, L. M., et al. *Physical Review B (R)* 101 (2020) 161409.
- [3] Bhowal, S. and S. Satpathy. *Physical Review B* 102 (2020) 035409.

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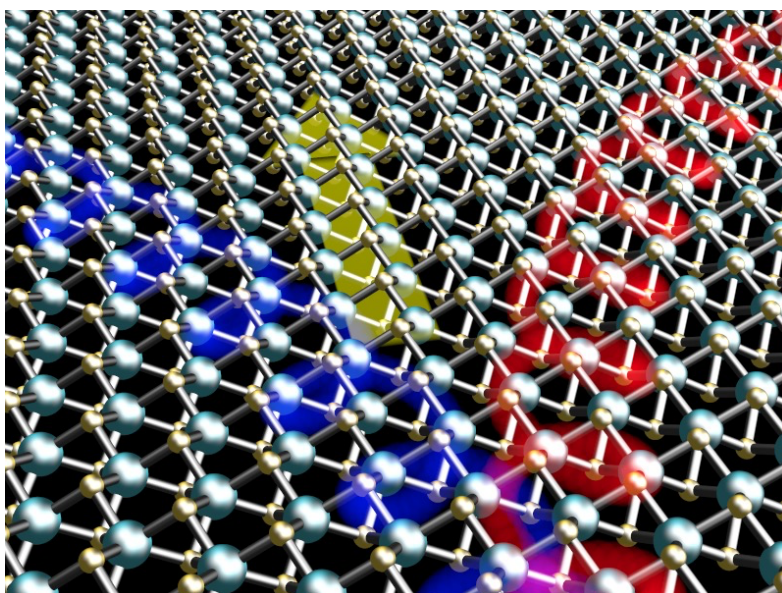


Figure 1: Schematic representation of the orbital-Hall effect in MoS₂.

Shell filling and trigonal warping in graphene quantum dots

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The investigation of the quantum dot ground states, excited states and addition spectra led to a complete understanding of the orbital and spin degeneracies of quantum dots in traditional semiconductors like InGaAs, GaAs and silicon, and hence made these quantum dots interesting as solid-state qubits. For vertical quantum dots etched into a circular geometry shell filling and Hund's rule spin filling was observed [1]. Another promising material for solid state qubits is graphene [2]. Graphene offers an environment with few nuclear spins (reducing hyperfine interactions compared to III-V semiconductors) and it is a light element (reducing spin-orbit effects even compared to silicon). Compared to other conventional semiconductors, electrons in bilayer graphene possess an additional valley degree of freedom and a non-trivial minivalley band-structure due to trigonal warping [3]. Applying a displacement field perpendicular to the bilayer graphene sheet opens a bandgap and forms three shallow minivalleys around the K and K' points, this allows to electrostatically define and control quantum dots [4]. However, the formation and relevance of the minivalleys for low-energy quantum dot states can be tuned by the band gap and the size of the quantum dot.

Here, we experimentally investigate shell filling effects in a nearly circular quantum dot in bilayer graphene [5]. Starting from the empty quantum dot we observe a successive bunching of four, eight and twelve conductance resonances, which becomes visible in the addition energy as shown in Fig. 1. We describe this observation in terms of a transition from a level scheme given by two-dimensional s- and p-shells for the first electrons to a level scheme dominated by mini-valleys with three-fold degeneracy.

REFERENCES

[1] S. Tarucha, D. G. Austing, T. Honda, et.al., *Phys. Rev. Lett.* **77**, 3613 (1996).

[2] B. Trauzettel, D. V. Bulaev, D. Loss, and G. Burkard, *Nature Physics* **3**, 192 (2007).

[3] A. Knothe and V. Fal'ko, *Phys. Rev. B* **98**, 155435 (2018).

[4] M. Eich, R. Pisoni, H. Overweg, et al., *Phys. Rev. X* **8**, 031023 (2018).

[5] R. Garreis, A. Knothe, C. Tong, et.al, arXiv preprint, arXiv:2011.07951 (2020).

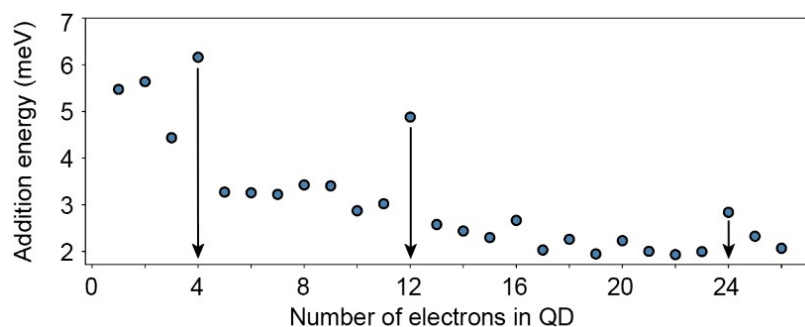


Figure 1: Addition energy for an extra electron versus number of electrons in the dot extracted from the separation between Coulomb resonances in a conductance trace.

Site selective oxidation of monolayered liquid-exfoliated WS₂ by shielding the basal plane through adsorption of a facial amphiphile

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Abstract:

In recent years, various functionalization strategies for transition metal dichalcogenides have been explored to tailor the materials' properties and to provide anchor points for the fabrication of hybrid structures. However, often functionalization approaches are carried out in the presence of additional components (e.g. stabilizers) other than the reagents which are often neglected. In this report,^[1] new insights into the role of the surfactant in functionalization reactions are described. Using the spontaneous reaction of WS₂ with chloroauric acid as a model reaction, the regioselective formation of gold nanoparticles on WS₂ is shown to be heavily dependent on the surfactant employed. A simple model is developed to explain the role of the chosen surfactant in this heterogeneous functionalization reaction. Variations in the surfactant coverage for classical and facial amphiphiles are identified as the crucial element that governs the dominant reaction pathway and therefore can severely alter the reaction outcome. This study shows the general importance of the surfactant choice and how detrimental or beneficial a certain surfactant can be to the desired functionalization.

REFERENCES

- [1] Angew. Chem. Int. Ed. 2020, 59, 13785–13792. doi.org/10.1002/anie.202005730 (Front Cover: 13665–13665. doi.org/10.1002/anie.202007849)

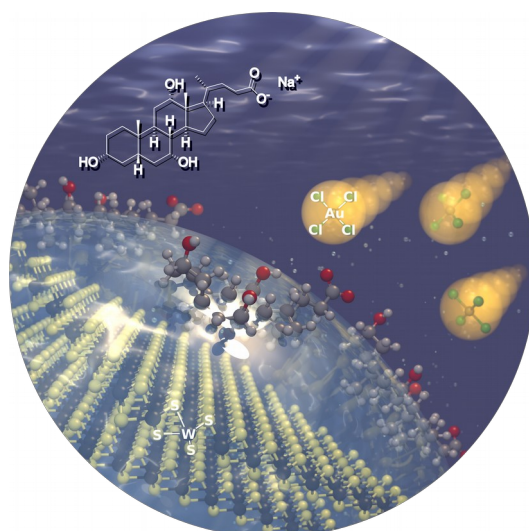


Figure 1: The heterogeneous reaction of chloroauric acid at the nanosheet-solution interface reveals that the employed surfactant plays a significant role in governing the reactivity of the nanomaterial and consequently on the functionalization outcome.

Spin-Orbit Torques in Magnetic Janus Transition Metal Dichalcogenides

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Modern magnetic applications rely on precise control of spins in the matter. In magnets, this quantum degree of freedom is very robust against external perturbations, and it is therefore valuable for memory devices. The downside nowadays is in the speed. To change the state in magnetic-based memory is quite slow and inefficient, as it requires polarizing an electronic current first, which will serve as a torque source for switching the magnetization later. A promising solution to this problem is to use spin-orbit torque (SOT) [1,2]. The spin-orbit torque is an effect where a nonmagnetic substrate exerts a torque on a magnetic material through its interface due to the spin-orbit coupling (SOC). The most relevant spin-orbit interaction for SOT is the Rashba SOC, which requires the presence of an electric field perpendicular to the interface [2]. The Janus structures are systems with opposite surfaces possessing different properties and are then intrinsically Rashbianic systems. A magnetic Janus monolayer will allow for Rashba SOC, Magnetism, and gate-tunability in a single system, making them very interesting for SOT-based memories. Transition metal dichalcogenides (TMDs) support the Janus phase [3] and magnetism[4-5], thus could be used for a mid-term realization of SOT-devices. In this work, I present large-scale numerical calculations of the torque efficiency in VSeTe within the linear-response theory. We demonstrate that these heterostructures support field-like and anti-damping torques of comparable magnitudes. Also, we report on the presence of a different torque source that does not obey any typical symmetry, which we deemed as unusual. We demonstrate that torque efficiency in these systems is comparable with heavy metals in magnitude with the added feature of gate-tunability. Finally, we will show the effect of disorder simulated in large-scale systems consisting of 100.000 atoms obtained from Density Functional Theory.

REFERENCES

- [1] A. Manchon, J. Železný, I. M. Miron, et al., Rev. Mod. Phys., 91, 035004 (2019).
- [2] A. Manchon and S. Zhang, Phys. Rev. B., 78, 212405 (2008).
- [3] A. Lu, H. Zhu, J. Xiao, et al. Nature Nanotech 12, 744–749 (2017).
- [4] D. J. O'Hara, T. Zhu, A.H. Trout, et al., Nano Lett. 2018, 18, 5, 3125-3131 (2018)

Reversible hydrogenation restores defected graphene to graphene

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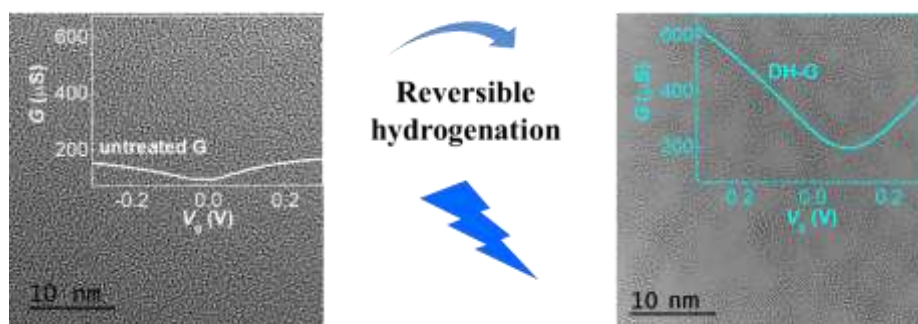
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Graphene as a two-dimensional material is prone to hydrocarbon contaminations, which can significantly alter its intrinsic electrical properties. Herein, we implement a facile hydrogenation-dehydrogenation strategy to remove hydrocarbon contaminations and preserve the excellent transport properties of monolayer graphene. Using electron microscopy we quantitatively characterized the improved cleanness of hydrogenated graphene compared to untreated samples. In situ spectroscopic investigations revealed that the hydrogenation treatment promoted the adsorption of water at the graphene surface, resulting in a protective layer against the redeposition of hydrocarbon molecules. Additionally, the further dehydrogenation of hydrogenated graphene rendered a more pristine-like basal plane with improved carrier mobility compared to untreated pristine graphene. Our findings provide a practical post-growth cleaning protocol for graphene with maintained surface cleanness and lattice integrity to systematically carry a range of surface chemistry in the form of a well-performing and reproducible transistor device.¹⁻⁴



References:

1. Jiang L, et al., Sci. China Chem., 2021, <https://doi.org/10.1007/s11426-020-9959-5>.
2. Jiang L, Fu W, Birdja YY, Koper MT, Schneider GF. Nat Commun, 2018, 9(1): 1-9.
3. Prydatko AV, Belyaeva LA, Jiang L, Lima LM, Schneider GF. Nat Commun, 2018, 9(1): 1-7.
4. Belyaeva LA, Jiang L, Soleimani A, Methorst J, Risselada HJ, Schneider GF. Nat Commun, 2020, 11(1): 1-11.

Multiscale Charge Transport in van der Waals Thin Films: Reduced Graphene Oxide as a Case Study

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Large area van der Waals (vdW) thin films are assembled materials consisting of a network of randomly stacked nanosheets. The multi-scale structure and the two-dimensional nature of the building block mean that interfaces naturally play a crucial role in the charge transport of such thin films.[1] While single or few stacked nanosheets (i.e. vdW heterostructures) have been the subject of intensive works,[2] little is known about how charges travel through multilayered, more disordered networks. Here we report a comprehensive study of a prototypical system given by networks of randomly stacked reduced graphene oxide 2D nanosheets, whose chemical and geometrical properties can be controlled independently,[3] permitting to explore percolated networks ranging from a single nanosheet to some billions with room temperature resistivity spanning from 10^{-5} to 10^{-1} $\Omega\cdot\text{m}$. We systematically observe a clear transition between two different regimes at a critical temperature T^* : Efros-Shklovskii variable range hopping (ES-VRH) below T^* and power law (PL) behavior above. Firstly, we demonstrate that the two regimes are strongly correlated with each other, both depending on the charge localization length ξ , calculated by ES-VRH model,[4] which corresponds to the characteristic size of overlapping sp^2 domains belonging to different nanosheets. Thus, we propose a microscopic model describing the charge transport as a geometrical phase transition, given by the metal-insulator transition associated with the percolation of quasi-1D nanofillers with length ξ ,[5,6] showing that the charge transport behaviour of the networks does neither depend on geometry nor on the defects of the nanosheets, ultimately suggesting a generalized description on vdW and disordered thin films.[7]

REFERENCES

- [1] Lin Z. et al., Nature Electronics, 2 (2019) 378 – 388
- [2] Geim A.K. et al., Nature, 499 (2013) 419 – 425
- [3] Liscio A. et al., 2D Materials, 4 (2017) 025017
- [4] Shklovskii B et al., *Electronic properties of doped semiconductors* (1984) Berlin, Germany
- [5] Stanley, H. *Introduction to Phase Transition and Critical Phenomena* (1971) Oxford, UK
- [6] Menon R. et al., Physical Reviews B, 48 (2003) 17685 – 17694
- [7] Kovtun A. et al., ACS Nano, 15 (2021) 2654 – 2667

FIGURE

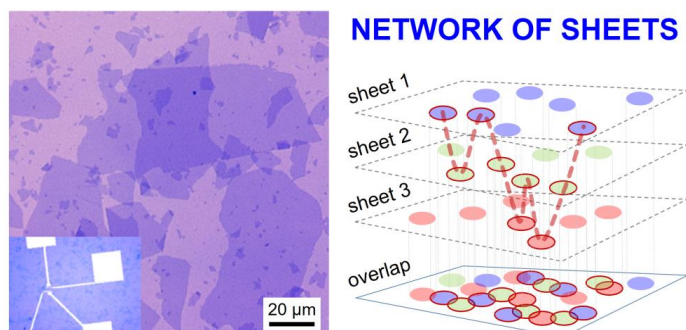


Figure: (Left) Optical image of a sparse network composed by few 2D RGO sheets in partial contact. Inset: Optical image showing the metal pad geometry used to measure CT in such samples; inset size: 1.7×1.2 mm^2 . (Right) Three-layer RGO thin film. Each plane is represented as a patchwork of isolated sp^2 domains (circles) separated by domain border defects. For sake of clarity, we distinguish each layer with a different colours. Dashed red line corresponds to a random path connecting overlapped disks.

Giant effective trion-polariton Zeeman splitting realized by spin-selective strong light-matter coupling

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Atomically thin quantum materials present a varied ecosystem in which to study emergence in condensed matter, where strongly interacting mixtures of fermions and bosons play host to novel and often unexpected collective phenomena. Here we study the relationship between spin polarization of a two-dimensional electron gas (2DEG) in a monolayer semiconductor (molybdenum diselenide, MoSe₂) and light-matter interactions modified by a zero-dimensional optical microcavity [1,2]. We find robust paramagnetism of the 2DEG to simultaneously enhance and suppress trion-polariton formation in opposite photon helicities, leading to observation of a giant effective Zeeman splitting between +K or -K valley trion-polaritons (g-factor >20), exceeding the purely trionic splitting (g-factor =4) by five times. We demonstrate tuning of the 2DEG susceptibility by application of weak continuous-wave laser illumination, allowing optical control of the effective polaritonic Zeeman splitting, amplified by a highly nonlinear response of the valley-specific Rabi splitting. Our experiments achieve the often elusive large mode splitting necessary to support highly unidirectional edge modes in topological polaritonics.

REFERENCES

[1] M. Sidler, et al. *Nature Physics* **13**, 255-261 (2017)

[2] J. G. Roch, et al. *Nature Nanotechnology* **14**, 432-436 (2019)

FIGURES

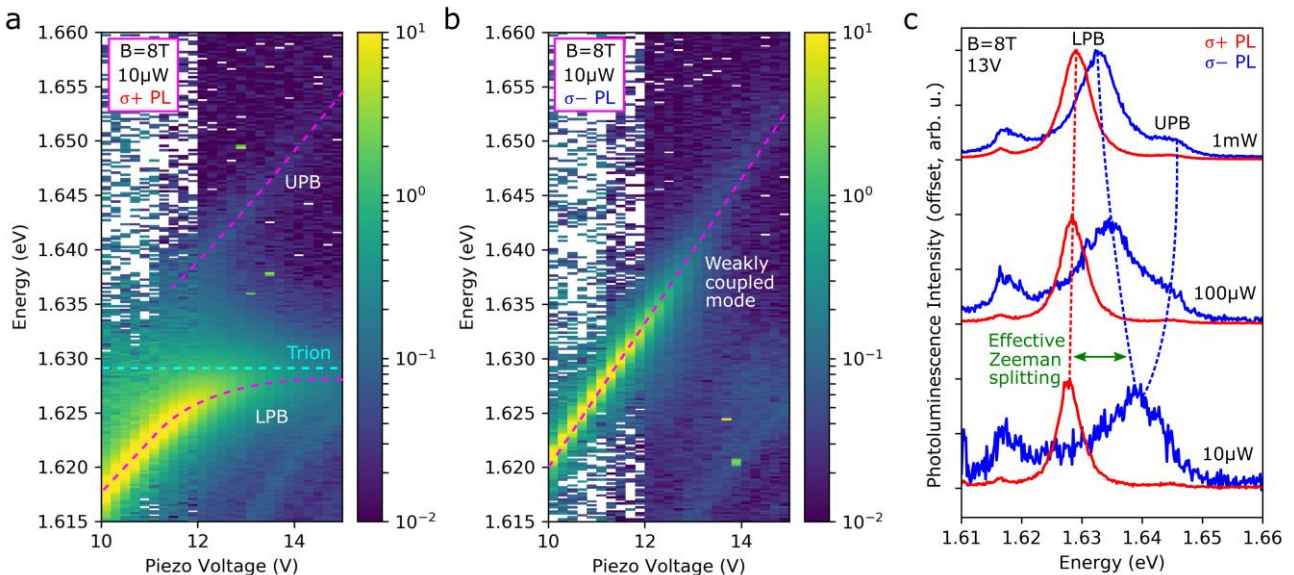


Figure 1: **a,b** Photoluminescence maps from monolayer MoSe₂ hosting a 2DEG embedded inside a tunable optical microcavity. Increasing the piezo voltage decreases the cavity length and tunes the 0-dimensional cavity mode through resonance with the trion state, forming trion-polaritons. At $B = 8$ T, the 2DEG is spin polarized, enhancing the Rabi splitting in σ^+ (**a**) while completely quenching strong coupling in σ^- (**b**). This leads to a giant effective Zeeman splitting (**c**) exceeding 10 meV. Applying higher laser powers depolarizes the 2DEG, allowing strong coupling in σ^- with associated tuning of the effective Zeeman splitting.

Local dielectric-function modulation and exciton recombination efficiency in monolayer WS₂ flakes

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Excitons dominate the light absorption and re-emission spectra of monolayer transition-metal dichalcogenides (TMD) [1]. Microscopic investigations of the excitonic response in TMD almost invariably focus on the radiative recombination, which only constitutes one-half of the picture. Here, we provide a comprehensive description of the excitonic effects in both the absorption and re-emission spectra of WS₂ flakes by originally combining state-of-the-art imaging ellipsometry (lateral resolution < 1 μm) and imaging photoluminescence spectroscopy (Figure 1). By relying on a proven methodology to maximize the amount of information extracted from ellipsometry data [2], for the first time we obtain the local dielectric function of monolayer WS₂, which constitutes a fundamental physical quantity to describe light-matter interaction on a microscopic scale.

By comparing the exciton-induced absorption and re-emission features, we observed correlated and uncorrelated spatial patterns, thus demonstrating that the two phenomena are not always proportional at a microscopic scale. Micro-structural modulations across the flakes, having a different influence on the absorption and re-emission of light, are deemed responsible for this effect. By revealing the possibility to locally decouple the exciton-induced absorption and emission properties, these findings advance the fundamental understanding of excitonic processes in TMD, and may be of use to engineer diverse optical properties within individual flakes.

REFERENCES

- [1] G. Wang, A. Chernikov, M. Glazov, T. Heinz, X. Marie, T. Amand, B. Urbaszek, Excitons in atomically thin transition metal dichalcogenides. *Rev. Mod. Phys.* 90:021001, 2018.
- [2] M. Magnozzi; M. Ferrera; G. Piccinini; S. Pace; S. Forti; F. Fabbri; C. Coletti; F. Bisio; M. Canepa, Optical dielectric function of two-dimensional WS₂ on epitaxial graphene. *2D Mater.* 7:025024, 2020.

FIGURES

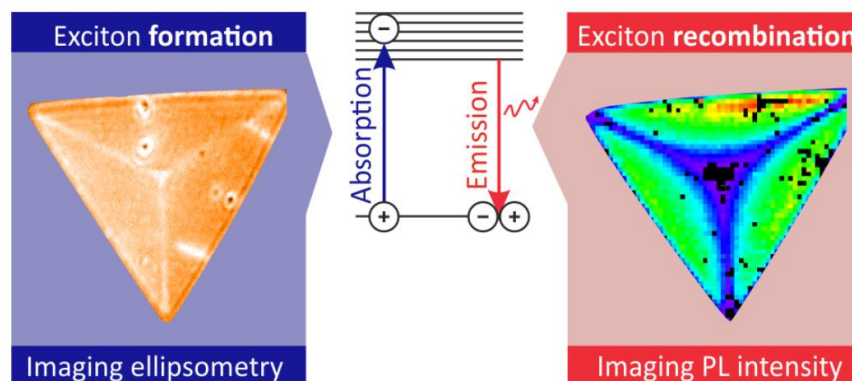


Figure 1: Microscopic spectral analysis of exciton formation (left) and recombination (right). We found that the two phenomena might lack spatial correlation within individual WS₂ flakes. Notably, the absorption and emission maxima may be located in different parts of the flake.

Atomically-precise Graphene Nanoarchitectonics

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Abstract

Nanostructuring graphene, or combining it in lateral heterostructures or stacks, can bring new and highly tunable functionalities, turning it from semimetal into semiconductor, inducing magnetism or superconductivity, or introducing tailored reactivity and permeability. However, one of the most obnoxious challenges have been to pattern graphene on a small scale where even atomic level of disorder can ruin its properties. On-surface reactions, via programmed interactions of molecular building blocks, has recently emerged as a promising route to synthesise atomically precise materials from the 'bottom-up'.

Here, I will discuss progress we have made in engineering 1D and 2D graphene nanoarchitectures with atomic precision. I will describe our recent results to synthesize atomically precise 2D nanoporous graphene [1,3], 1D functionalized nanoribbons[4,5], superlattices [2] and hybrid heterostructures. Finally, we demonstrated its implementation in electronic devices and advanced filters and sensing systems.

REFERENCES

1. C. Moreno, et al. Science 360, 199-203 (2018)
2. C. Moreno, et al. Chem. Comm. 54, 9402-9405 (2018)
3. C. Moreno, et al. Chemistry of Materials 31(4), 331-341 (2019)
4. J. Li, et al. ACS Nano 14 (2), 1895-1901 (2020)
5. Panighel et al., ACS Nano 14 (9), 11120–11129 (2020)

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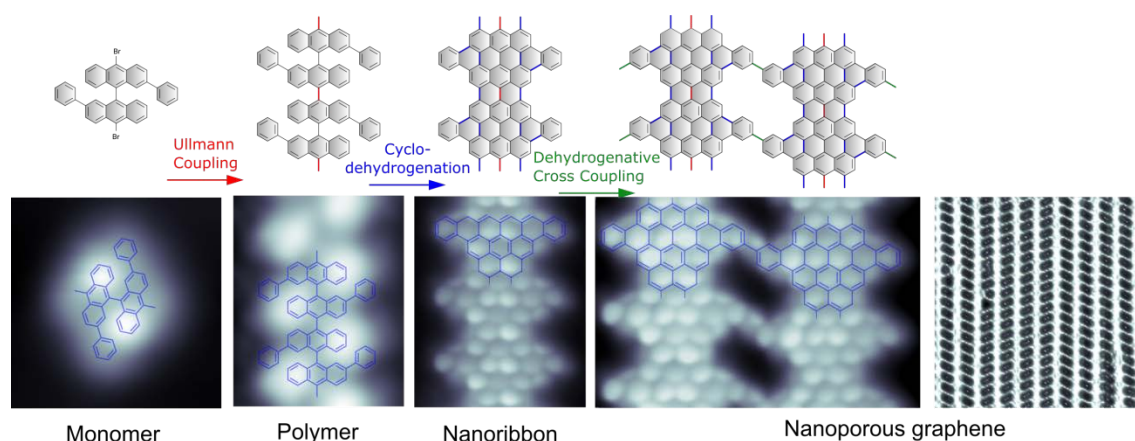


Figure 1: STM images tracking the on-surface reaction towards the synthesis of atomically-precise nanoporous graphene.

Electronic localization in small-angle twisted bilayer graphene

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ABSTRACT:

Owing to the outstanding and nicely tunable properties, twisted bilayer graphene (TBLG) systems display many fascinating features, especially, related to the electronic flat bands and the corresponding strong electronic localization observed when the twist angle is close to magic angles. Indeed, superconductivity, correlated insulating states, magnetism, and quantized anomalous Hall states have been explored in magic-angle TBLGs [1], thus giving rise to the nascent research field of “twistronics”. In such context, a comprehensive and accurate understanding of the intrinsic electronic properties of TBLG is very mandatory. However, while the electronic properties of large-angle TBLG at large twist angles down to $\sim 1.1^\circ$ have been well clarified, there are still discrepancies between theoretical explorations and experimental observations for small-angle TBLGs. In particular, the recent studies [2] have theoretically predicted a recurrent series of magic angles $\lesssim 1.1^\circ$. However, only the first magic angle at $\sim 1.1^\circ$ has been experimentally demonstrated [3,4] but there is no evidence pointing to the existence of smaller ones. In this work [5], using a tight-binding framework performed on fully relaxed TBLG lattices, the twist angle $\sim 1.1^\circ$ is found to be a unique magic angle and concurrently is the critical case where the electron localization is maximum, thus separating TBLGs into two classes with clearly distinct electronic properties (i.e., as illustrated in Fig. 1). For large twist angles $> 1.1^\circ$, low-energy Dirac fermions are preserved. For small-angles ($\lesssim 1.1^\circ$), TBLG systems present common features such as large spatial variation and strong electron localization in the AA stacking regions. The global electronic localization (maximum at $\sim 1.1^\circ$) is shown to monotonically reduce when the twist angle decreases, confirming that isolated electronic flat bands (as observed at 1.1°) can no longer be observed for smaller angles. In very good agreement with recent nano-Raman/STM/STS spectroscopies [4,6], our study clarifies essentially the reasons of the absence of magic angles below 1.1° as previously reported, and on the other hand, provide a more comprehensive and accurate understanding of the electronic properties of small-angle ($\lesssim 1.1^\circ$) TBLG systems.

REFERENCES: [1] E. Y. Andrei and A. H. MacDonald, Nat. Mater. 19, 1265-1275 (2020). [2] R. Bistritzer and A. H. MacDonald, PNAS 108, 12233-12237 (2011); G. Tarnopolsky *et al.*, Phys. Rev. Lett. 122, 106405 (2019); Y. Ren *et al.*, Phys. Rev. Lett. 126, 016404 (2021). [3] Y. Cao *et al.*, Nature 556, 43-50 (2018); *ibid.* 556, 80-84 (2018). [4] A. C. Gadelha *et al.*, Nature 590, 405-409 (2021). [5] V.-H. Nguyen *et al.*, [arXiv:2102.05376](https://arxiv.org/abs/2102.05376). [6] A. Kerelsky *et al.*, Nature 572, 95-100 (2019); I. Brihuega *et al.*, Phys. Rev. Lett. 109, 196802 (2012); S. Huang *et al.*, Phys. Rev. Lett. 121, 037702 (2018).

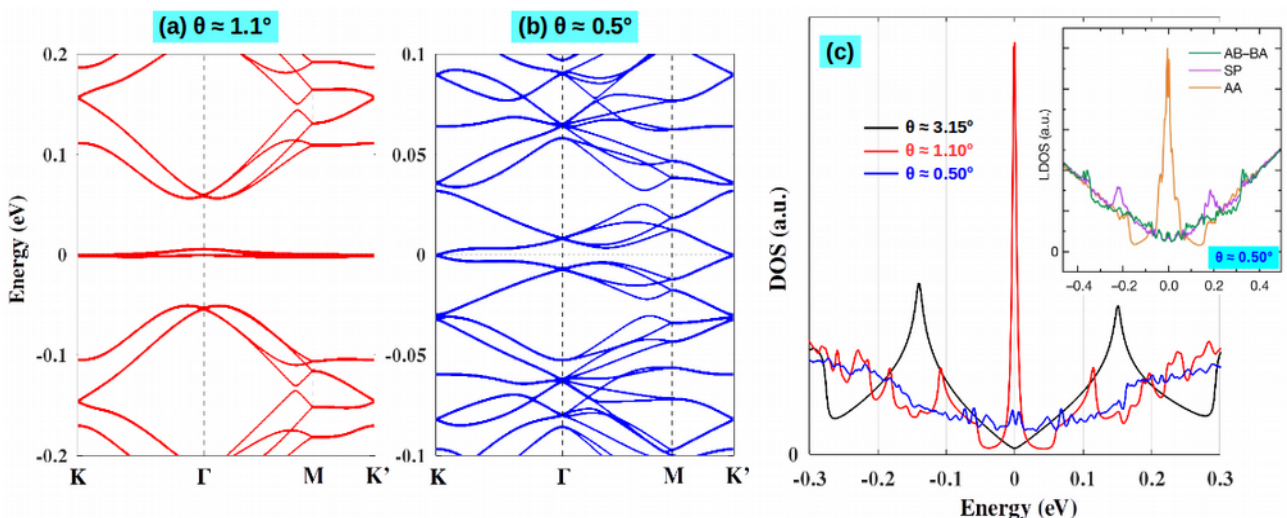


Fig.1: Electronic bandstructure of TBLG at 1.1° (a) and 0.5° (b) predicted in [2] to be the first and second magic angles, respectively. (c) Density of electronic states (DOS) at different twist angles and local DOS at 0.5° in different stacking regions (see the inset).

Controlling the photoluminescence of liquid phase exfoliated γ -InSe nanosheet thin films by centrifugation-based size selection

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ABSTRACT

Indium selenide (γ -InSe) is a layered III-VI semiconductor with a thickness dependent direct bandgap in the near-infrared region. In this project we performed liquid phase exfoliation of phase-pure γ -InSe in *N*-Methyl-2-pyrrolidone (NMP) and aqueous surfactant dispersions. With the aid of liquid-cascade centrifugation, we isolate nanosheets of different sizes and thicknesses. We establish quantitative metrics for layer number and lateral size based on optical spectroscopy in combination with a statistical evaluation of the nanosheet dimension and study the thickness-dependent photoluminescence in dispersion and in thin films (Figure 1B). While we find that the nanosheets are stable in NMP, some degradation occurs in the aqueous surfactant solution. In order to prevent reaggregation effects during film deposition, nanosheets were assembled at liquid-liquid interfaces prior to the deposition on glass substrates. Film morphologies were studied via optical microscopy and AFM. Using a TCSPC setup, we investigate the PL lifetime and find two contributions to the radiative decay which we attribute to intrinsic emission and defect-induced photoluminescence. Also lifetime parameters show size-dependent trends. The herein utilized protocol allows for a straight forward, large scale production of homogenous InSe thin-films from nanosheet dispersions with defined mean thicknesses, and thereby allows to control their PL emission in the n-IR.

FIGURES

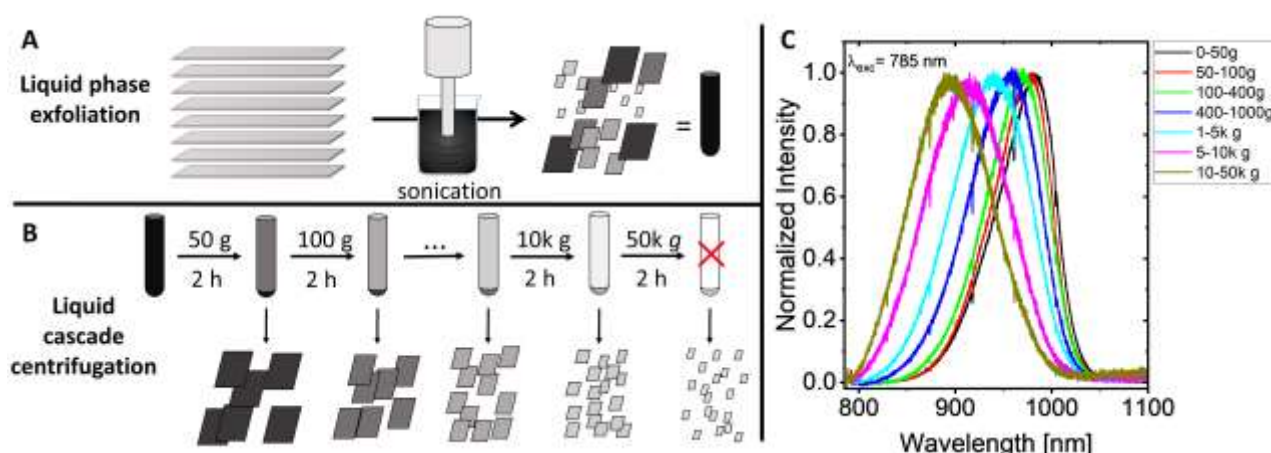


Figure 1: A): Schematic of Liquid-Phase Exfoliation of layered materials using tip sonication, followed by liquid cascade centrifugation (B) for size selection of nanosheets. C): Dispersions of γ -InSe show a thickness dependent shift in their photoluminescence upon excitation with a 785 nm laser.

Manipulating valley currents in graphene nanostructures

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Two-dimensional materials are promising valleytronic candidates due to the K and K' valleys at the Dirac points. All-electronic control is particularly desirable for device applications. Many proposed setups exploit strain-induced pseudomagnetic fields which act oppositely in the K and K' valleys, e.g. graphene nanobubbles can filter or split a charge current into its different valley components [1]. Experimental approaches in this direction are advancing, but promising signatures of valley-dependent phenomena have also emerged from graphene/hexagonal boron nitride heterostructures.

Large non-local resistance signals here have been interpreted in terms of a valley Hall effect (VHE) driven by a bulk Berry curvature [2], which in turn emerges from a finite, global mass term. A complete understanding of such measurements in terms of either bulk [3]- or edge-driven [4] mechanisms is very much an open question.

Here [5] we demonstrate the emergence of bulk, valley-polarized currents in graphene-based devices, driven by spatially varying regions of broken sublattice symmetry, and revealed by non-local resistance (RNL) fingerprints. Using a combination of quantum transport formalisms, the presence of a non-uniform local bandgap is shown to give rise to valley-dependent scattering and a finite Fermi surface contribution to the valley Hall conductivity, related to RNL characteristics. Our findings suggest both an alternative mechanism for the generation of valley Hall effect in graphene, and a route towards valley-dependent electron optics, by materials and device engineering.

REFERENCES

- [1] M. Settnes et al, Physical Review Letters 117, 276801 (2016).
- [2] R. Gorbachev et al., Science 346, 448 (2014).
- [3] Y. D. Lensky et al, Physical Review Letters 114, 256601 (2015).
- [4] J. M. Marmolejo-Tejada et al, Journal of Physics: Materials 1 (1), 015006 (2018).
- [5] T. Aktor et al, Physical Review B 103, 115406 (2021).

FIGURES

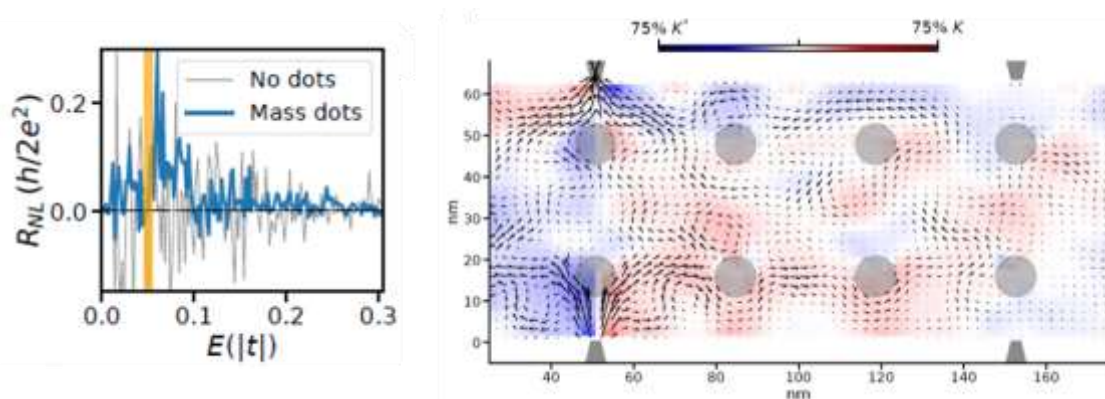


Figure 1: Nonlocal resistance and valley-dependent current flow in a graphene Hall bar with periodic mass dots [5].

Systematic study of the thermal conductivity of MoSe₂ as a function of thickness — from bulk to monolayer

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Semiconducting 2D materials, such as transition metal dichalcogenides (TMDs), show great potential in the fields of thermoelectricity and thermal management, which requires understanding their heat transport properties. The electrical, optical, and thermal properties of many atomically thin, two-dimensional materials have been found to differ from their bulk counterparts [1]. However, the thickness-dependent thermal properties of TMDs are still under extensive scientific debate [2]–[4]. Here we present the results of systematic study of the thermal conductivity of MoSe₂ as a function of flake thickness, down to the monolayer limit. We use Raman Thermometry as a tool to study the in-plane thermal conductivity (κ) of MoSe₂ single crystals suspended on large (15 μm), circular apertures. We first discuss some of the experimental effects that can occur in these type of measurements that can give rise to an apparent κ that does not correspond to the intrinsic material property. In particular, we point out the importance of: (i) the efficiency of the heat sink with a well-defined geometry; (ii) the effective suppression of additional cooling channels (e.g. convection to air); and (iii) the sufficiently large ratio between the suspended and probed areas. For our final results, we study a large batch of suspended MoSe₂ flakes, with >15 samples in the 1- to 7-layer regime, showing highly reproducible κ values. Our results expose a weak thickness-dependence of MoSe₂ thermal conductivity for the entire thickness range, with less than a factor 2 difference between several tens of nm- and monolayer-flakes. These findings are important for reaching a thorough understanding of heat flow in 2D layered materials.

REFERENCES

- [1] Y. Zhao, Y. Cai, L. Zhang, B. Li, G. Zhang, and J. T. L. Thong, “Thermal Transport in 2D Semiconductors—Considerations for Device Applications,” *Adv. Funct. Mater.*, vol. 30, no. 8, p. 1903929, Feb. 2020, doi: 10.1002/adfm.201903929.
- [2] X. Zhang *et al.*, “Measurement of Lateral and Interfacial Thermal Conductivity of Single- and Bilayer MoS₂ and MoSe₂ Using Refined Optothermal Raman Technique,” *ACS Appl. Mater. Interfaces*, vol. 7, no. 46, pp. 25923–25929, Nov. 2015, doi: 10.1021/acsami.5b08580.
- [3] E. Easy *et al.*, “Thermal Conductivities and Interfacial Thermal Conductance of 1- to 3-Layer WSe₂,” Oct. 2020, Accessed: Mar. 12, 2021. [Online]. Available: <http://arxiv.org/abs/2011.00730>.
- [4] H. Zobeiri, R. Wang, T. Wang, H. Lin, C. Deng, and X. Wang, “Frequency-domain energy transport state-resolved Raman for measuring the thermal conductivity of suspended nm-thick MoSe₂,” *Int. J. Heat Mass Transf.*, vol. 133, pp. 1074–1085, Apr. 2019, doi: 10.1016/j.ijheatmasstransfer.2019.01.012.

Room temperature spin Hall effect in CVD graphene/Pt heterostructures

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Spin to charge interconversion driven by the spin Hall (SH) and spin galvanic effects have emerged as promising phenomena for spin-logic operations without ferromagnets [1]. The SH effect has been studied in metals, possessing large spin-orbit coupling like Pt and more recently in graphene-based devices, showing an unprecedented electrical gating control at room temperature [2,3]. These results provide the building blocks for efficient spin manipulation using spin Hall phenomena in van der Waals heterostructures and pave the way towards development of ultra- compact memory devices.

In this work, we use high quality CVD graphene/Pt heterostructures, exhibiting large signals to study the spin Hall effect [4]. By using a carefully designed device, we characterise spin transport properties and extract precisely the spin Hall angle (SHA) at room temperature. Remarkably, we obtain large SHAs with a lower limit of 0.2, which stems from the good spin properties and interface quality in our devices. Our findings provide an efficient and systematic approach to characterise spin Hall phenomena in two dimensional devices.

REFERENCES

- [1] J. Sinova, S.O. Valenzuela, J. Wunderlinch, C. H. Back Rev. Mod. Phys. 87, 1213 (2015)
- [2] W. Savero Torres *et al.* 2D. Mater. 4 041008 (2017)
- [3] L.A. Benitez, W. Savero Torres *et al.* Nat. Mat. 19, 170–175(2020)
- [4] W. Savero Torres *et al.* To be published.

Charge Transport in Multilayer Graphene Oxide: Bulk Diffusion versus Device Properties

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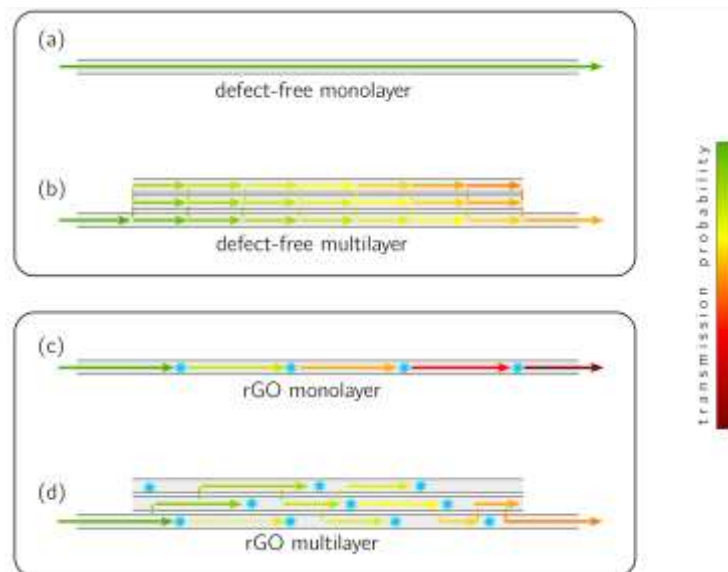
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Charge transport in multi-layered van der Waals materials has become an attractive and challenging problem, in the perspective of both fundamental and applied research on these structures. [1-2] We report a theoretical study of the effect on interlayer interaction in charge transport for chemically disordered graphene multilayer compounds. Using molecular dynamics and tight-binding Hamiltonian, layered disordered graphene sheets containing random distribution of epoxide and hydroxyl defects as well as divacancies and Stone-Wales type defects are modelled and their bulk and device transport properties are analysed. Bulk transport is found to become damaged by increasing the number of layers. In sharp contrast, when computing quantum transport using a device geometry and including contact effects, a different scenario is obtained, supporting the positive contribution of layer-layer interaction in increasing the effective sp^2 spatial area and favouring enhanced delocalization of electronic states. This sheds some new light on recent experimental features. [3]

REFERENCES

- [1] C.Ferrari, A. et al. *Nanoscale* 2015, 7, 4598–4810.
- [2] Mohan, V. B.; Lau, K.-t.; Hui, D.; Bhattacharyya, D. *Composites Part B: Engineering* 2018, 142, 200–220.
- [3] Kovtun, A.; Candini, A.; Vianelli, A.; Boschi, A.; Dell'Elce, S.; Gobbi, M.; Kim, K. H.; Lara Avila, S.; Samor, P.; Affronte, M.; Liscio, A.; Palermo, V. *ACS Nano* 2021, 15, 2654–2667.

FIGURES



Anatomy of 2D materials based memristors: the role of each type of defect

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Abstract

In the race of fabricating solid-state nano/micro-electronic devices using two-dimensional (2D) layered materials (LMs), achieving high yield and low device-to-device variability are the two main challenges [1-4]. Electronic devices that drive currents in-plane along the 2D-LMs (i.e. transistors, memtransistors) are strongly affected by local defects (i.e. grain boundaries, wrinkles, thickness fluctuations, polymer residues), as they create inhomogeneities and increase the device-to-device variability, resulting in a poor performance at the circuit level [5-6]. Here we show that memristors are insensitive to most types of defects in 2D-LMs, even when fabricated in academic laboratories that do not meet industrial standards. The reason is that the currents produced in these devices, which flow out-of-plane across the 2D-LM, are always driven locally by the most conductive locations. Consequently, we conclude that it is much easier to fabricate 2D-LMs based solid-state nano/micro-electronic circuits using memristors than transistors or memtransistors, not only due to the inherent simpler fabrication process (i.e. less lithography steps), but also because the local defects do not degrade the yield and variability of memristors considerably.

REFERENCES

- [1] D. Akinwande, C. Huyghebaert, C. Wang, M. I. Serna, S. Goossens, L. Li, H.-S. P. Wong, F. H. L. Koppens, *Nature*, 2019, 573, 507-518.
- [2] M. Li, S. Su, H. S. P. Wong, L. Li, *Nature*, 2019, 567, 169-170.
- [3] H. Lee, V. K. Sangwan, W. A. Gavia Rojas, H. Bergeron, H. Y. Jeong, J. Yuan, K. Su, M. C. Hersam, *Adv. Funct. Mater.* 2020, 30, 2003683.
- [4] N. C. Wang, E. A. Carrion, M. C. Tung, E. Pop, *Appl. Phys. Lett.* 2017, 110, 223106.
- [5] K. Xu, P. Cao, J. R. Heath, *Nano Lett.* 2009, 9, 12, 4446-4451.
- [6] J. W. Suk, W. H. Lee, J. Lee, H. Chou, R. D. Piner, Y. Hao, D. Akinwande, R. S. Ruoff, *Nano Lett.* 2013, 13, 4, 1462–1467.

Graphene-based materials as platforms for skin disease treatment

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Abstract

Skin diseases are one of the leading causes of global disease burden, affecting millions of people worldwide. In the United States of America (USA), nearly 85 million people are seen by a physician for at least 1 skin disease every year. Guidelines for treatment of Psoriasis, Atopic Dermatitis (AD), and Vitiligo include as first or second line options phototherapy with ultraviolet radiation combined or not with drugs while for Basal Cell Carcinoma (BCC), photodynamic therapy (PDT) with photosensitizers activated by near-infrared (NIR) radiation are listed in the first line of treatments. [1-3] However, these treatments still present limitations due to the low stability, toxicity, and skin penetration of commonly used drugs. Graphene-based materials (GBM) properties allow targeted drug delivery, sustained release, improved biostability and, low toxicity. In addition, they possess a high coefficient extinction in near-infrared (NIR) region making them good candidates to act as photothermal agents. [4]

In this study, we propose the use of nanographene oxide (GON) and reduced nanographene oxide (rGON) as platforms for skin diseases treatment. GO was produced from graphite (Gt) powder through the modified Hummer's method, [4] and further sonicated and centrifuged to obtain GON. This material was later photo-reduced to obtain rGON. Gt water dispersions stabilized with Pluronic P-123 (Gt-P-123) were also prepared. Particle size and morphology were evaluated by transmission electron microscopy (TEM), optic microscopy, and using a zetasizer; zeta potential was also measured. Absorbance spectra (200-850 nm) were obtained using a UV-Vis spectrophotometer. GON and rGON were irradiated with a LED source of 812 nm (150 mW cm⁻²) and temperature increase recorded using a thermocouple. GON and rGON biocompatibility with primary human fibroblasts (HFF-1) was evaluated using the Alamar Blue assay. The permeability of GON, rGON and Gt-P-123 water suspensions through human skin was determined using a Franz cell system.

Single layer GON and rGO were obtained with average lateral dimensions below 200 nm. GON and rGON dispersions showed colloidal stability with zeta potential values of -39.4 ± 1.8 and -37.8 ± 1.2 mV (neutral pH), respectively. rGON temperature reached 59.4 °C after 30 min irradiation, around 1.3-fold higher than GON heating. GON and rGON (100-500 µg mL⁻¹) did not affect HFF-1 cell viability after 24 h of incubation. Both materials were able to cross epidermis and dermis in a time-dependent manner. Skin permeability of rGON revealed to be lower and slower than GON permeability, during the 1st hour of contact with the skin. After 6 h, the amount of rGON that permeated to the receptor compartment was 1.2-fold lower than for GON. Gt-P-123 presented sizes between a few to hundreds (agglomerates) of microns. Due its large size, no skin permeation was observed for Gt-P-123.

These results demonstrate for the first time the potential of GBM for use in skin disease treatment, as biocompatible photothermal agents able to penetrate deep into skin.

Acknowledgements

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REFERENCES

- [1] Eichenfield, L.F., et al., J Am Acad Dermatol, 70 (2014) 338-351.
- [2] Taieb, A., et al., Brit J Dermatol, 168 (2013) 5-19.
- [3] Menter, A., et al., J Am Acad Dermatol, 58 (2008) 826-850.
- [4] Costa-Almeida, R., et al., Polymers, 12 (2020), 1840.

GRAPHENE AND 2DM ONLINE CONFERENCE (GO2021)

Switch RF based on 2d materials

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Recently, nonvolatile switching has been observed in various monolayer and multilayer 2D materials. Besides memory applications, resistive switching is promising for analogue RF switches because of the favorable scaling with the area compared to other emerging technologies [1]. The RF switches are metal-insulator-metal structures consisting of a vertical junction made of metal electrodes separated by a 2D material. In this work, we investigate RF switches made with hBN and MoS₂ for 5G and 6G data communication applications. We first fully characterized the devices at DC and RF, then we demonstrated their potential in a real-life scenario by routing a live stream of a full-HD video across the RF switch. The devices are embedded in a coplanar waveguide for RF measurements. The DC measurements show that the switch is in a high-resistance state until the application of a SET voltage (~2V for the MoS₂ device), which brings the device into a low-resistance state. This state persists until a negative bias is applied to RESET the switch to its high-resistance state. We used S-parameter characterization covering the frequency range 0.25-320GHz to extract the small equivalent circuit of the device. From S-parameters, we deduced two main figures of merit of the RF switch: the insertion loss (the power loss due to the device with the switch in the ON state) and the isolation (the attenuation of the power across the switch in the OFF state). The device is non-volatile, with a state retention exceeding 3 months [2]. Finally, we used the switch for data communication experiments at carrier frequency $f_c=100\text{GHz}$, demonstrating a high data-rate of 8.5 Gbit.s^{-1} and the routing of a raw (uncompressed) HD-TV data stream.

REFERENCES

[1] R. Ge et al., Nano Lett. 2018, 18, 434–441

[2] M. Kim et al., Nat. Elec., 2020, 3, 479–485

Dielectric susceptibility of graphene due to its out-of-plane polarizability

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Although atomically thin, graphene monolayer has a significant out-of-plane polarizability that is important for self-consistent quantitative analysis of gating of both Bernal-stacked and twisted graphene multilayers. The out-of-plane electric field is screened by both the charge redistribution among the layers and by polarizability of orbitals in each of the layers. We show how to consistently implement both screening mechanisms, taking into account that layers are not polarized by the field from their own charges, Fig.1. For bilayer this leads to the equation (see Fig 1 for the notations):

$$U_t - U_b = \frac{e d}{\epsilon_0} \left[\frac{D}{\epsilon_z} - e \frac{1 + \epsilon_z^{-1}}{2} \left(\frac{n_b - n_t}{2} \right) \right].$$

To determine ϵ_z , we combine the DFT analysis of out-of-plane polarizability of monolayer graphene, producing $\epsilon_z = 2.65$, with the available experimental data [3-5], fitted with self-consistent tight-binding model calculations of electronic band structure in electrically gated Bernal-stacked and twisted bilayers, Fig.2. Upon comparison, we find a good agreement with the theoretically computed $\epsilon_z = 2.65$.

REFERENCES

- [1] Sergey Slizovskiy, Aitor Garcia-Ruiz, Neil Drummond, Vladimir I. Fal'ko, arXiv:1912.10067
- [2] B. Fallahazad, Y. Hao, K. Lee, S. Kim, R. S. Ruoff, and E. Tutuc, Phys. Rev. B **85**, 201408 (2012)
- [3] J. D. Sanchez-Yamagishi, T. Taychatanapat, K. Watanabe, T. Taniguchi, A. Yacoby, and P. Jarillo-Herrero, Phys. Rev. Lett. **108**, 076601 (2012)
- [4] L. Ju, L. Wang, T. Cao, T. Taniguchi, K. Watanabe, S. G. Louie, F. Rana, J. Park, J. Hone, F. Wang, and P. L. McEuen, Science **358**, 907–910 (2017)

FIGURES

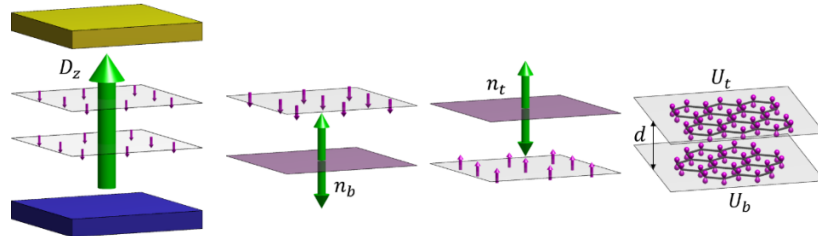


Figure 1: Dielectric polarisation of graphene layers, induced by external displacement field [left panel] and by the charges on the bottom and top layers [two central panels]. Right: Notations for layer potentials.

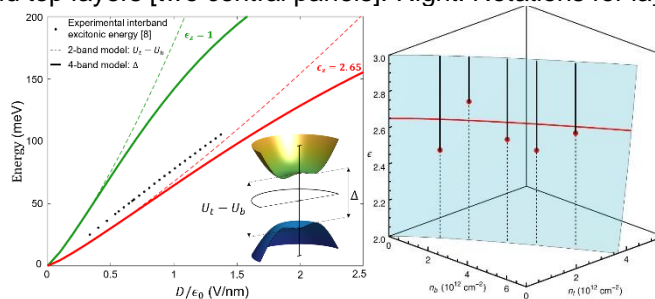


Figure 2: Left: Calculated gap in Bernal graphene bilayer compared with exciton spectrum measured in [4]. Right: Calculation of layer densities for single-gated twisted graphene bilayer (cyan surface) is compared with experiment [2] (black lines) for different values of ϵ_z .

Spectroscopy and Charge-Sensing using Defects Embedded in Waals Tunnel Barriers

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We study electronic transport in vertical structures where naturally occurring defects, found in exfoliated hexagonal Boron Nitride and transition metal dichalcogenides thin flakes, assist tunneling processes when those flakes serve as tunnel barriers. In our typical geometry, electrons tunnel from a source electrode, through the defect-bound state, to the drain. In this geometry, the defect exhibits transport features typical of single-charge tunneling through quantum dots with very high charging energies. We operate that the defect-bound dots in a number of transport regimes: (i) A defect-dot coupled to a superconductor (NbSe₂) reveals sub-gap Andreev bound states (ABS). Analogous to nanowire systems, ABS related to defect-dots exhibit a magnetic-field driven singlet-to-doublet transition. (ii) We show that using graphene as a source electrode, the defect energy can be gate-tuned using electric field which penetrates the graphene. In this system, the dot serves as a stable spectral probe for graphene at high magnetic fields, and can also be used as a local compressibility probe. The local nature of the dot allows it to detect transitions between compressible and incompressible behavior at the broken-symmetry regime in graphene quantum Hall. (iii) Finally, we demonstrate that a gated dot, when coupled to a superconductor, can be energy tuned, and is thus used as a sensitive spectrometer. We demonstrate this by showing how defect-dot states couple to both superconducting gaps of NbSe₂. Our results demonstrate the utility of defect-bound states as highly local and precise sensors.

Built-in atomically sharp superlattice heterojunctions from hybrid Nanoporous Graphene

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Bottom-up synthesis has shown to be a very efficient method to build graphene nanoarchitectures with atomic precision. The most illustrative example is the plethora of graphene nanoribbons (GNR) that have been created practically à la carte. Despite such impressive advances in 1D homostructures, going beyond in structural complexity has turned to be a tough challenge. In particular, the synthesis of heterostructures has been limited to 1D, with no control on size and distribution of fusing components [1].

Here we report a hierarchical on-surface synthesis method for the fabrication of graphene-based superlattice heterojunctions by laterally coupling alternating doped/undoped graphene nanoribbons. For that we harness our ability to create parallelly-aligned graphene nanoribbons superlattices [2] in order to guide the synthesis of a second GNR component, in this case an N-doped isostructural counterpart, within the empty channels of the superlattice. The final step consists on fusing the hybrid GNR array into a hybrid nanoporous graphene (h-NPG) [3]. Interestingly, the electronic structure of the final product preserves the one dimensional character of the individual components, with a rigid downshift of 0.2 eV for the N-doped GNR. The resulting structure can therefore be considered as a type II superlattice heterojunction.

Our hierarchical strategy fuses the concepts of 2D nanoporous graphene nanostructures, heteroatom doping and hybrid arrays in a single, novel graphene-related material, which we expect to seed new initiatives to synthesize other complex graphene nanoarchitectures with atomic precision.

REFERENCES

1. J. Cai et al., *Nat. Nano.*, 9, (2014) 896-900
2. C. Moreno et al., *Chem. Comm.*, 54, (2018) 9402 – 9405
3. C. Moreno et al., *Science*, 360, (2018) 199-203

FIGURES

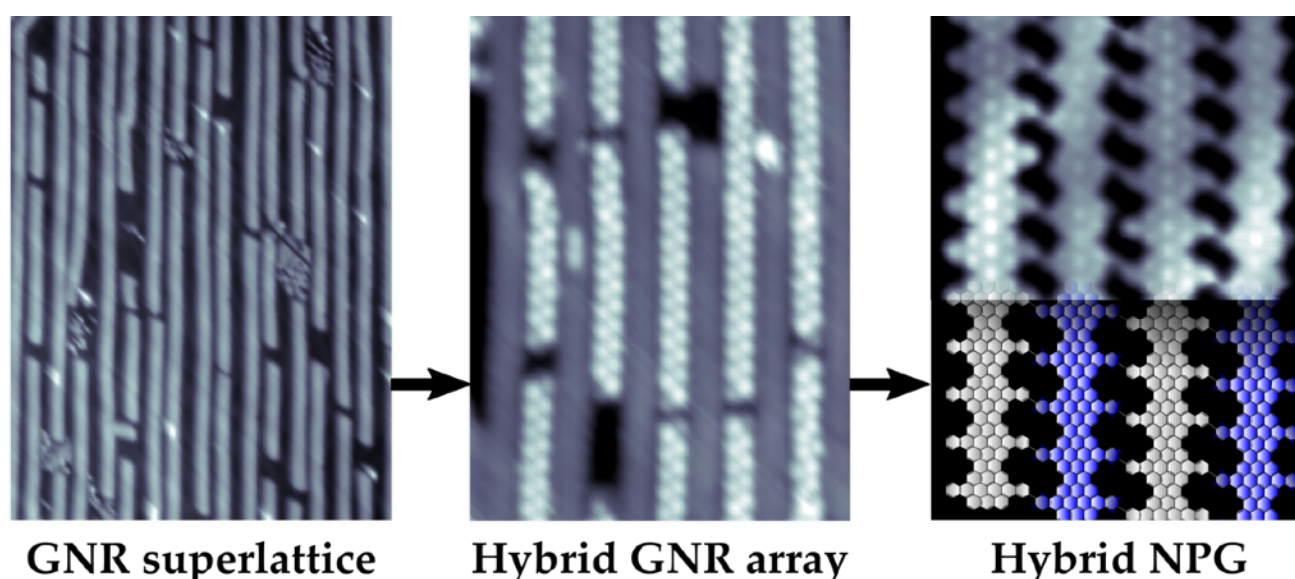


Figure 1: STM images of the on-surface synthesis of graphene superlattice heterojunctions

Graphene for nonlinear THz photonics and thermal management

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Graphene has been suggested as a game-changer material for many types of applications. Here, we highlight two such applications that we identified recently.

In the first part of this talk, we will discuss the highly efficient generation of terahertz (THz) harmonics, facilitated by hot carriers in graphene. This effect was first observed in 2018 [1], and recently we combined graphene with a metallic grating in order to make this process even more efficient [2]. We will show that this grating-graphene metamaterial gives third-harmonic generation with a power that is enhanced by more than 3 orders of magnitude compared to graphene without metallic grating, has a harmonic field conversion efficiency of 1%, as well as gives rise to generation of higher harmonics (up to the ninth). These results are promising for the development of on-chip THz nonlinear photonic applications.

In the second part, we will discuss diffusion of electronic heat in graphene, which we have studied using a novel spatiotemporal thermoelectric microscopy technique with femtosecond temporal and sub-100 nm spatial control. With this technique we follow electronic heat flow in space and time at room temperature, and observe electronic heat flow consistent with charge flow in the “normal” diffusive regime. In the hydrodynamic time window before momentum relaxation occurs, and under Dirac-fluid conditions, we observe much more significant heat spreading. Importantly, we show that heat spreading is so efficient that the thermal conductivity of the electron system can be larger than the already record-high thermal conductivity of the phonon system of graphene. This result is relevant for thermal management applications where heat needs to be extracted as fast as possible from sub-micron-sized local hot spots.

REFERENCES

- [1] H. Hafez et al. Nature, 561 (2018) 507
- [2] J.C. Deinert et al., ACS Nano, 15 (2021) 1145
- [3] A. Block et al., Arxiv 2008.04189 (2020), *under review*

FIGURES

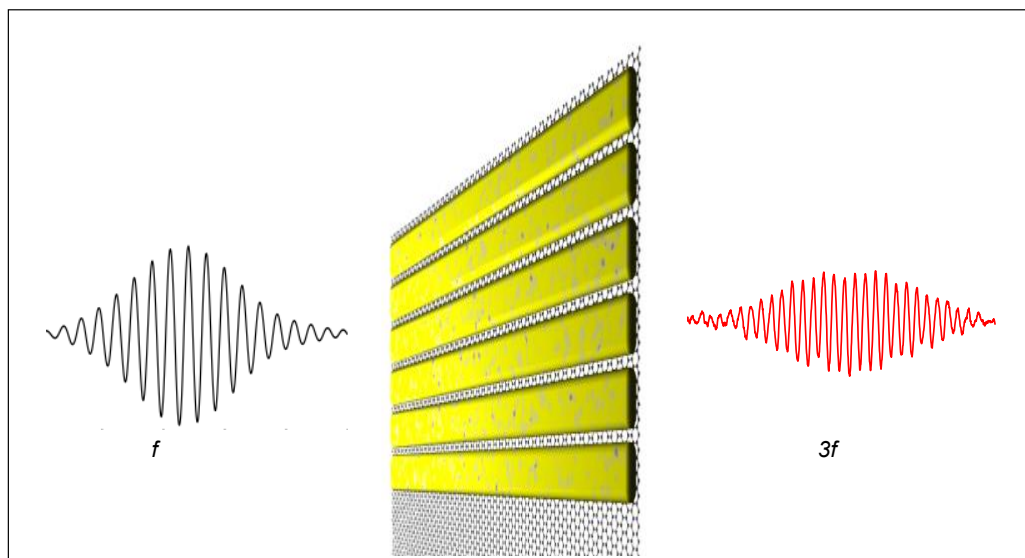


Figure 1: Terahertz third-harmonic generation using a grating-graphene metamaterial [2].

Microscopic theory of plasmon-enabled resonant terahertz detection in bilayer graphene

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The electron gas hosted in a two-dimensional solid-state matrix under external driving supports the propagation of plasma waves.[1] Nonlinear interactions between plasma waves generate a constant density gradient which can be detected as a dc potential signal at the boundaries of the system. This phenomenon is at the heart of a plasma-wave photodetection scheme which was first introduced by Dyakonov and Shur for electronic systems with a parabolic dispersion [2] and then extended to the massless Dirac fermions in graphene.[3]

Motivated by a recent experimental breakthrough in the resonant detection of plasma waves in double-gated bilayer graphene, [4] we develop the theory of plasma-wave photodetection in such geometry, [5] where the dispersion relation depends locally and dynamically on the intensity of the plasma wave. We show that quantum capacitance effects, arising from the local fluctuations of the electronic dispersion, modify the intensity of the photodetection signal. An external electrical bias, e.g. induced by top and bottom gates, can be used to control the strength of the quantum capacitance corrections, and thus the photoresponse.

REFERENCES

- [1] A.N. Grigorenko, M. Polini, and K.S. Novoselov, *Nature Photon.* **6**, 749 (2012).
- [2] M.I. Dyakonov and M.S. Shur, *IEEE Trans. Electron Devices* **43**, 380 (1996); *ibid.* **43**, 1640 (1996).
- [3] A. Tomadin and M. Polini, *Phys. Rev. B* **88**, 205426 (2013).
- [4] D.A. Bandurin *et al.*, *Nature Commun.* **9**, 5392 (2018).
- [5] A. Tomadin, M. Carrega, and M. Polini, *Phys. Rev. B* **103**, 085426 (2021).

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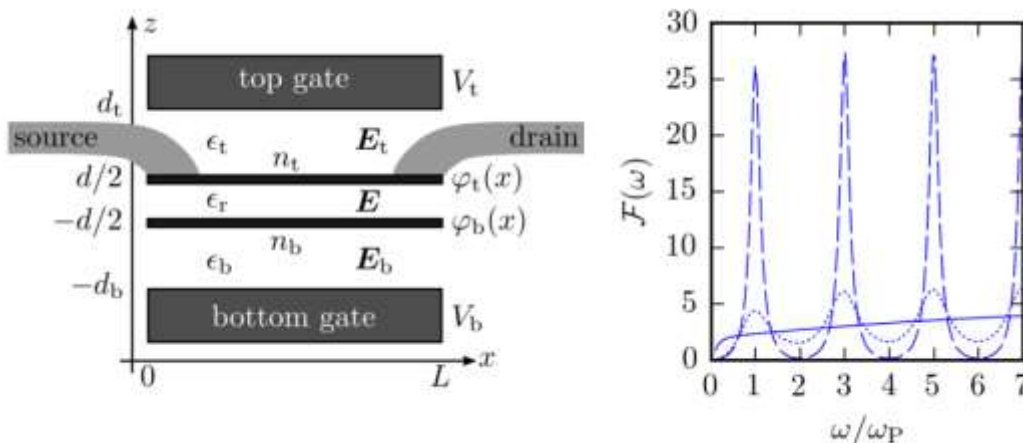


Figure 1: Schematics of the double-gated bilayer graphene setup (left) and photoresponse as a function of the driving frequency (right) for several carrier densities $n = 0.1$ (solid), 1.0 (dotted), and 5.0 (dashed) $\times 10^{12} \text{ cm}^{-2}$.

A novel technique to measure thermal diffusion of thin films

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Understanding heat transport at the nanoscale is of great importance to fundamental science and the development of efficient electronic devices. A precise understanding and control of the transport mechanisms is important for enabling thermoelectric, optoelectronic, and medical applications. For these reasons, there is great interest in the development of tools to study nanoscale heat transport through electrical [1,2] and optical [3,4] techniques. However, there lacks a technique that meets the following requirements: (i) minimal sample fabrication, (ii) high sensitivity to small temperature changes, (iii) simple mathematical modelling and (iv) few input parameters.

Here we address these challenges and demonstrate a novel method for quantifying thermal diffusivity (D) in nanometre thick materials by spatiotemporally probing a temperature-dependent optical resonance using visible light. Our experimental setup combines two femtosecond laser pulses in a pump-probe configuration: one to excite the sample (pump) and the other to probe the pump-induced changes in reflectivity [5]. By raster scanning the probe over the pump spot we resolve the spatial profile of the reflection signal with nanometre spatial precision. We achieve femtosecond temporal resolution by delaying the arrival of one pulse with respect to the other.

Over picosecond timescales we observe the diffusion of the electronic excitation in which the spatial profile broadens by 10's of nanometres. However, on much longer timescales (>10 ns) we observe a significantly broadened profile which we attribute to the diffusion of heat carried by phonons. We determine the thermal diffusivity of the sample using a simple model based on the heat equation where the only input parameter is the initial width of the spatial profile. As a proof of concept we measure the diffusivity of suspended transition metal dichalcogenide flakes and find excellent agreements with reported literature values of heat capacity and thermal conductivity [6].

References

- [1] Cahill D G 1990 Thermal conductivity measurement from 30 to 750 K: The 3w method *Rev. Sci. Instrum.* **61** 802–8
- [2] Yamane T, Katayama S I and Todoki M 1996 Analysis of ac temperature wave during the measurement of thermal diffusivity of two-layered platelike samples *J. Appl. Phys.* **80** 2019–26
- [3] Malekpour H and Balandin A A 2018 Raman-based technique for measuring thermal conductivity of graphene and related materials *J. Raman Spectrosc.* **49** 106–20
- [4] Jiang P, Qian X and Yang R 2017 Time-domain thermoreflectance (TDTR) measurements of anisotropic thermal conductivity using a variable spot size approach *Rev. Sci. Instrum.* **88**
- [5] Block A, Liebel M, Yu R, Spector M, Sivan Y, García De Abajo F J and Van Hulst N F 2019 Tracking ultrafast hot-electron diffusion in space and time by ultrafast thermomodulation microscopy *Sci. Adv.* **5** 1–8
- [6] Zobeiri H, Wang R, Wang T, Lin H, Deng C and Wang X 2019 Frequency-domain energy transport state-resolved Raman for measuring the thermal conductivity of suspended nm-thick MoSe₂ *Int. J. Heat Mass Transf.* **133** 1074–85

Spin dynamics in the topological, low-symmetry MoTe₂ and WTe₂

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Recently, the low-symmetry phases (1T_d and 1T') of transition metal dichalcogenides (TMDs) have attracted great attention for their spintronics potential and topological properties. In this talk, I will theoretically show unconventional forms of the spin Hall effect and the quantum spin Hall effect in monolayers of MoTe₂ and WTe₂. Due to the low crystal symmetry, the spin polarization of electrons in these TMDs displays a momentum invariant (persistent) spin texture fixed in a direction along the yz plane (Figure 1, left), and as a result, the spin transport displays anisotropic spin relaxation. The spin Hall effect exhibits an unconventional component, with spin accumulation generated in the plane, which together with the conventional out-of-plane polarization, forms an oblique or canted spin Hall effect. The spin relaxation length and the spin Hall angle are gate-tunable, being both maximum at the bottom of the conduction band, leading to a charge-to-spin interconversion figure of merit of 1-50 nm, largely superior to conventional spin Hall effect materials [1]. When the Fermi level is placed in the topologically nontrivial gap, the canted spin Hall effect is predicted to transition into a canted quantum spin Hall effect (Figure 1, right) [2]. The corresponding topologically protected edge states are robust to disorder and carry spins polarized in the same canted direction as the persistent spin texture found at the bottom of the conduction bands. Remarkably, these predictions have been recently confirmed experimentally [3]. Overall, our findings open new perspectives to predict and scrutinize spin transport in topological, low-symmetry two-dimensional materials.

REFERENCES

[1] Marc Vila, Chuang-Han Hsu, Jose H. Garcia, L. Antonio Bentez, Xavier Waintal, Sergio O. Valenzuela, Vitor M. Pereira, and Stephan Roche, Charge-to-Spin Interconversion in Low-Symmetry Topological Materials, arXiv:2007.02053, Submitted, (2020).

[2] Jose H. Garcia, Marc Vila, Chuang-Han Hsu, Xavier Waintal, Vitor M. Pereira, and Stephan Roche, Canted Persistent Spin Texture and Quantum Spin Hall Effect in WTe₂, Phys. Rev. Lett., 125, (2020), 256603.

[3] W. Zhao, E. Runburg, Z. Fei, J. Mutch, P. Malinowski, B. Sun, X. Huang, D. Pesin, Y.-T. Cui, X. Xu, J.-H. Chu, and D. H. Cobden, arXiv:2010.09986 ; C. Tan, M.-X. Deng, F. Xiang, G. Zheng, S. Albarakati, M. Algarni, J. Partridge, A. R. Hamilton, R.-Q. Wang, and L. Wang, arXiv:2010.15717

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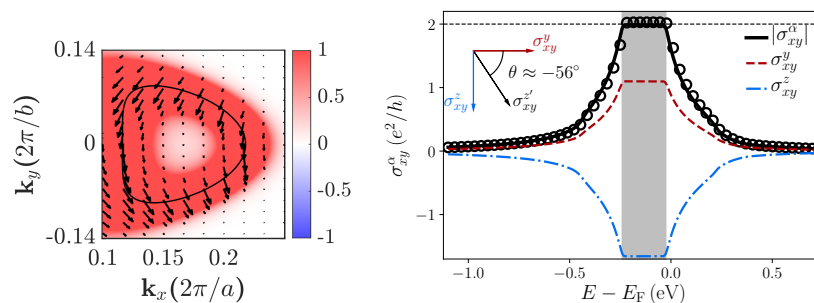


Figure 1: Left: Persistent spin texture in the yz plane of MoTe₂. Right: Spin Hall conductivity of WTe₂ displaying a canted quantum spin Hall effect.

Reversing of humidity response of MoS₂- and WS₂-based sensors with metal coatings

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Abstract

Two-dimensional materials, such as transition metal dichalcogenides, have been identified as attractive candidates for sensing applications due to their high surface-to-volume ratio, chemically active edges and good electrical performance. However, their electrical response to humidity is still under debate and the experimental reports still remain inconclusive. For instance, the impedance of the MoS₂-based sensors decreases or increases with increasing humidity, compromising the use of MoS₂ for humidity sensing. In this work we focus on understanding the interaction between water and the transition metal dichalcogenides. We fabricated and studied humidity sensors based on MoS₂ and WS₂ coated with copper and silver metals. The devices exhibited high chemical stability and excellent humidity sensing performance in relative humidity between 4 and 80%, with response and recovery times of 2 and 40 seconds, respectively. We have systematically investigated the humidity response of the materials as a function of the type and amount of metal coating and observed the reverse action of sensing mechanisms. This phenomenon is explained based on a detailed structural analysis of the samples considering the Grotthuss mechanism in the presence of charge trapping, which was verified by simulations of an appropriate lumped-element model. Our findings open up a possibility for tuning of the electrical response in a facile manner and without compromising the high performance of our sensor.

Effect of metal deposition on atomically h-BN

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Abstract

Metal deposition is a standard process in semiconductors industry to fabricate electronic devices. However, it has been suggested that electron beam evaporation of metals can damage the surface of two-dimensional (2D) layered materials, producing partial local etching and resulting in multiple dangling bonds that can reduce the performance of the devices. However, how the effect of metal deposition will influence h-BN has never been studied. Here we present statistical analyses that compare the effect of metal deposition (electron beam evaporation and sputtering) on multilayer hexagonal boron nitride (h-BN) produced by mechanical exfoliation and metal organic chemical vapour deposition (MOCVD) h-BN. Our experiments indicate that both deposition methods damage the surface of the h-BN, as the h-BN protected with materials deposited at low energy (e.g. spin-coated photoresist, inkjet printed metals and transferred electrodes) do not exhibited this damage.

Fully inkjet printed h-BN memristors

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Abstract

Layered hexagonal boron nitride (h-BN) has been proved to show switching behaviour for both information storage and neuromorphic computing [1-3]. However, synthesis methods like mechanical exfoliation and transfer after chemical vapor deposition (CVD) growth limit its industrial applications [4,5]. In this work, we introduce inkjet printing technology [6] to fabricate h-BN based memristors to achieve low cost and scalable mask-free fabrication. We have first synthesized inks containing h-BN nanoflakes, and then produced (at a low fabrication temperature <100 °C) fully inkjet printed Ag/h-BN/Pt and Ag/h-BN/Ag devices. The devices show stable bipolar resistive switching behavior with high on-off ratio of 10^7 , retention time $>10^5$ s at 85 °C, and operation voltages less than ± 1 V. The devices also show potential for multilevel data storage controlled by current limitation. This study indicates that inkjet printing is one promising fabrication method for large-scale memristor fabrication, especially for flexible electronics.

REFERENCES

- [1] S. Chen et al, Nat. Electron. 3 (2020) 638.
- [2] Y. Shi et al, Nat. Electron. 1 (2018) 458.
- [3] C. Pan et al, Adv. Funct. Mater. 27 (2017) 1604811.
- [4] L. Sun et al, Nat. Commun. 10 (2019) 3161.
- [5] K. Zhu et al, ACS Appl. Mater. Interfaces 11 (2019) 37999.
- [6] G. Vescio et al, ACS Appl. Mater. Interfaces 11 (2019) 23659.



**ABSTRACTS
FLASH POSTERS**

Hydrogen isotopes functionalization of nano-porous graphene: attainment of stable and low-defect free-standing *graphane*

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Achievement of semiconducting *graphane* [1] through hydrogen isotopes adsorption on semi-metallic graphene is a big challenge in terms of the quality and stability of the hosting graphene. High quality and low-defect free-standing nano porous graphene (NPG), synthesized by a nano-porous Ni based chemical vapour deposition (CVD) method [2], is an outstanding hosting graphene template for enhancing the loading of hydrogen (H) stable isotopes due to its large surface to volume ratio [3] and the absence of any holding substrate.

We here with present achievement of H- and deuterium- (D) free-standing *graphane* based on low-energy ion irradiation (6 eV) and hot-temperature cracked molecule irradiation in ultra-high-vacuum (UHV), resulting in low-defect non-destructive adsorption, and high H and D coverage on NPG. X-ray photoelectron spectroscopy (XPS) reveals the high H (and D) up-load through the sp^3 -distorted component in the C 1s core level, pointing out H-C (and D-C) covalent bonding [4-6]. Raman spectroscopy presents remarkably low-defect and clean H- and D-functionalized NPG. The synthesized H- and D- functionalized NPGs are very stable at unprecedented high temperatures, up to 800 K, with complete desorption only above 920 K. Moreover, ultraviolet photoelectron spectroscopy (UPS) shows an energy band gap opening in the valence band, indicating the H stable isotopes functionalization of NPG. Consequently, this low-defect and highly-loaded H- and D-functionalized NPG with high chemical and temperature stabilities paves not only the way towards fabricating semiconducting *graphane* on large-scale, but it may also represent a guidance for tritium (T, the radioactive isotope of H) functionalization of graphene for futuristic advanced detectors for the β - spectrum analysis [7].

REFERENCES

- [1] J.O. Sofo et al., Phys. Rev. B 75 (2007) 153401.
- [2] Y. Ito, et al., Angew. Chem. Int. Ed. 53 (2014) 4822-4826.
- [3] X. Sha, et al., Surf. Sci. 496 (2002) 318-330.
- [4] P. Ruffieux, P., et. al, Phys. Rev. B 66 (2002) 245416.
- [5] M. M. S. Abdelnabi et. al., Nanotechnology 32(3) (2020) 035707.
- [6] M. M. S. Abdelnabi et al., Nanomaterials 11(1) (2021) 130.
- [7] M.G Betti, et al., Prog. Part. Nucl. Phys. 106 (2019) 120-131.

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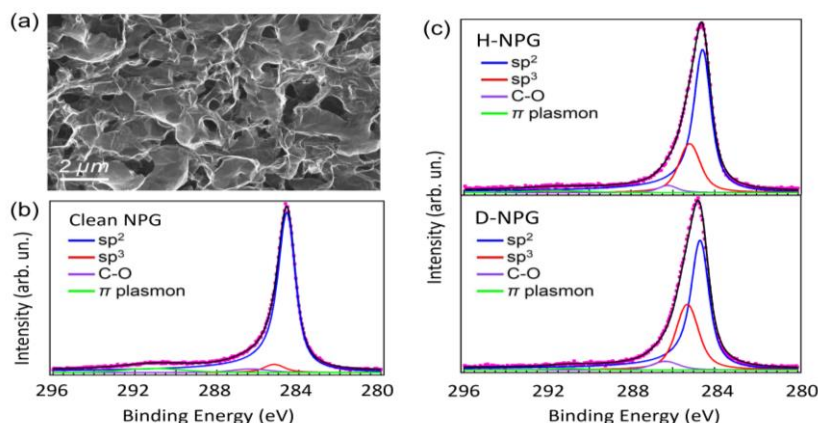


Figure 1: (a) SEM image of the NPG sample; (b) C 1s XPS spectrum of clean NPG; (c) C 1s XPS spectra of NPG exposed to saturation coverage of H (top spectrum) and D (bottom spectrum) using low-energy ion irradiation source.

Solution-processed photoelectrochemical (PEC)-type photodetectors based on layered GaSe and GeSe nanoflakes

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The photoelectrochemical (PEC) devices, such as self-powered photodetectors and water splitting cells, represent powerful tools to convert the electromagnetic radiation into chemical fuels and electricity.[1] To achieve efficient PEC systems, it is mandatory to develop photocatalytic materials that efficiently absorb light in the desired spectral range (UV/visible for energy conversion systems), creating free charge carriers with suitable energies to carry out the oxidation-reduction (redox) reactions before they recombine.[2] In this context, two-dimensional (2D) materials are continually attracting utmost interest as potential advanced photo(electro)catalysts,[2] and recently, 2D group-III and group-IV transition metal monochalcogenides (MCs) have been theoretically predicted to be low-cost and eco-friendly photocatalyst. [3] Among them, gallium selenide (GaSe) and germanium selenide (GeSe), are promising material candidates for optoelectronic devices due to their properties: tuneable electronic structure, strong visible-light absorbance, photoresponse and environmental stability.[4] Here, we report the first experimental characterization of the PEC water splitting activity of single-/few-layer flakes of GaSe and GeSe produced in inks form by scalable liquid-phase exfoliation method in non-toxic solvent (*i.e.*, 2-propanol).[5] The PEC behaviour of monochalcogenides(MCs)-based photoelectrodes, obtained by spray coating approach,[6] were evaluated in different aqueous media, ranging from acidic to alkaline solutions and under different illumination wavelengths, *i.e.*, 455, 505 and 625 nm. The obtained performances (responsivity and external quantum efficiency up to 0.32 A/W and 86.3%) are superior to those of several self-powered and low-voltage solution-processed photodetectors, approaching the ones of their commercial UV–Vis counterparts. Finally, we demonstrate the use of MCs-based photoelectrodes as photoanodes or photocathodes for water splitting reactions under simulated sunlight.

REFERENCES

- [1] Bellani, S., Ghadirzadeh, A., Meda, L., Savoini, A., Tacca, A., Marra, G., Meira, R., Morgado, J., Di Fonzo, F. and Antognazza, M.R., *Adv. Funct. Mater.*, (2015), 25(28), 4531-4538.
- [2] M. I. Zappia, G. Bianca, S. Bellani, M. Serri, L. Najafi, R. Oropesa-Nuñez, B. Martín-García, D. Bouša, D. Sedmidubský, V. Pellegrini, Z. Sofer, A. Cupolillo, F. Bonaccorso, *Adv. Funct. Mater.*, (2020), 1909572.
- [3] H. Cai, Y. Gu, Y.-C. Lin, Y. Yu, D. B. Geohegan, K. Xiao, *Appl. Phys. Rev.* (2019), 6, 041312.
- [4] Zhuang L., Hennig R. *Chemistry of Materials* (2013), 25, 15, 3232-3238
- [5] G. Bianca, M. I. Zappia, S. Bellani, M. Serri, L. Najafi, B. Martín-García, R. Oropesa-Nuñez, T. Hartman, D. Sedmidubský, V. Pellegrini, Z. Sofer, A. Cupolillo and F. Bonaccorso, *ACS Appl. Mater. Interfaces*, 12, 43, (2020), 48598–48613.
- [6] F. Bonaccorso, A. Bartolotta, J. N. Coleman, C. Backes, *Adv. Mater.*, 29, (2016), 6136-6166.

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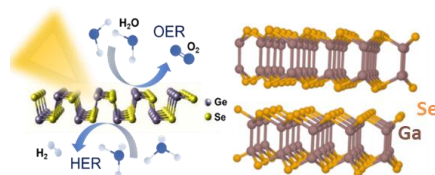


Figure: Crystal structure of monochalcogenides and schematic processes of PEC water splitting

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Is solar going indoors?

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Recent developments in the field of photovoltaics and their prospective role in the internet of things (IoT) applications indicate a clear need to leverage on their ability to operate indoors. Low-light harvesters are particularly interesting, as they can provide a driving source for low-power sensor nodes used in various IoT systems [1,2]. In this work, we propose a facile, low-cost solar cell fabrication approach towards efficient indoor light harvesters based on graphene/n-Si Schottky-junction. The cells exhibit the efficiency of 6% and only 0.2% in indoor and outdoor conditions, respectively; demonstrating a 30 times increase in efficiency indoors [3]. With Raman spectroscopy and thermovision we validate the operational stability of such devices over a period of 48 months and identify critical structural points responsible for performance degradation during the ageing process [4]. The high efficiency under indoor light is caused by large shunt (parallel) and serial resistances. As we used high quality c-Si which is very stable over many years and graphene that becomes more stable with time, we can conclude that the Ag contact degradation mostly impacts the cell performance. The cells are produced from liquid phase exfoliated graphene made by Langmuir-Schaefer assembly [5]. In addition, cells were annealed (A cells) and then functionalized for 5 min by UV/ozone (AO cells). We found that AO cells exhibit a better performance than A cells even though they have a lower EQE. The main reason is the existence of a small E_{gap} in AO. We assume that our cells are better in dark than light conditions because of intense recombination owing to the highly doped Si. Those cells have high concentrations of carriers leading to efficient photo conversion, but more light results in more carriers and a higher recombination rate, consequently reducing the efficiency of the cells. A good performance at low light intensities could significantly extend the usage of Si solar cells in indoor light conditions. Finally, the low cost solution production process of the graphene films will have an important impact on faster adoption of these devices.

REFERENCES

- [1] Addanki Venkateswararao et al., *Materials Science and Engineering: R: Reports* 139, (2020), 100517.
- [2] Ian Mathews et al., *Joule* 3 (2019), 1415-1426.
- [3] Djordje Jovanović et al., *Proc. NanoBio 2018 conf.* 1 (2018), 119 (abstract).
- [4] Djordje Jovanović et al., in preparation (2021).
- [5] Tijana Tomašević-Ilić et al. *Applied Surface Science* 458 (2018) 446-453

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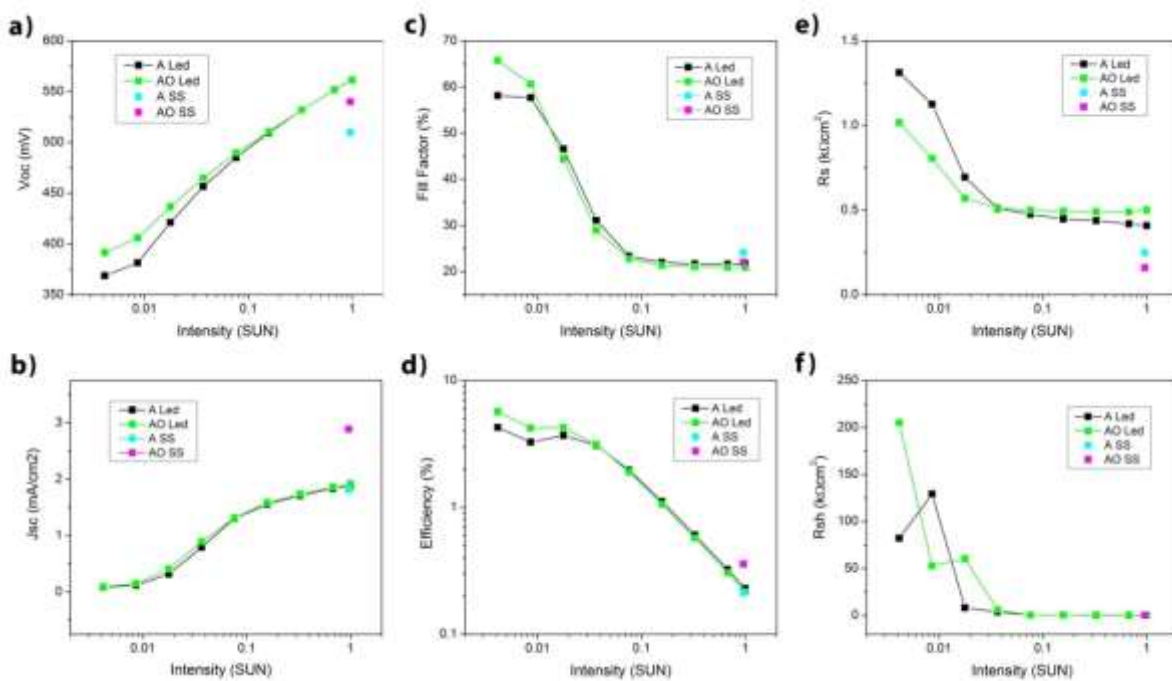


Figure 1: Solar cell parameters of pristine A and AO cells for different light intensities (indoor to outdoor) from LED (4200K, 0.004-1Sun) and Solar Simulator AM 1.5G (0.96Sun) light sources.

Graphene Nanostructures Integration in Nanophotonic Biosensors

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Biosensors are profiled as next-generation diagnostics devices, offering point-of-care rapid testing with excellent performance. Among them, the Bimodal Waveguide (BiMW) interferometric biosensor has demonstrated outstanding sensitivities, multiplexing capabilities, and high potential for integration in compact and user-friendly devices [1]. One of the major challenges in the advance of biosensor technology is the reproducible biofunctionalization of the sensing area. The lack of precise control during the arrangement of the biorecognition interface severely limits the detection selectivity and reliability of actual devices, hampering the mass-production and implementation in the clinical field. By proposing an advanced method to produce functionalized graphene nanostructures with atomic precision, we aim to develop a universal sensor biofunctionalization protocol, which will facilitate a biorecognition molecular template control at the nanometer scale.

Here, we combine the possibility to functionalize graphene building blocks with atomic precision via a bottom-up synthesis approach to support the production of different graphene nanoarchitectures (i.e., graphene nanoribbons and nanoporous graphene) containing selective anchoring groups such as amine, carboxyl and epoxy groups. The quality of the functionalized graphene template is dictated by the on-surface synthesis approach carried out in UHV conditions [2]. Additionally, the graphene successful integration on the BiMW biosensor is obtained by a direct transfer to preserve the stability of the graphene under flow conditions. Finally, as a proof of concept, nucleic acids biomarkers will be detected applying a universal biofunctionalization protocol for the early, non-invasive diagnostic of melanoma cancer.

REFERENCES

(1) M.C. Estevez et al., *Laser & Photonics Reviews*, 6(4), (2012) 463 – 487

(2) C. Moreno et al., *Science*, 360, (2018) 199 – 203

FIGURES

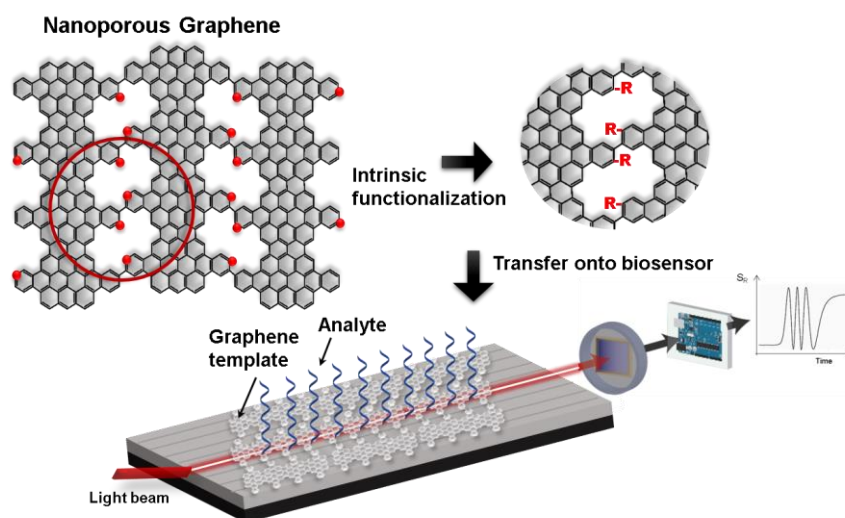


Figure 1: Nanoporous graphene (NPG) template presents the functional groups arranged in the porous sites. At the biosensor area the DNA analyte is monitored while bonding to the graphene template.

Valley and Spin Blockade in Graphene Quantum Dots

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The Pauli blockade effect manifests itself in coupled quantum dots by forbidding transitions between states with non-matching quantum numbers, conserved in inter-dot tunneling processes. The prohibition of transitions between spin singlet and triplet states [1] is the foundation of successful manipulation of spin qubits [2]. In our bilayer graphene quantum dots, we observe robust Pauli spin blockade at high perpendicular magnetic field $B > 600\text{mT}$ rather than at zero magnetic field, and valley blockade at low field. This unusual behaviour arises from the peculiar two-particle spin-triplet ground state of a single quantum dot, at low magnetic field [3]. The spin blockade leakage current is more than 50 times, and the valley blockade leakage current five times smaller than the non-blockaded current. This advancement prepares graphene quantum dots for spin (and valley) qubits [2]. The observation of blockade demonstrates the superb quality that the graphene quantum dots have reached, brought about by recent progress in fabrication technology.

REFERENCES

- [1] K. Ono, D.G. Austing, Y. Tokura, and S. Tarucha, *Science* **297** (2002), 1313–1317.
- [2] J.R. Petta, A.C. Johnson, J. M. Taylor, E.A. Laird, A. Yacoby, M.D. Lukin, C.M. Marcus, M.P. Hanson, and A.C. Gossard, *Science* **309** (2005), 2180–2184.
- [3] A. Kurzmann, M. Eich, H. Overweg, M. Mangold, F. Herman, P. Rickhaus, R. Pisoni, Y. Lee, R. Garreis, C. Tong, et al., *Phys. Rev. Lett.* **123** (2019), 026803.

FIGURES

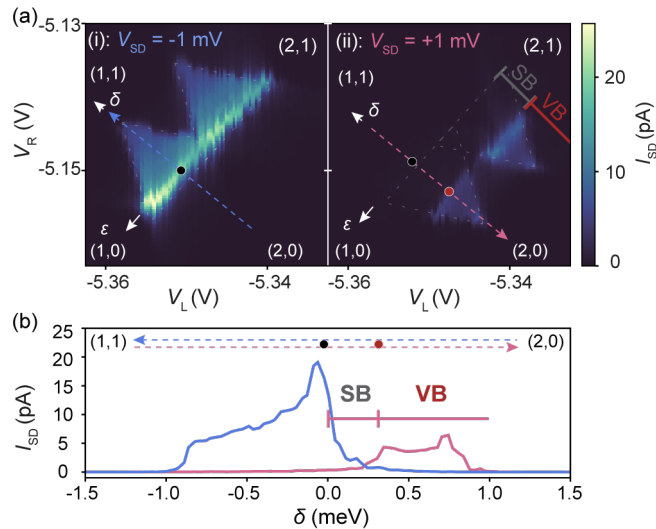


Figure 1: (a) DC current maps of finite-bias triangles at $B = 800\text{mT}$ with (i) negative bias $V_{SD} = -1\text{ mV}$ [electron transport $(2,0) \rightarrow (1,1)$], and (ii) positive bias $V_{SD} = +1\text{ mV}$ [electron transport $(1,1) \rightarrow (2,0)$], with the same gate voltage window. (b) Line-cuts along the δ -axis, at $\epsilon = 0$ where current peaks are labeled by circles. Valley blockade (VB) and spin blockade (SB) effects suppress the current in the negative bias direction. Here the VB leakage current is five times smaller than the current in the non-blockaded bias direction. The SB leakage current is masked by measurement noise $\sim 300\text{fA}$, and is therefore more than 50 times smaller than the non-blockaded current.

Transition metal dichalcogenide photonic dimer nano-antenna with ultra-small gap

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In the past decade, transition metal dichalcogenides (TMDs) have drawn large scientific interest involving their integration with nano-photonic structures [1, 2]. However, the use of TMDs in these studies was limited to single and few-layer samples coupling to resonances and cavity modes in different material systems. Recently, TMDs have emerged as promising materials for fabrication of nano-photonic resonators due to their large refractive index and low absorption within a large portion of the visible spectrum. Another advantage of this material family is their compatibility with a wide variety of substrates owing to their van-der-Waals attractive forces. Recent reports have demonstrated WS₂ nano-disk Mie resonators where strong light-matter coupling [3] and second harmonic generation (SHG) enhancement [4] were observed. However, further uses for this material family within the nano-photonic field have been in short supply.

In our work we study the nano-photonic capability of TMDs by fabricating single (monomer) and double (dimer) nano-pillar antennas in a circular, square or novel zigzag-terminated hexagonal geometries with potentially atomically sharp edges and vertices. We probe the structures with dark field spectroscopy followed by second harmonic generation experiments, in which we induce polarization-dependent enhancement due to coupling with an anapole mode. In order to achieve ultra-small dimer gaps and rotate the relative orientation of individual nano-pillars, we introduce a post-fabrication atomic force microscopy (AFM) step, achieving gaps limited by our spatial resolution. The smallest dimer gap we measured (10±5 nm shown in middle inset of Fig. 1) confirms that we have reached the fabrication limit of focused ion beam milling, yet we provide a more precise and less damaging method for controlling the photonic properties of these structures.

Simulations of such nano-antennas yield electric field intensity enhancements of more than 10³ at hotspots surrounding the edges of the fabricated hexagonal geometry. We calculate a Purcell factor as high as 157 for single photon emitters (SPEs) positioned within these hotspots (right image of Fig. 1). A route to the modulation of these values by varying the gap separation and relative rotations of the nano-pillars is also readily available. Optical trapping simulations for such small gaps result in attractive forces of >350 fN for colloidal quantum dots (QDs) (left image of Fig. 1) and > 70 fN for protein-like, polystyrene beads. These results surpass previous reports of dielectric nano-antennas by a factor of >83 for QDs [5] and >40 for PBs [6].

References

- [1] Luo, Y. et al. *Nature Nanotechnology*, 13(2018), 1137-1142.
- [2] Sortino, L. et al. *Nature Communications*, 10(2018).
- [3] Verre, R. et al. *Nature Nanotechnology*, 14(2019), 679-683.
- [4] Busschaert, S. et al. *ACS Photonics*, 7(2020), 2482-2488.
- [5] Xu, Z. et al. *Optics Express*, 27(2019), 4034-4045.
- [6] Xu, Z. et al. *ACS Photonics*, 5(2018), 4993-5001.

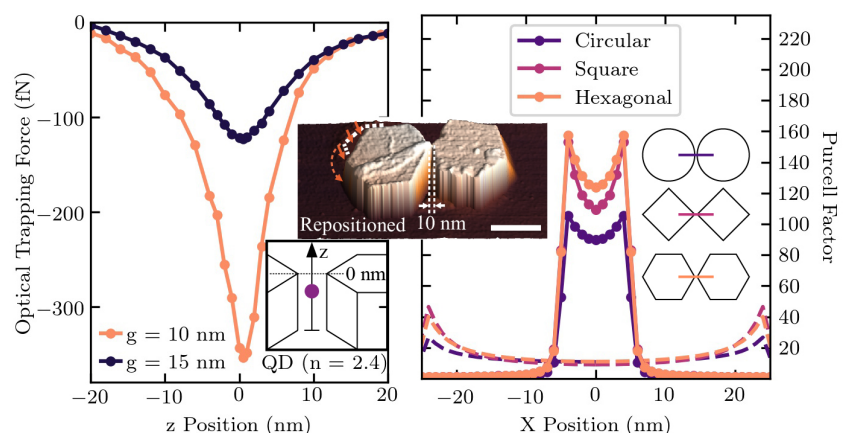


Figure 1: Simulations for a repositioned WS₂ hexagonal dimer nano-antenna. Left plot: Optical trapping force for a 10 nm QD translated across the z-axis in the middle of the dimer gap (g) for 10mW/μm pump intensity. Bottom right inset shows positions of QD. Right plot: Purcell factor for a SPE placed along the dimer axis 0.5 nm above the surface of nano-antennas with different geometries. Solid lines: g = 10 nm. Dashed lines: g = 50 nm. Right inset shows positions of SPE for different geometries. Inset middle: AFM scan of a repositioned WS₂ hexagonal dimer nano-antenna.



ABSTRACTS
ePOSTERS

Towards synthesis and characterization of heterogeneously doped graphene nanostructures

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ABSTRACT

Graphene and its nano-functionalization are hot research topic. Besides the promising mechanical and electronic properties of pristine graphene [1], various possibilities for the functionalization of graphene through e.g., structural defects, [2] such as vacancies and single atom impurities or chemical adsorption [3], are reported to enhance its the chemical activity and tune its electronic properties. Functionalized graphene is predicted to have potential applications as gas sensors [4] or nanoelectronics [5], serving as energy efficient conversion material or stable nanostructured semiconductors. Although various theoretical studies predict high potential of such materials [6], their synthesis remains challenging and effective extension to large-scale synthesis is missing. The direct incorporation of heteroatoms into the graphene mesh was extensively reported for B and N but, to our knowledge, only Ni [9], Pt and Au [7] metals were reported to replace a carbon atom in the honeycomb structure of graphene. Nevertheless, theoretical calculations predict that several transition metal single atoms can be used to tune the graphene properties, for example Co can be added to enhance its activity towards HER [8]. In this work we investigated a new route to produce by means of a potentially scalable method a single graphene layer where a sizable amount (few %) of single Co atoms are trapped in the mesh. The Co-doped layer is characterized by means of variable temperature scanning tunneling microscopy (STM), x-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED).

REFERENCES

- [1] Rodríguez-Pérez, L., et al., Chemical Communications 49.36 (2013): 3721-3735
- [2] Banhart, F., et al., ACS nano 5.1 (2011) 26-41
- [3] Liu, H., et al., Journal of Materials Chemistry 21.10 (2011) 3335-3345
- [4] Yang, S., et al., Appl. Phys. Rev. 4 (2017) 021304
- [5] Berger, C., et al., The Journal of Physical Chemistry B 108.52 (2004): 19912-19916
- [6] Krasheninnikov, A. V., et al., Physical Review Letters 102.12 (2009): 126807
- [7] Gan, Y., et al., Small 4, No. 5, (2008) 587–591
- [8] Qiu, H.-J., et al., Angew. Chem. Int. Ed. 54 (2015) 14031–14035

Graphene and Boron-doped Graphene by Pulsed Laser Deposition

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Among various physical vapor deposition (PVD) processes used to produce graphene as an alternative route to chemical vapor deposition (CVD) processes, pulsed laser deposition (PLD) is a versatile process to synthesize graphene materials, mainly for dopant incorporation in a controlled and reproducible way to modulate the graphene properties. By considering a short review on graphene synthesis by PLD [1-4], the present contribution is focused on the synthesis and characterization of few-layer graphene and boron doped-graphene films obtained by vacuum thermal heating (500-900°C) of thin amorphous carbon-based films (a-C, a-C:B) synthesized by PLD in the presence of a nickel catalyst. The growth mechanism is highlighted on the basis of *in situ* XPS investigations during graphene growth [5]. The film characteristics are discussed mainly in terms of layer nano-architecture, lateral homogeneity and boron chemistry, on the basis of Raman, XPS/AES and HRTEM/EELS investigations [6-7]. The effect of boron doping on graphene electronic or electrochemical properties is investigated. It will be shown that PLD can produce few-layer graphene (within 2-5 layers) with tunable electrochemical properties through an accurate control of the boron doping concentration [8].

REFERENCES

- [1] Y. Bleu, F. Bourquard, T. Tite, A.-S. Loir, C. Maddi, C. Donnet, F. Garrelie, *Frontier in Chemistry* 6 (2018) 572 (18 pp)
- [2] F. Bourquard, C. Donnet, F. Garrelie, A.-S. Loir, F. Vocanson, V. Barnier, C. Chaix, C. Farre, N. Jaffrezic-Renault, F. Lagarde, G. Raimondi, *Handbook of Graphene*, B. Palys (ed.), Scrivener Publishing LLC, Vol. 6 (2019) 483-508
- [3] Y. Bleu, F. Bourquard, A.-S. Loir, V. Barnier, F. Garrelie, C. Donnet, *J. of Raman Spect.* 50 (2019) 1630-1641
- [4] Y. Bleu, F. Bourquard, V. Gartiser, A.-S. Loir, B. Caja-Munoz, J. Avila, V. Barnier, F. Garrelie, C. Donnet, *Mat. Chem. Phys.* 238 (2019) 121905
- [5] Y. Bleu, V. Barnier, F. Christien, F. Bourquard, A.-S. Loir, F. Garrelie, C. Donnet, *Carbon* 155 (2019) 410-420
- [6] Y. Bleu, F. Bourquard, V. Barnier, Y. Lefkir, S. Reynaud, A.-S. Loir, F. Garrelie, C. Donnet, *Applied Surface Science* 513 (2020) 145843
- [7] Y. Bleu, F. Bourquard, J.-Y. Michalon, Y. Lefkir, S. Reynaud, A.-S. Loir, V. Barnier, F. Garrelie, C. Donnet, *Applied Surface Science*, in press, <https://doi.org/10.1016/j.apsusc.2021.149492>
- [8] Y. Bleu, F. Bourquard, C. Farre, C. Chaix, J. Galipaud, A.-S. Loir, V. Barnier, F. Garrelie, C. Donnet, *Diamond and Related Materials* 115 (2021) 108382

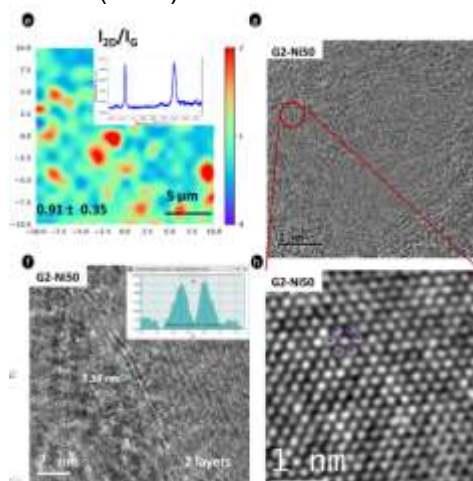


Figure 1: Raman and HRTEM images of as-synthesized graphene from PLD, using a 50 nm thick nickel catalyst film. From [7].

A simple model relating gauge factor to filler loading in nanocomposite strain sensors

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Piezoresistive polymer nanocomposites are typically filled with conductive nanomaterials such as graphene [1], carbon nanotubes [2] and other 2D materials [3]. These nanocomposites often display significant changes in resistance when deformed, and display sensitivities, or gauge factors, far beyond what is achievable with traditional metal foil strain gauges. This, coupled with a soft and flexible polymer matrix makes them ideal candidates as strain sensors in areas such as human health monitoring and robotics. However a challenge still remains in understanding the physical mechanisms underlying nanocomposite sensors and hence optimizing their performance. We have developed a simple model which yields equations for nanocomposite gauge factors as a function of both filler volume fraction and composite conductivity. These equations can be used to fit experimental data, outputting figures of merit, or predict experimental data once certain physical parameters are known. We have found these equations to match data, measured from our own experimental work and extracted from the literature, extremely well. Importantly, the model shows the response of composite strain sensors to be more complex than previously thought and shows factors other than the effect of strain on the interparticle resistance to be performance limiting [4].

REFERENCES

- [1] Boland et al., *Science* 2016, 354, 6317, 1257-1260
- [2] Hu et al., *Carbon* 2010, 48, 680 – 687
- [3] Bicca et al., *ACS Nano* 2019, 13 (6), 6845– 6855
- [4] J R Garcia et al., *ACS Appl. Nano Mater.* 2021, 4, 3, 2876–2886

FIGURES

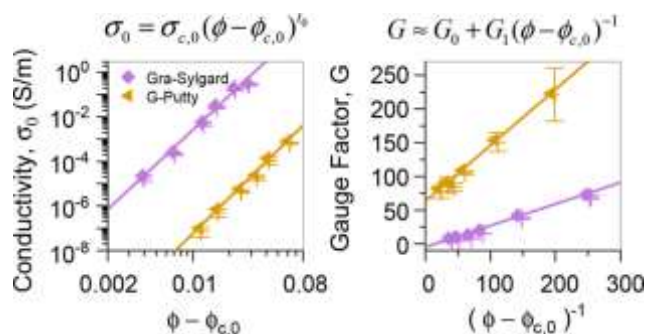


Figure 1: Percolation data and fits to graphene based polymer nanocomposites (Left). Gauge factor / Conductive filler data and model (Right).

Few-layered mesoporous graphene obtained through high energy dry ball-milling.

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Graphene-based materials (GBMs), such as graphene oxide (GO), few-layered graphene (FLG) or graphene nanoplatelets (GNPs), differ from graphene in physical and chemical properties and synthesis methods. Several techniques have been developed for a scalable and potential GBMs production since the yields obtained from the original tape method is reduced and limited to lab use. Although these techniques present their corresponding benefits and drawbacks, none of them has yet accomplished the large-scale production requirements [1].

In this work, we used a high energy dry ball-milling method to obtain few-layered mesoporous graphene (FLMG). We tested different milling conditions and times ranging from 20 to 300 minutes. FLMG was studied using XRD, SEM, TEM, UV-vis absorption and confocal Raman spectroscopy. The characterization revealed homogeneous nanoparticle size distributions with non-oxidized aggregations of few-layered graphene domains (for example, a mean value of 132(2) is obtained for the 100 min. sample). This top-down technique uses no additives or post-treatments, unlike wet ball-milling, making it low-cost, environmental-friendly, and suitable for large-scale production. The FLMG obtained by this method demonstrated an excellent performance as NO₂ sensing material [2]. Further applications such as electromagnetic shielding and polymer-based composite materials are worth exploring [3, 4].

REFERENCES

- [1] N. Kumar et al., FlatChem, 27 (2021) 100224
- [2] D. Matatagui et al., Sensors and Actuators: B. Chemical, 335 (2021) 129657
- [3] F. Meng, Composites Part B, 137 (2018) 260–277
- [4] V. B. Mohan et al., Composites Part B, 142 (2018) 200–220

FIGURES

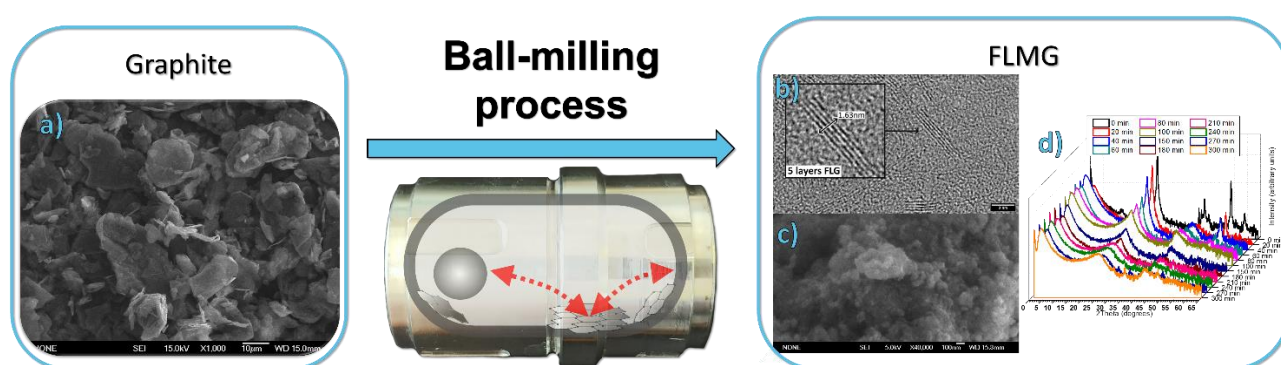


Figure 1: Representation of the ball-milling process including a) SEM image of the precursor, b) TEM and c) SEM images of the material obtained after 240 min of milling and d) XRD spectra showing the evolution of the materials crystallography with the milling time.

Diamane and diamanoids as new non-vdW 2D materials

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Diamane and diamanoid are promising new wide band-gap semiconducting materials for electronics, photonics and medical devices. Diamane was prepared from the exposure of bi-layer (2LG) graphene to H radicals produced by the hot-filament process at low pressure and low temperature [1,2]. A sharp sp^3 -bonded carbon stretching mode was observed in UV Raman spectra at around 1344 - 1367 cm^{-1} while no sp^2 -bonded carbon peak was simultaneously detected (Figure 1). By replacing 2LG with few-layer graphene (FLG), diamanoid/graphene hybrids were formed from the partial conversion of FLG [2,3]. Raman spectroscopy, electron diffraction and Density Functional Theory calculations show that partial conversion generates twisted 2LG located at the interface between the upper diamanoid domain and the non-converted graphenic domain underneath. C-H bonding in the basal plane of hydrogenated FLG, where carbon is bonded to a single hydrogen over an area of $150\text{ }\mu\text{m}^2$, is directly evidenced by Fourier Transform Infrared microscopy and possible full hydrogenation of diamane is supported by first principle calculations. The results are comprehensively discussed. They open the door to large-scale production of diamane, diamanoids and diamanoid/graphene hybrids, as new carbon 2D materials.

[1] F. Piazza, K. Cruz, M. Monthieux, P. Puech, I. Gerber, Carbon, 169 (2020) 129

[2] F. Piazza, M. Monthieux, P. Puech, I.C. Gerber, K. Gough, C, 7 (2021) 9

[3] F. Piazza, M. Monthieux, P. Puech, I.C. Gerber, Carbon, 156 (2020) 234

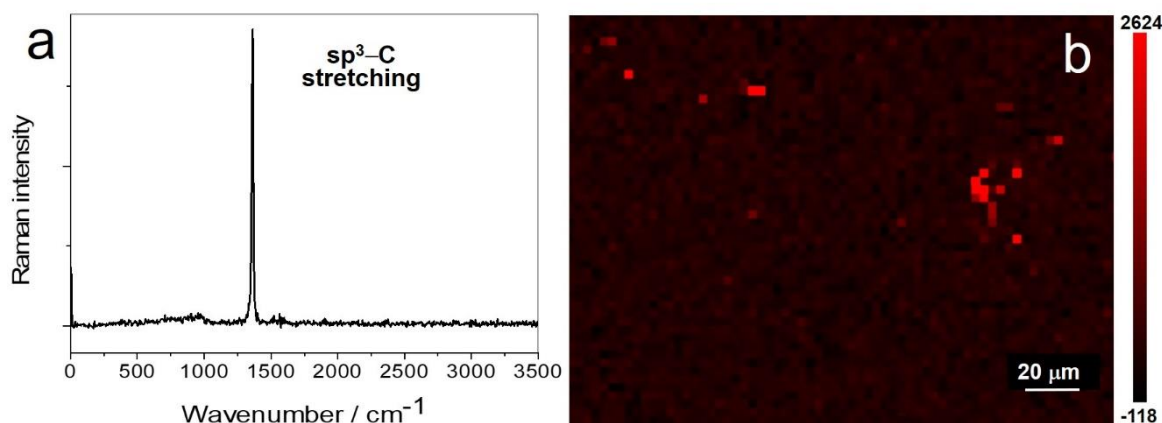


Figure 1. Typical UV Raman data for 2LG exposed to the hot-filament-promoted hydrogenation process. **(a)** Example of spectrum; **(b)** example of intensity map of the sp^3 -C stretching mode.



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