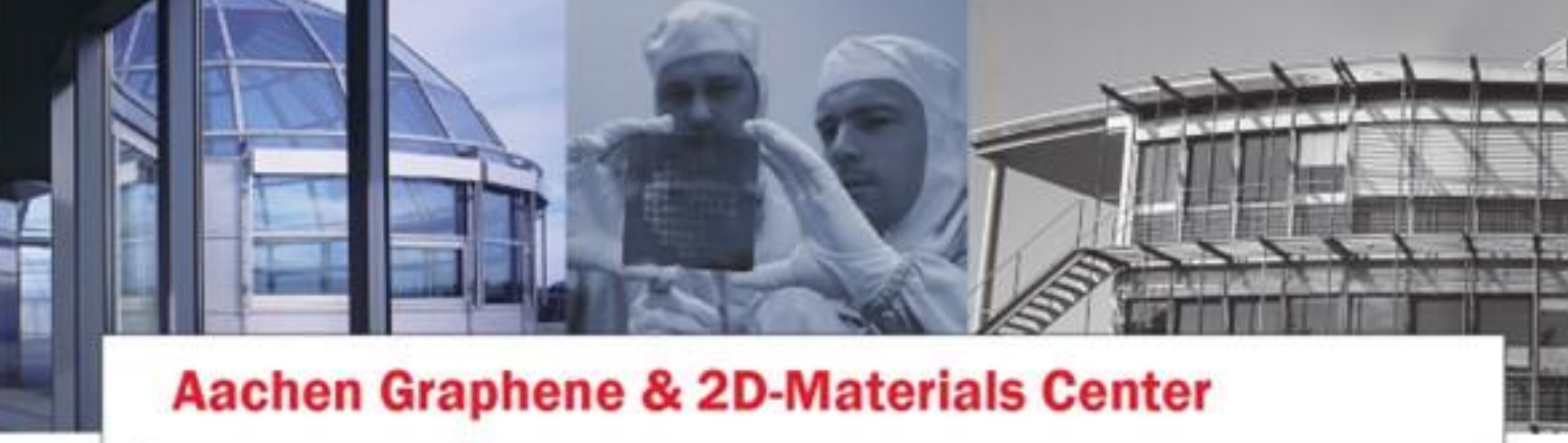
Graphene 2022

July 05 - 08

Aachen (Germany)

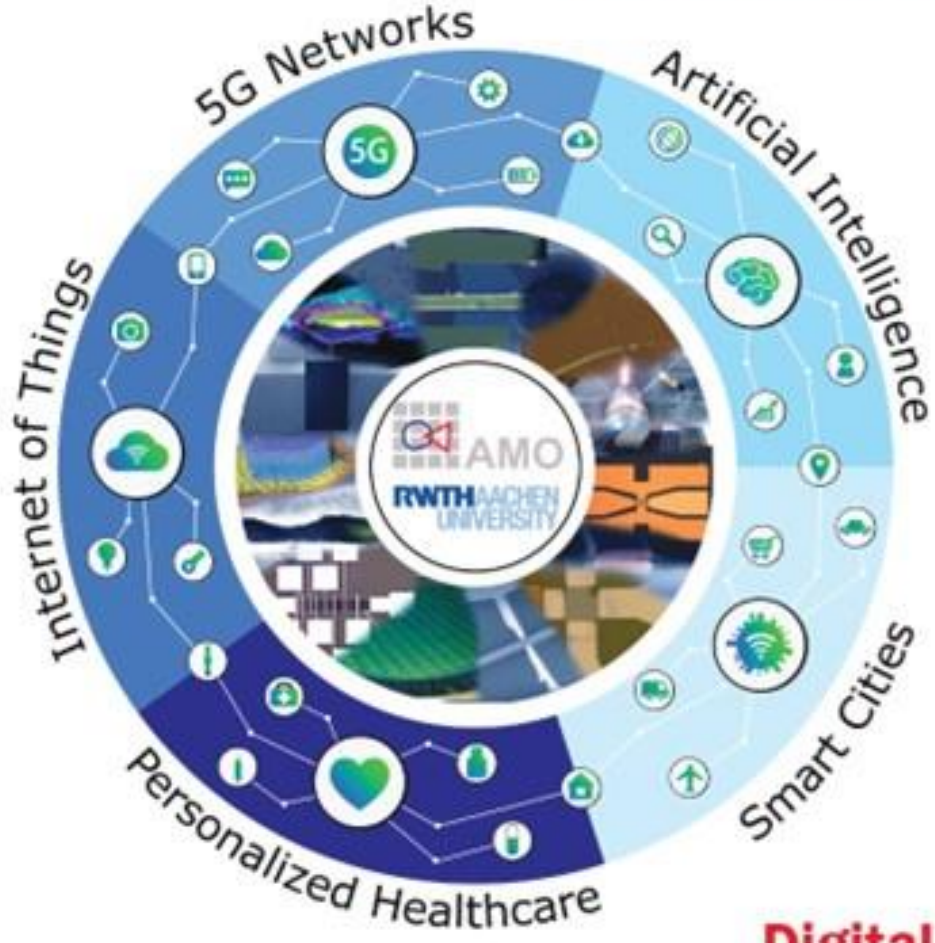
ORGANISERS PHANTOMS foundation ICN2 IDREA UCLouvain AMO TECHNISCHE UNIVERSITÄT DRESDEN RWTH AACHEN UNIVERSITY

PARTNERS GDR



Aachen Graphene & 2D-Materials Center

From basic research to innovation



Digital Hardware

- Electronics for neuromorphic computing
- Sensor technology for autonomous driving and IoT
- Optoelectronics for high speed data communication
- Electronics for wearables and implantables

AMO

AMO GmbH
Otto-Blumenthal-Straße 25 ▪ D-52074 Aachen ▪ Germany
Phone +49 241 88 67-125 ▪ Fax +49 241 88 67-571
services@amo.de ▪ www.amo.de

FOREWORD

On behalf of the Organising and the International Scientific Committees we take great pleasure in welcoming you to Aachen for the 12th in-person edition of the Graphene and 2D Materials International Conference & Exhibition (Graphene2022).
Over the past 11 editions, the Graphene Conference strengthened its position as one of the main meeting points of the Graphene community Worldwide. Graphene2022 is now an established event, attracting global participant's intent on sharing, exchanging and exploring new avenues of graphene-related scientific and commercial developments.

Graphene2022 Highlights:

- Expected attendance: 550 participants in-person
- 77 Plenary, Keynote & Invited Speakers
- More than 140 posters
- Nearly 170 oral contributions
- More than 30 Exhibitors
- 6 Parallel Workshops covering the whole value chain of "Graphene and 2D Materials innovation"
- 2-days Industrial Forum in parallel to get an updated understanding of Graphene based technologies from worldwide industries.

We are also indebted to the following Scientific Institutions, Companies and Government Agencies for their help and/or financial support:
AIXTRON, OXFORD Instruments, HORIBA Scientific, AMO GmbH, ULISSES, AEOLUS, RWTH Aachen University and GDR-I Graphene & CO – HOWDI.

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

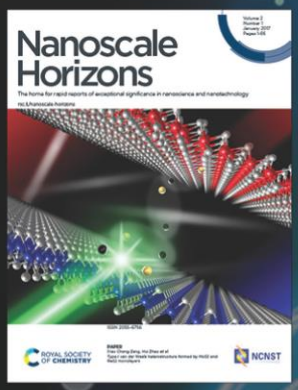
We truly hope that Graphene2022 serves as an international platform for communication between science and business.

Hope to see you again in the next edition of Graphene2023 to be held in Manchester (UK).

Graphene2022 Organising Committee

ROYAL SOCIETY OF CHEMISTRY

A home for all your nano research



Nanoscale Horizons

Extraordinary innovation in nanoscience and nanotechnology

Editorial Board Chair
Katharina Landfester Max Planck Institute for Polymer Research, Germany

Impact factor 2020: 10.989, median time to first decision (peer reviewed articles only): 34 days*

rsc.li/nanoscale-horizons

Nanoscale

At the core of the global nanoscience community

Editors-in-Chief

Chunli Bai Institute of Chemistry, Chinese Academy of Sciences, China
Dirk Guldi Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Impact factor 2020: 7.790, median time to first decision (peer reviewed articles only): 35 days*

rsc.li/nanoscale

Nanoscale Advances

Open developments in nanoscience and nanotechnology

Editors-in-Chief

Chunli Bai Institute of Chemistry, Chinese Academy of Sciences, China
Dirk Guldi Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Impact factor 2020: 4.553, median time to first decision (peer reviewed articles only): 30 days*

rsc.li/nanoscale-advances

Submit your work today

rsc.li/nano-science

Fundamental questions
Elemental answers

Visit rsc.li/metrics-explainer for more information
Registered charity number: 207890

INDEX

RamanFest Paris | FRANCE

www.ramanfestconf.com

September | 15-16, 2022

ORGANISERS

PHANTOMS foundation

HORIBA

PLENARY


Anne De Paepe


Andrea Ferrari

KEYNOTE


Silke Christiansen

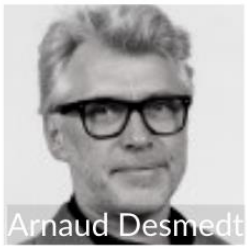

Thomas Nuytten


Hervé Rigneault

INVITED


Anthony Boulange


Marc Chaigneau

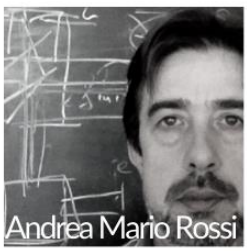

Arnaud Desmedt


Naresh Kumar


Van-Hoan Le


Alex Morata Garcia


Ioannis Paradisanos


Andrea Mario Rossi


Pierre-Yves Sacré


Iwan Schie


Ivan T. Lucas

MORE SPEAKERS

DEADLINES

ABSTRACT SUBMISSION ORAL REQUEST

JULY **15** 2022

EARLY BIRD REGISTRATION FEE

JULY **25** 2022

GENERAL INFO

Free WiFi

Ask for details at registration desks

Exhibition & Poster Area

Europa Hall

Coffee Breaks

Check the program for timetables
Location: Exhibition & Poster Area

Cocktail Lunch

Offered by Graphene2022 organisers
Tuesday July 05
Thursday July 07

Location: Exhibition & Poster Area

Conference Dinner*

Wednesday July 06, 19:30
Coronation Hall
Aachen Rathaus (Town Hall)
Markt
52062 Aachen

Posters Schedule

Session A: From Tuesday morning (July 05) to Wednesday (July 06) just after lunch. Topics: Advances in hBN growth, characterization and device integration / Chemistry of 2D materials / Composites for Energy applications / Devices for Electronic Applications (flexible displays, high frequency devices, sensors, etc...) / Quantum transport, magnetism and spintronics

Session B: From Wednesday (July 06) just after lunch to Thursday (July 07) end of the day. Topics: Health and Medical Applications / Photonics and Plasmonics / Growth, synthesis techniques and integration methods / Spectroscopies (Optics, Raman, EELS) and microscopies (HRTEM, STM, AFM) / Theory and Simulation / Topological and Exotic Physics in van Der Waals Heterostructures

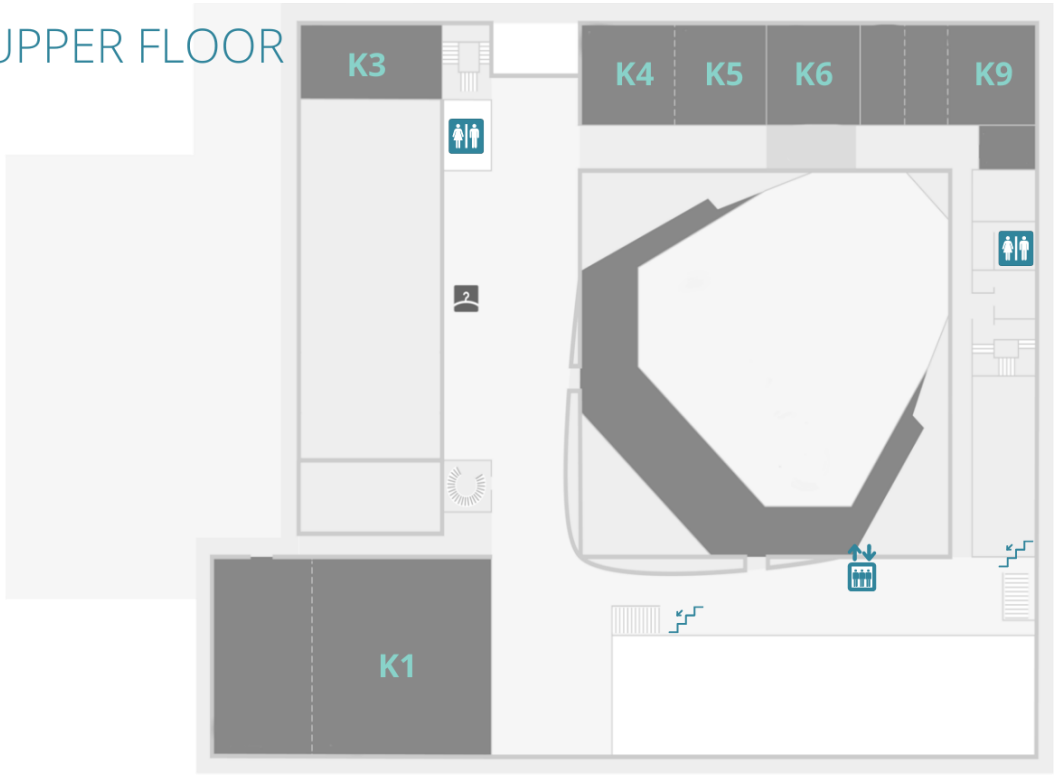
* Conference dinner NOT included in Exhibition and Industrial Forum Passes. Included only in FULL conference passes.
If you wish to attend, contact the organisers at the registration desks.

Scan the QR for Graphene 2022 PROGRAM

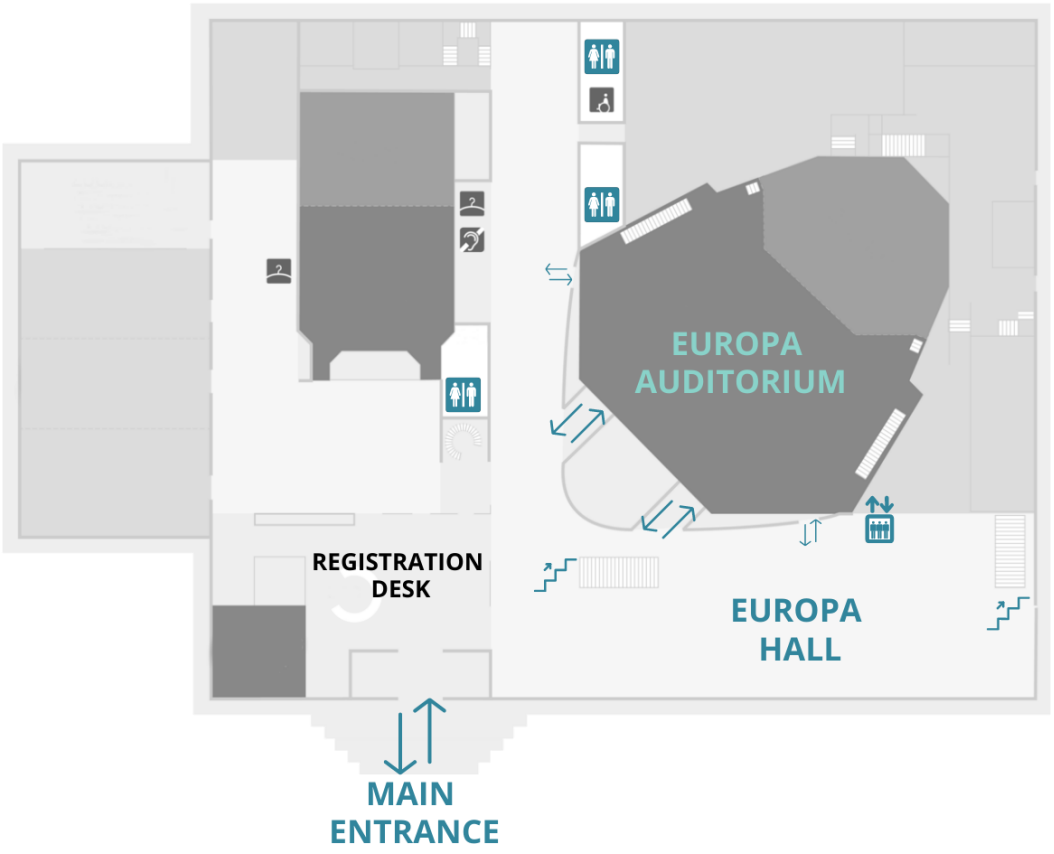
www.grapheneconf.com/Files/Graphene2022_Program.pdf

LOCATION

UPPER FLOOR



GROUND FLOOR



AGENDA & LOCATION**

Tuesday – July 05	Room	Time
Graphene2022 Plenary Session	Europa Auditorium	08:45 - 18:30
Exhibition & Poster Sessions	Europa Hall	-
Cocktail Lunch (offered by the organisers) - Poster session - Exhibition	Europa Hall	13:00 - 14:30
Wednesday – July 06	**Room**	**Time**
Workshop 1: Twistronics and Topological Phenomena	K3	09:00 - 16:15
Workshop 2: 2D Materials for Quantum Technologies	K6	09:00 - 12:15
Workshop 3: Chemistry of 2D Materials & Energy	K9	09:00 - 18:15
Workshop 4: Theory of 2D Materials and Devices Simulation	K4	09:00 - 18:15
Workshop 5: 2D Materials for Health & Medical Applications	K6	14:00 - 16:15
Workshop 6: Advanced Characterization of 2DM and Heterostructures	K5	09:00 - 17:45
Industrial Forum	K1	09:00 - 18:30
Exhibition & Poster Sessions	Europa Hall	-
Conference dinner	Coronation Hall	19:30
Thursday – July 07	**Room**	**Time**
Graphene2022 Plenary Session	Europa Auditorium	09:00 - 13:00
Parallel Session PhD Students Track 1	K3	14:30 - 16:40
Parallel Session PhD Students Track 2	K6	14:30 - 16:40
Parallel Session PhD Students Track 3	K9	14:30 - 16:40
Parallel Session Orals Track 4	K4	14:30 - 16:50
Parallel Session Orals Track 5	K5	14:30 - 16:50
Industrial Forum	K1	09:00 - 18:30
Graphene2022 Plenary Session	Europa Auditorium	17:15 – 18:30
Exhibition & Poster Sessions	Europa Hall	-
Cocktail Lunch (offered by the organisers) - Poster Session - Exhibition	Europa Hall	13:00 - 14:30
Friday – July 08	**Room**	**Time**
Graphene2021 Plenary Session	Europa Auditorium	09:00 - 13:30
Poster Awards Ceremony	Europa Auditorium	To be announced

** Rooms & time table subject to change

Share with us your vision of the conference.
Post your photos and comments
#Grapheneconf

@GrapheneConf

PLENARY SPEAKERS

- **Andrea Ferrari** (CGC, University of Cambridge, UK)
- **Yury Gogotsi** (Drexel University, USA)

KEYNOTE SPEAKERS

- **Jordi Arbiol** (ICREA / ICN2, Spain)
- **Adrian Bachtold** (ICFO, Spain)
- **Larysa Baraban** (HZDR, Germany)
- **Cinzia Casiraghi** (University of Manchester, UK)
- **Gianni Ciofani** (IIT,Italy)
- **Lucia Gemma Delogu** (University of Padua, Italy)
- **Vladimir Falko** (NGI, University of Manchester, UK)
- **Coskun Kocabas** (University of Manchester, UK)
- **Elena Martínez Fraiz** (IBEC, Spain)
- **Rodrigo Martins** (NOVA University Lisbon, Portuga)
- **Virgilio Mattoli** (IIT, Italy)
- **Mariana Medina Sánchez** (IFW Dresden, Germany)
- **Pablo Orejón** (ICN2, Spain)
- **Michal Otyepka** (CATRIN, Czech Republic)
- **Sibel Ayþýl Özkan** (Ankara University, Turkey)
- **Janez Plavec** (NIC/NMR, Slovenia)
- **Kevin Plaxco** (UC Santa Barbara, USA)
- **Beatriz Prieto-Simon** (ICREA/URV, Spain)
- **Daniel Ruiz-Molina** (ICN2-CSIC, Spain)
- **Oliver Schmidt** (TU Chemnitz, Germany)
- **Carsten Sönnichsen** (University of Mainz, Germany)
- **Clivia Sotomayor** (ICN2, Spain)
- **Klaas-Jan Tielrooij** (ICN2, Spain)
- **Sergio O. Valenzuela** (ICREA / ICN2, Spain)

CALL FOR ABSTRACTS

ABSTRACT SUB.
ORAL REQUEST
JULY **15**
2022

EXHIBITION & SPONSORSHIP OPPORTUNITIES

36 KEYNOTE & INVITED SPEAKERS CONFIRMED

ORGANISERS

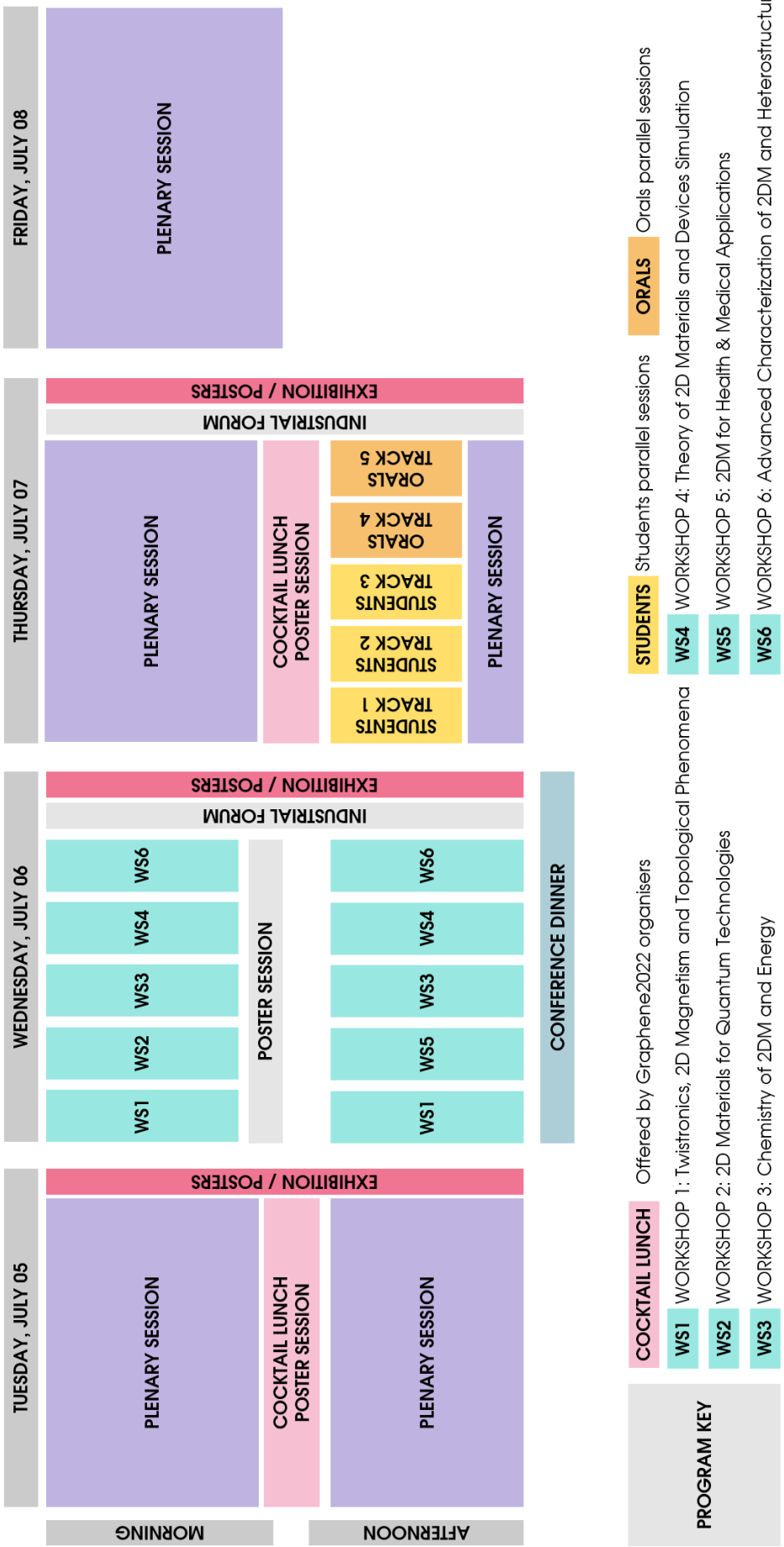
PHANTOMS foundation

ICN2 Institut Català de Nanociència i Nanotecnologia

LOCAL ORGANISERS

NanoAlb

PROGRAM AT A GLANCE



COMMITTEES

	Organising Committee
Phantoms Foundation (Spain)	**Chairperson: Antonio Correia**
Bedimensional (Italy)	**Francesco Bonaccorso**
Université Catholique de Louvain (Belgium)	**Jean-Christophe Charlier**
TU Dresden (Germany)	**Xinliang Feng**
AMO GmbH / RWTH Aachen (Germany)	**Max Lemme**
ICREA/ICN2 (Spain)	**Stephan Roche**
	Local Organising Committee
RWTH Aachen (Germany)	**Julia Floehr**
AMO GmbH (Germany)	**Federica Haupt**
AIXTRON (Germany)	**Michael Heuken**
AMO GmbH (Germany)	**Michael Hornung**
AMO GmbH (Germany)	**Herbert Kleinjans**
AMO GmbH (Germany)	**Maike Mayer-Amjadi**
University of Wuppertal (Germany)	**Daniel Neumaier**
AMO GmbH (Germany)	**Birgit Teschner**
	International Scientific Committee
The University of Manchester / NGI (UK)	**Chairperson: Vladimir Falko**
RWTH (Germany)	**Co-chairperson: Christoph Stampfer**
Yonsei University (South Korea)	**Jong-Hyun Ahn**
CFM (CSIC-UPV/EHU) (Spain)	**Sara Barja**
Universidade Franciscana (Brazil)	**Solange Binotto Fagan**
KAIST (South Korea)	**Sung-Yool Choi**
CNRS (France)	**Alessandro Cresti**
University of Rome "Tor Vergata" (Italy)	**Aldo Di Carlo**
University of Chile (Chile)	**Luis Foa-Torres**
FORTH/ ICE-HT and University of Patras (Greece)	**Costas Galiotis**
TU Wien (Austria)	**Tibor Grasser**
DTU (Denmark)	**Antti-Pekka Jauho**
Universidade Federal de Minas Gerais (Brazil)	**Ado Jorio**
Aalto University (Finland)	**José Lado**
Ohio State University (USA)	**Jeanie Lau**
ONERA (France)	**Annick Loiseau**
IMM-CNR (Italy)	**Vittorio Morandi**
NIMS (Japan)	**Shu Nakaharai**
University of Wuppertal (Germany)	**Daniel Neumaier**
Tohoku University (Japan)	**Taiichi Otsuji**
Warsaw University of Technology (Poland)	**Iwona Pasternak**
University of California Santa Cruz (USA)	**Yuan Ping**
ENS/CNR (France)	**Bernard Plaçais**
Université Paris Saclay (France)	**Rebeca Ribeiro-Palau**
University of Chemnitz (Germany)	**Thomas Seyller**
ENS Paris (France)	**Christophe Voisin**
KAIST (South Korea)	**Young-Woo Son**
University Münster (Germany)	**Ursula Wurstbauer**
	Industrial International Committee (I2C)
The University of Texas at Dallas (USA)	**Chairperson: Luigi Colombo**
AMO GmbH (Germany)	**Co-chairperson: Max Lemme**
Bedimensional (Italy)	**Francesco Bonaccorso**
BGI (China)	**Yunqiao Fu**
TUDresden / Sixonia (Germany)	**Martin Lohe**
CGIA (China)	**Minyang Lu**
AIXTRON (UK)	**Oliver Whear**

SPONSORS

Diamond Sponsor

AIXTRON

www.aixtron.com

The AIXTRON Group is a leading provider of deposition equipment to the semiconductor industry. The Company was founded in 1983 and is headquartered in Herzogenrath (Aachen City Region), Germany, with subsidiaries and representative offices in Asia, the USA, and Europe. The company's products are used worldwide by a wide range of customers to manufacture high-performance components for electronic and optoelectronic applications based on compound or organic semiconductor materials. These components are used in a variety of innovative applications, technologies and industries. These include, for example, LED and display technology, data transmission, sensor technology, energy management and conversion, communication, signal and lighting technology, and many other sophisticated high-tech applications.

Platinum Sponsor

https://plasma.oxinst.com

Oxford Instruments develops, delivers, and supports high-technology tools and systems with a focus on research and industrial applications. Innovation has been the driving force behind Oxford Instruments' growth and success for 60 years, supporting its core purpose of addressing some of the world's most pressing challenges. Our market-leading atomic-level fabrication solutions provide reproducible and scalable process layers that enable the integration of graphene in electronics, optoelectronics and sensors. The wide range of Oxford Instruments Plasma Technology includes high-temperature chemical vapor deposition of 2D materials, dielectrics integration and encapsulation, device pattern etching, atomic layer etching, low-temperature atomic layer deposition and more. Through the product lines of WITec GmbH and Asylum Research, the Oxford Instruments Group also supplies leading-edge nanoanalysis and nanomanipulation capabilities that are ideally suited to 2D materials research. WITec's Raman imaging and correlative microscopes can chemically characterise graphene samples and visualise layer number, strain, doping and defects, while Asylum's atomic force microscopes can investigate film quality and determine electrical and mechanical properties simultaneously with topography at sub-angstrom resolution.

Gold Sponsor

www.horiba.com

The HORIBA Group of worldwide companies provides an extensive array of instruments and systems for applications ranging from automotive R&D, process and environmental monitoring, in-vitro medical diagnostics, semiconductor manufacturing and metrology, to a broad range of scientific R&D and QC measurements. Proven quality and trustworthy performance have established widespread confidence in the HORIBA Brand.

Silver Sponsors

www.amo.de

AMO's mission as a non-profit SME is to bridge the gap between university research and industrial application. In joint projects and in bilateral cooperation, research and development results are transferred to industry for the preservation and creation of jobs. The potential of nanotechnology is thus tapped in fields of application such as information technology, biotechnology and environmental technology. AMO operates a state-of-the-art 400 m² clean room under the direction of Prof. Lemme and offers a rang of services from consulting to prototype development.

Silver Sponsors

www.ulisses-project.eu

ULISSES will develop an integrated optical gas sensor and the networking technology required to bring it onto the Internet of Things (IoT). ULISSES will deliver the wafer-scale mass production methods necessary to enable production volumes of millions of sensors per year, and thus provide an order of magnitude reduction of sensor module cost.

https://aeolusproject.eu/

AEOLUS aims to be the first to provide a field-tested holistic air quality solution that is affordable, cloud-connected and 'smart' as well as facilitating and encouraging citizen engagement and its widespread deployment into our communities, to meet the needs of Smart City applications and ultimately pave the way to affect necessary changes in our lives.

www.thermofisher.com

Thermo Fisher Scientific produces a wide range of instruments for materials analysis. Our range of X-ray photoelectron spectroscopy instruments are designed to deliver high quality results, quickly and easily. Systems can be configured with other surface analysis and materials analysis techniques, including Raman spectroscopy to enable maximum understanding with minimum effort. Contact us to learn about our surface analysis products, and the huge range of other instrumentation for materials science, including electron microscopy and molecular spectroscopy.

Other Sponsor

www.rwth-aachen.de

RWTH Aachen University is one of the leading universities of technology in Germany with a tradition dating back to 1870 when it was founded as an institution to provide technological innovation. The university is divided into 9 faculties and approximately 45,000 students are enrolled in more than 150 courses of study. The number of foreign students (~10,000) substantiates the university's international orientation. Every year about 7,000 graduates and doctoral graduates leave the university. Approximately 500 professors work at RWTH Aachen University and the university budget amounts to more than 900 million Euros of which about 350 million Euros are third-party expenditures. RWTH Aachen is also participating in the IDEA League, a network of the leading Universities of Technology in Europe, which defines standards for degree programs and academic.

PhD Grants Sponsor

http://gdr-howdi.org/

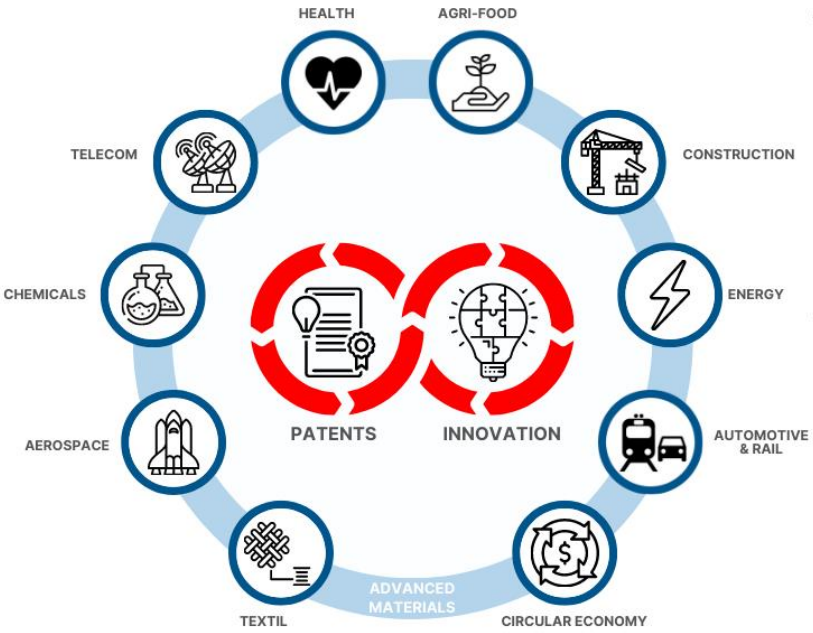
The "HOWDI" research group: Van der Waals hetero-structures of low dimensionality "is both a national research group (GDR 2112) and an international coordination network (IRN" Graphene and co). The ambition of the GDR is to bring together and interact with teams interested in the study of all the physical properties that emerge from these van der Waals assemblies.

Awards Sponsors

P4I PATENTS for INNOVATION

October 26-27, 2022 • Madrid (Spain)

International Summit & Expo



The 1st edition of the "Patents for Innovation" International Summit & Expo (P4I 2022) aims to become the largest European meeting point in Innovation and Tech Transfer.
P4I 2022 is born as a forum for technological innovation and also as a patent fair, thus allowing the creation of a market for the transfer of research results and the purchase and sale of scientific patents.

BECOME A **SPONSOR EXHIBITOR**

Universidad Autónoma de Madrid
PHANTOMS foundation
BeAble CAPITAL
Madrid K·node knowledge-based innovation ecosystem

@P4Iexpo
p4iexpo.com

EXHIBITORS


AIXTRON

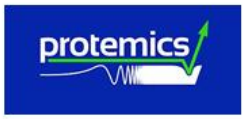

OXFORD
INSTRUMENTS


HORIBA
Scientific


NanoLockin
ADVANCED THERMAL IMAGING


LAYTEC
MEMBER OF THE NYNOMIC GROUP


attocube
WITTENSTEIN Group


protemics


AMO


HEIDELBERG
INSTRUMENTS
The power of direct writing


BRUKER


Grapheal


ANL
Applied Nanolayers


SPECS™


EDINBURGH
INSTRUMENTS


hq graphene


GRAPHENE
LAYERS


ICN2
Institut Català
de Nanociència
i Nanotecnologia


ACCURION


Park
SYSTEMS


FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA


2D-MAT-NET
Network to establish new value chains
based on 2D materials
www.2dmatnet.uni-jena.de/en/


AMO
tronics


nb technologies
consulting engineers


SIEGERT WAFER
Wafer Specialist


microlight3D


micro resist
technology


LayerOne
Advanced Materials


BE DIMENSIONAL


iit
GRAPHENE
ISTITUTO ITALIANO
DI TECNOLOGIA


ANNEALSYS
IN SEARCH OF EXCELLENCE


Ra


BeeGraphene


ThermoFisher
SCIENTIFIC

SKEAKERS LIST

Proton Transport through 2D Crystals

Andre K Geim
University of Manchester, United Kingdom
geim@manchester.ac.uk

I shall review our group's ongoing work [1-4] on proton transport through graphene and other two-dimensional materials, focusing on fundamental aspects of this phenomenon but also discussing possible applications including those in fuel cells, hydrogen production, hydrogen-isotope separation, etc.

References

[1] S. Hu et al. Proton transport through one-atom-thick crystals. Nature 516 (2014) 227-230
[2] M. Lozada-Hidalgo et al. Sieving hydrogen isotopes through two-dimensional crystals. Science 351 (2016) 68-70
[3] L. Mogg et al. Atomically thin micas as proton-conducting membranes. Nature Nano 14 (2019) 962-966
[4] P. Z. Sun et al. Limits on gas impermeability of graphene. Nature 579 (2020) 229-232

The Magic of Moiré Quantum Matter

Pablo Jarillo-Herrero
MIT, USA
pablodjh@gmail.com

The understanding of strongly-correlated quantum matter has challenged physicists for decades. The discovery four years ago of correlated phases and superconductivity in magic angle twisted bilayer graphene has led to the emergence of a new materials platform to investigate strongly correlated physics, namely moiré quantum matter. These systems exhibit a plethora of quantum phases, such as correlated insulators, superconductivity, magnetism, Chern insulators, and more. In this talk I will review some of the recent advances in the field, focusing on the newest generation of moiré quantum systems, where correlated physics, superconductivity, and other fascinating phases can be studied with unprecedented tunability. I will end the talk with an outlook of some exciting directions in this emerging field.

Advances in Organic 2D Crystals

Xinliang Feng
Center for Advancing Electronics Dresden & Faculty of Chemistry and Food Chemistry, Technische Universitaet Dresden; Max Planck Institute of Microstructure Physics, Germany
Xinliang.feng@tu-dresden.de

Abstract

In contrast to the tremendous efforts dedicated to the exploration of graphene and inorganic 2D crystals such as metal dichalcogenides, boron nitride, black phosphorus, metal oxides, and nitrides, there has been much less development in organic 2D crystalline materials, including the bottom-up organic/polymer synthesis of graphene nanoribbons, 2D metal-organic frameworks, 2D polymers/supramolecular polymers, as well as the supramolecular approach to 2D organic nanostructures. One of the central chemical challenges is to realize a controlled polymerization in two distinct dimensions under thermodynamic/kinetic control in solution and at the surface/interface. In this talk, we will present our recent efforts in bottom-up synthetic approaches towards novel organic 2D crystals with structural control at the atomic/molecular level and beyond. On-water surface synthesis represents a powerful synthetic platform. We will introduce a surfactant-monolayer assisted interfacial synthesis (SMAIS) method that is highly efficient to promote programmable assembly of precursor monomers on the water surface and subsequent 2D polymerization in a controlled manner. 2D conjugated polymers and coordination polymers belong to such materials classes. The unique 2D crystal structures with possible tailoring of conjugated building blocks and conjugation lengths, tunable pore sizes and thicknesses, as well as impressive electronic structures, make them highly promising for a range of applications in electronics, optoelectronics and spintronics. Other physicochemical phenomenon and application potential of organic 2D crystals, such as in membranes, will also be discussed.

Opportunities and Challenges of Graphene Neurotechnology in Neuroscience and Medical Applications

Jose A Garrido
Catalan Institute of Nanoscience and Nanotechnology, (ICN2), CSIC and BIST, Barcelona, Spain
ICREA, Barcelona, Spain
joseantonio.garrido@icn2.cat

Establishing a reliable bidirectional communication interface between the nervous system and electronic devices is crucial for exploiting the full potential of neurotechnology. Despite recent advancements, current technologies evidence important shortcomings, e.g. challenging high density integration of sensors, low signal-to-noise ratio, etc. Thus, efforts to explore novel materials are essential for the development of next-generation neural interfaces. Graphene and graphene-based materials possess a very attractive set of physicochemical properties holding great potential for biomedical applications, in particular for implantable neural interfaces. This presentation provides an overview on fundamentals and applications of several graphene-based technologies and devices aiming at developing an efficient bidirectional communication with the nervous system. The main goal of this talk is to discuss opportunities of graphene-based neurotechnologies in neuroscience and implantable medical applications, and at the same time to identify the main challenges ahead.

MXenes Expand the Range of 2D Materials for Electronics, Optics and Communication Beyond Graphene

Yury Gogotsi
A.J. Drexel Nanomaterials Institute, and Department of Materials Science and Engineering,
Drexel University, Philadelphia, PA 19104, USA
gogotsi@drexel.edu

Discovery of new materials provides moments of inspiration and shifts in understanding, shaping the dynamic field of materials science. Following the graphene breakthrough, many other 2D materials emerged. Although many of them remain subjects of purely academic interest, others have jumped into the limelight due to their attractive properties, which have led to practical applications. Among the latter are 2D carbides and nitrides of transition metals known as MXenes [1]. The family of MXenes has been expanding rapidly since the discovery of Ti_3C_2 in 2011 [2]. More than 30 different stoichiometric MXenes have been reported, and the structure and properties of numerous other MXenes have been predicted. Moreover, the availability of solid solutions on M and X sites, multi-element high-entropy MXenes, control of surface terminations, and the discovery of out-of-plane ordered double-M *o*-MXenes (e.g., Mo_2TiC_2), as well as in-plane ordered *i*-MAX phases and their *i*-MXenes offer a potential for producing dozens of new distinct structures. This presentation will describe the state of the art in the manufacturing of MXenes, their delamination into single-layer 2D flakes and assembly into films, fibers and 3D structures. Synthesis-structure-properties relations of MXenes will be addressed on the example of Ti_3C_2. The versatile chemistry of the MXene family renders their properties tunable for a large variety of applications. In particular, the interaction of MXenes with electromagnetic waves can be controlled via their composition and structure. Many MXenes offer high electronic conductivity and outstanding electromagnetic interference shielding. They can also be used in telecommunication, energy, medical and electronic device applications.

References

1. A. VahidMohammadi, J. Rosen, Y. Gogotsi, The World of Two-Dimensional Carbides and Nitrides (MXenes), *Science*, 372, eabf1581 (2021)
2. M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J.-J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum, Two-Dimensional Nanocrystals Produced by Exfoliation of Ti_3AlC_2, *Advanced Materials*, 23, 4248-4253 (2011)
3. X. Li, Z. Huang, C. E. Shuck, G. Liang, Y. Gogotsi, C. Zhi, MXene chemistry, electrochemistry, and energy storage applications, *Nature Reviews Chemistry*, (2022)

Figures

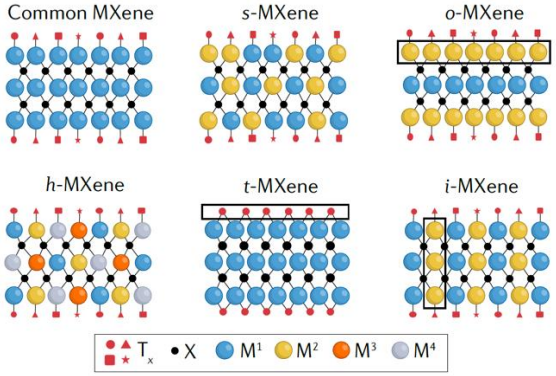


Figure 1. Six key types of MXenes (side view): common MXenes with identical M and hybrid T_x; random solid-solution MXenes (s-MXene) with hybrid M and T_x; out-of-plane ordered MXenes (o-MXene) with hybrid M and T_x; in-plane ordered MXenes (i-MXene) with hybrid M and T_x; isostoichiometric MXenes (t-MXene) with identical M and T_x; high-entropy MXenes with
many M elements (h-MXene).

Visualizing Electron Localization and Minibands in Moiré Superlattices

Alessandra Lanzara
University of California, Berkeley, USA
alanzara@lbl.gov

The ability to engineer flattened electronic bands by controlling interlayer effects in moiré superlattices of two-dimensional materials has opened the door for material physicists to understand and control correlated electron phenomena in an unprecedentedly broad class of materials. In this talk I will present our work on different van der Waals heterostructure, from graphene to the heterobilayer WS¬2/WSe2 family to study the evolution of the electronic structure from weakly interacting regime to strongly localized regime by using angle resolved photoemission spectroscopy with spatial resolution. I will discuss how correlation develops and its effect on the band structure and electron self-energy as well as the significant role of interlayer physics and hybridization in driving electron localization.

2D Materials: The Critical Infrastructure for the Future of Technology

Tomás Palacios
Massachusetts Institute of Technology
77 Massachusetts Ave, Bldg. 39-567, Cambridge, MA 02139, USA
tpalacios@mit.edu

The recent shortage of semiconductor chips has highlighted the critical role that semiconductors play in the world. We are at the most exciting (and challenging) time for microelectronics, the engine that powers modern society, in its entire history. Applications ranging from electric vehicles to security, high performance computing and advanced medical devices all rely of relentless improvements in semiconductor device performance. The performance of silicon-based electronics is however saturating as Si reaches its intrinsic scaling limit. Fortunately, two-dimensional materials are quickly maturing, and getting ready to take the baton. This talk will describe recent work our group at MIT has done to improve the performance of Silicon microchips by leveraging the unique properties of single-layer transition metal dichalcogenides (TMD). In particular, we will discuss the growth and integration technology of TMD materials and devices at the back-end-of-the-line of silicon technology, and its huge impact on the future of microsystems.

Gaining control over liquid-exfoliated nanosheets and their networks

Claudia Backes
Physical Chemistry of Nanomaterials and CINSaT, University of Kassel, Heinrich Plett Str. 40, 34132 Kassel
backes@uni-kassel.de

Liquid phase exfoliation (LPE) has become an important production technique giving access to single and few-layered nanosheets in colloidal dispersion. It has been shown to be applicable to a whole host of inorganic crystals with the nanosheet morphology being defined by the in plane and out of plane binding strength in the parent crystal.[1] In addition to layered inorganic crystals, organic materials such as 2D polymers,[2] metal organic frameworks[3] or even organic molecular crystals such as rubrene[4] can be exfoliated this way continuously increasing the palette of available materials. While size selection by centrifugation can be used to gain control over nanosheet size and thickness distributions, it is still challenging to fabricate nanosheet networks of high optical quality where the properties of the individual constituents are retained.
Here, we show progress in the deposition of nanosheets after preassembly at the liquid-liquid interface through a Langmuir-Schaefer type technique. In contrast to deposition by spraying or printing which produces porous networks, the nanosheets are well aligned parallel to the substrate. Due to the minimal overlap between the sheets, optical properties such as fluorescence of monolayer transition metal dichalcogenides is retained in the film. Subsequent stacking, also of different types of nanosheets is feasible, giving rise to the possibility to build up thicker films or heterostructures. We show the potential of this strategy by embedding WS_2 nanosheets in optical microcavities and the observation of the formation of exciton polaritons.
Further, we explore possibilities to further control the nanosheet dimensions by chemical means. Particular emphasis is given to increasing the length thickness aspect ratio. Following our work on site selective oxidation of WS_2 nanosheets in the presence of certain surfactants,[5,6] we now show that reaction parameters for MoS_2 can be tuned in such a way to achieve selective destruction of few-layers over monolayers resulting in increased length/thickness aspect ratio of the mono-layered constituents.

References

[1] *ACS Nano* **2019**, 13 (6), 7050-7061.
[2] *Angew. Chem. Int. Edit*. **2020**, *59*, 5683 –5695
[3] J. Gosch, K. Synnatschke, N. Stock, C. Backes, *Chem. Commun.* **2022**, submitted.
[4] *ACS Nano* **2021**, 15 (12) 20466-20477.
[5] *Angew Chem Int Edit* **2020,** *59* (33), 13785-13792.
[6] *Adv. Mater.* **2021,** *33* (42), 2102883.

Water-based, defect-free and biocompatible 2D material inks enabled by supramolecular chemistry

Cinzia Casiraghi
Department of Chemistry, University of Manchester, Oxford Road, Manchester, UK
cinzia.casiraghi@manchester.ac.uk

Solution processing of 2D materials [1] allows simple and low-cost techniques, such as ink-jet printing, to be used for fabrication of heterostructure-based devices of arbitrary complexity. Our group has developed highly concentrated, defect-free, inkjet printable and water-based 2D crystal formulations, by exploiting non-covalent functionalization of 2D materials with pyrene derivatives [2]. Examples of printed heterostructures, such as arrays of photosensors, programmable logic memories, capacitors and transistors will be discussed [3-5]. Furthermore, inkjet printing can be easily combined with materials produced by chemical vapor deposition, allowing simple and quick fabrication of complex circuits on paper, compatible with CMOS technology [6-7]. Finally, I will show that the use of pyrene derivatives as supramolecular receptors enables to easily tune the surface chemistry of the material making it suitable for biomedical applications [8-9] and gas sensing.

References

[1] Coleman et al, Science 331, 568 (2011)
[2] Xu et al, Nanoscale 13, 460 (2021)
[3] McManus et al, Nature Nano, 12, 343 (2017)
[4] Worsley et al, ACS Nano, 2018, DOI: 10.1021/acsnano.8b06464
[5] Lu et al, ACS Nano, 13, 11263 (2019)
[6] Conti et al, Nature comms, 11 (1), 1-9 (2020)
[7] Brunetti et al, npj 2D Materials and Applications 5, 1-6 (2021)
[8] Shin et al, Faraday Discussion, 2021, https://doi.org/10.1039/C9FD00114J
[9] Shin et al, Nanoscale, 2020, DOI: 10.1039/D0NR02689A

Synthesizing high-quality 2D materials and (twisted) heterostacks: from surface science to industrial applications

Camilla Coletti
Center for Nanotechnology Innovation @ NEST and Graphene Labs, Istituto Italiano di Tecnologia, P56127 Pisa, Italy
Camilla.coletti@iit.it

To make graphene appealing for several applications at high technology readiness levels, requirements such as high-quality, scalability and contamination control have to be satisfied. In this talk, I will present our approaches in this direction and how we adopt surface science to impact technology of 2D materials. I will present wafer-scale growth approaches of high-quality graphene via chemical vapor deposition (CVD) [1,2] and show how this material can be integrated on existing photonic platforms [3,4]. Furthermore, I will present results on the field of twistronics - such as large and small angle twisted bilayer CVD graphene [5,6] - and I will discuss heterostacks containing 2D gold and 1T'-MoTe2 [7,8], exciting playgrounds for fundamental studies.

References

1. V. Miseikis, F. Bianco, J. David, M. Gemmi, V. Pellegrini, M. Romagnoli, C. Coletti, 2D Materials 4 (2), 2017.
2. N Mishra, S Forti, F Fabbri, L Martini, C McAleese, B Conran, PR Whelan, A Shivayogimath, BS Jessen, L Buß, J Falta, I Aliaj, S Roddaro, JI Flege, P Bøggild, KBK Teo, C Coletti, Small 15 (50), 2019.
3. V. Mišeikis, S. Marconi, M.A. Giambra, A. Montanaro, L. Martini, F. Fabbri, S. Pezzini, G. Piccinini, S. Forti, B. Terrés, I. Goykhman, L. Hamidouche, P. Legagneux, V. Sorianello, A.C. Ferrari, F.H.L. Koppens, M. Romagnoli, C. Coletti, ACS Nano 14 (9), 2020.
4. M.A. Giambra, V. Mišeikis, S. Pezzini, S. Marconi, A. Montanaro, F. Fabbri, V. Sorianello, A.C. Ferrari, C. Coletti, M. Romagnoli, ACS nano 15 (2), 2021.
5. S. Pezzini, V. Miseikis, G. Piccinini, S. Forti, S. Pace, R. Engelke, F. Rossella, K. Watanabe, T. Taniguchi, P. Kim, C. Coletti, Nano Letters 20 (5), 2020.
6. G. Piccinini, V. Miseikis, P. Novelli, K. Watanabe, T. Taniguchi, M. Polini, C. Coletti, S. Pezzini, https://arxiv.org/pdf/2203.15422.pdf.
7. S. Pace, L. Martini, D. Convertino, D.-H. Keum, S. Forti, S. Pezzini, F. Fabbri, V. Mišeikis, C. Coletti, ACS nano 15 (3), 2021.
8. S. Forti, S. Link, A. Stöhr, Y. Niu, A.A. Zakharov, C. Coletti, U. Starke, Nature Communications 11 (1), 2020.

The research leading to these results has received funding from the European Union's Horizon 2020 research and innovation program under grant agreements no. 785219-Graphene Core2 and 881603-Graphene Core3.

Emerging Device Applications of 2D Materials

Steven J. Koester
University of Minnesota, ECE Department, 200 Union St. SE, Minneapolis, USA
skoester@umn.edu

Two-dimensional (2D) materials, crystalline materials characterized by strong in-plane bonds and weak out-of-plane bonds, have been intensively studied for the better part of the past two decades. 2D materials have many remarkable properties, but the applications for which they are best suited remains an open question. In this talk, I will describe the efforts in our group to identify new applications for 2D materials, with a focus on the ones where their unique properties can best be utilized. I will first discuss our work on graphene and how its high mobility, monolayer thickness and unique band structure can enable a new class of high-speed, non-volatile tuning elements [1] and compact read heads for magnetic storage [2]. I will also describe the characteristics of selected 2D semiconductors, including transition metal dichalcogenides (TMDCs) and black phosphorus, and show how their properties can be used to realize ultra-scaled dynamic memories [3], and ultra-low power and reconfigurable electronic circuits. Finally, I will show recent results [4] on semi-metallic contacts to the TMDC, WS_2, that provide strong evidence that 2D materials have tremendous potential to realize high-performance MOSFETs for VLSI logic circuits with ultimate scalability.

References

[1] J. Wen, V. R. S. K. Chaganti, and S. J. Koester, IEEE Elect. Dev. Lett., vol. 43 (2022), pp. 820-823.
[2] J. Hu, G. Stecklein, D. A. Deen, Q. Su, P. A. Crowell, and S. J. Koester, IEEE Trans. Elect. Dev., vol. 66 (2019), pp. 5003-5010.
[3] C. U. Kshirsagar, W. Xu, Y. Su, M. C. Robbins, C. H. Kim, and S. J. Koester, ACS Nano, vol. 10 (2106), pp. 8457–8464.
[4] L. Jin, and S. J. Koester, IEEE Elect. Dev. Lett., vol. 43 (2022), pp. 639-642.

Figures

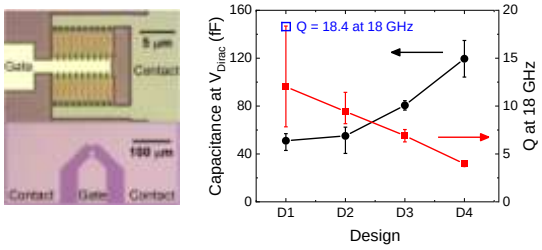


Figure 1: High-speed graphene varactor showing high-Q at 18 GHz. [1].

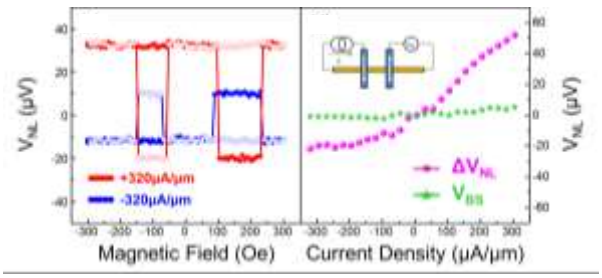


Figure 2: Results from narrow graphene spin valves showing low background signal [2].

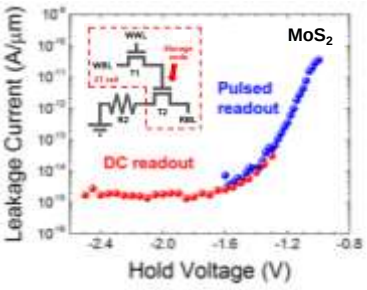


Figure 3: Results showing long retention time in MoS_2 two-transistor DRAM [3].

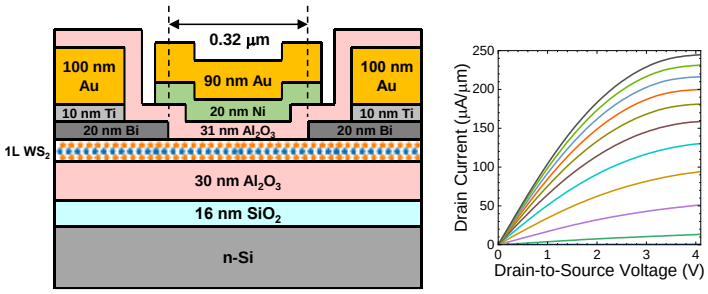


Figure 4: Dual-gated, single-layer CVD-grown WS_2 MOSFET with Bi contacts. [4].

Synthesisand, properties and applications of 2D amorphous carbon & nanoporous graphene foam

Barbaros Oezyilmaz
Co-Authors (Century Gothic 10)
barbaros@nus.edu.sg

Scalability, Reliability and process compatibility are key challenges in commercializing 2D materials. I will discuss our approach in addressing these challenges for atomically thin amorphous graphene and nonporous graphene foam. I will give two potential for applications.
Atomically thin amorphous thin films are essential for enabling semiconducting device scaling, increase data storage densities. Similarly, such films are expected to boost the performance of supercapacitors performance. Here I will discuss their synthesis, by laser-assisted chemical vapour deposition [1] and spark plasma sintering, respectively [2]. In the first part of my talk I will show, that the excellent physical properties of such stable, free-standing monolayer amorphous carbon are ideal as diffusion barriers in applications such as heated assited magnetic recording and copper interconnects. They can be directly grown on SiO2 and their performance exceeds the 10-years lifetime industry requirement based on time-dependent dielectric breakdown measurements. Furthermore, directly grown MAC on Cu lines with cross section of 80 nm by 200 nm not only preserve device integrity but also leads to 25% reduction in line resistance. In the second part of my talk I will discuss the synthesis of a novel nanoporous graphene foam. This structure is a monolithic, layered composite of 3 carbon allotropes, consisting of a stiff, sp3-rich backbone, covered by a conductive graphite layer, followed by an outermost layer of micropore-rich graphene. This monolithic carbon foam (MCF) hosts a hierarchy of 3D pores, ranging in size and providing high pore accessibility. MCF exhibits electrical conductivity as large as 120 S/cm, exceeding conventional carbon-based electrode performance and a Vickers hardness of over 900 MPa exceeding that of nuclear graphite allowing for a wide range of applications such as energy storage, filtration and catalysis. As a proof of concept, we demonstrate a supercapacitor with ten times longer device life time when compared to commercial devices. Last not but least, I will discuss a new route to synthesize 2D magnetic semiconductors based on interstial doping on black phosphorus with cobolt.

References

[1] Synthesis and properties of free-standing monolayer amorphous carbon; Chee-Tat Toh, Hongji Zhang, Junhao Lin, Alexander S. Mayorov, Yun-Peng Wang, Carlo M. Orofeo, Darim Badur Ferry, Henrik Andersen, Nurbek Kakenov, Zenglong Guo, Irfan Haider Abidi, Hunter Sims, Kazu Suenaga, Sokrates T. Pantelides & Barbaros Özyilmaz ; Nature (Jan 2020).

Finite momentum pairing in an MoS_2 bilayer

Jurgen H. Smet
Dong Zhao, Lukas Debbeler, Matthias Kühne, Sven Fecher, Nils Gross
Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany
j.smet@fkf.mpg.de

Abstract

2D materials with strong spin orbit interactions are an intriguing platform for the study of exotic superconductivity. This is particularly true, if the symmetry properties of the 2D material vary with the layer number. A transition metal dichalchogenide such as MoS2 serves as an excellent example. The behavior at high doping levels has been studied for the hexagonal phase in the monolayer regime. The monolayer possess in-plane mirror symmetry, but lacks inversion symmetry. As a result, a large non-zero in-plane crystal field exists that produces a strong out of plane spin orbit effective magnetic field. It splits the spin states due to spin orbit interaction in opposite directions for the two different valleys. As a result, spin singlet pairs with zero momentum of opposite spin from both valleys can form. This gives rise to Ising superconductivity with an exceptional resilience against pair breaking from an in-plane magnetic field [1,2], since the effective spin orbit field, as large as 100 T, needs to be overcome first. In a bilayer, each layer is non-centrosymmetric and possesses an in-plane crystal field in opposite directions, but globally inversion symmetry is restored. The spin, valley and layer degrees of freedom are all coupled. The layer degree of freedom enlarges significantly the number of possible superconducting channels and an unusual hitherto unobserved variant of finite momentum pairing may manifest according to theory [3]. A fascinating aspect of this non-uniform superconducting ground state is that the Fermi surface can be fully gapped and can entirely participate in pairing. This is in contrast to previous instances of finite momentum pairing where just segments of the Fermi surface as can contribute. Access to this superconducting state requires that both layers are doped in a balanced/symmetric fashion, while simultaneously retaining high sample quality to ensure that interlayer coherence is maintained down to the lowest temperature. The very potent electrolyte gating technique typically used to achieve the required doping levels is not capable of accomplishing this as only the layer closest to the electrolyte accumulates charges and a strong perpendicular electric field modifies the symmetry and generates an undesirable in-plane Rashba field. In addition, the strain fluctuations caused by an electrolyte drop on the active device area is detrimental for the material quality. Here we have overcome these shortcoming of electrolyte gating by using "remote" intercalation. Our observations are consistent with this new and unusual instance of finite momentum pairing in which the full Fermi surface can participate at small interlayer coupling.

References

[1] J. Lu, O. Zheliuk, I. Leermakers, N.F. Yuan, U. Zeitler, K.T. Law, J. Ye, Science **350**, 1353 (2015).

[2] Y:Saito, Y. Nakamura, M.S. Bahramy, Y. Kohama, J. Ye, Y. Kashara, Y. Nakagawa, M. Onga, M. Okunga, T. Nojima, Y. Yanase, Y. Iwasa, Nature Physics **12**, 144 (2016).

[3] C.X. Liu, Physical Review Letters **118**, 087001 (2017).

Growth of Single-Crystal Hexagonal Boron Nitride by Chemical Vapor Deposition

Hyeon Suk Shin
Department of Chemistry, UNIST, Ulsan 44919, Republic of Korea
shin@unist.ac.kr

Large-area single-crystal monolayers of two dimensional (2D) materials such as graphene, hexagonal boron nitride (hBN) and transition metal dichalcogenides have been successfully grown. Among them, hBN has been demonstrated to be the "ideal" dielectric substrate for 2D materials-based field effect transistors (FETs) – offering the potential for extending Moore's law. Although hBN thicker than a monolayer is more desirable as substrate for 2D semiconductors, the growth of highly uniform and single-crystal few- or multi-layer hBN has not yet been demonstrated. Here we report the epitaxial growth of wafer-scale single-crystal tri-layer hBN by a chemical vapour deposition method. Uniformly aligned tri-layer hBN islands are found to grow on a 2 cm × 5 cm single-crystal Ni (111) at early stage of growth and finally to coalesce into a single-crystal film. Cross-sectional transmission electron microscopy (TEM) results show that a $Ni_{23}B_6$ interlayer is formed (during cooling) between the single-crystal tri-layer hBN film and Ni (111) substrate by boron dissolved in Ni (111) and that there is epitaxial relationship between tri-layer hBN and $Ni_{23}B_6$ and between $Ni_{23}B_6$ and Ni (111). We further find that the tri-layer hBN film acts as a protective layer that remains intact during catalytic evolution of hydrogen – suggesting continuous and uniform single-crystal tri-layer hBN in large area. This tri-layer hBN transferred onto the SiO_2 (300 nm)/Si wafer acts as a dielectric layer to reduce electron doping from the SiO_2 substrate in MoS_2 FETs. Our results demonstrate that it is possible to achieve high quality multi-layered hBN over large areas by CVD – opening up new pathways for making it a ubiquitous substrate for 2D semiconductors and other purposes.

High-dimensional immune analyses towards 2D materials applications

Lucia Gemma Delogu
University of Padua, Italy
Luciagemma.delogu@unipd.it

Abstract

We recently depicted the "Nano-immunity-by-design" where the characterization of 2D materials is not solely based on their physical-chemical parameters but also their immune profiling. [1] The immune profiling can be revealed in its complexity in unique, informative ways: high dimensional approaches. [2,3] We exploited high-dimensional approaches, such as single-cell mass cytometry and imaging mass cytometry on graphene and other novels two-dimensional materials, such as transition metal carbides/carbonitrides (MXenes). [4-6]
We revealed that the amino-functionalization of graphene oxide increased its immuno-compatibility. [4] Moreover, we combined graphene with $AgInS_2$ nanocrystals, enabling its detection by single-cell mass cytometry on a large variety of primary immune cells. [5] Recently, we reported the immune modulation of specific MXenes, $Ti_3C_2T_x$ in particular, in combination with their antiviral properties against SARS-CoV-2 again by single-cell mass cytometry and other high dimensional approaches. [6]
Together with our published works, I will present unpublished results from the EU projects G-IMMUNOMICS and CARBO-IMMAP, in a broader variety of novel 2D materials, MXenes, MoS_2, WS_2, and bismuthene on human immune cell subpopulations, as well as on mice and swine models.
Our results conceptualize that chemical and immunological designs of 2D materials offer new strategies for their safe exploitation in biomedicine.

References

[1] Gazzi A et al… and **Delogu LG***. Graphene, other carbon nanomaterials and the immune system: toward nanoimmunity-by-design. J Phy Mat (2020).
[2] Fusco L et al… and **Delogu LG***. Graphene and other 2D materials: a multidisciplinary analysis to uncover the hidden potential as cancer theranostics. Theranostics (2020).
[3] Weiss C et al… and **Delogu LG***. Toward Nanotechnology-Enabled Approaches against the COVID-19 Pandemic. ACS Nano (2020)
[4] Orecchioni M et al… and **Delogu LG*.** Single-cell mass cytometry and transcriptome profiling reveal the impact of graphene on human immune cells. Nature Communications (2017).
[5] Orecchioni M et al… and **Delogu LG*.** Toward High-Dimensional Single-Cell Analysis of Graphene Oxide Biological Impact: Tracking on Immune Cells by Single-Cell Mass Cytometry. Small (2020).
[6] Unal MA et al. and Gogotsi Y*, **Delogu LG*,** Yilmazer A*. Nanotoday (2021).

Plethora of Many-Body Ground States in Magic Angle Twisted Bilayer Graphene

Dmitri K. Efetov
LMU Munich, Germany
Dmitri.Efetov@icfo.eu

Twist-angle engineering of 2D materials has led to the recent discoveries of novel many-body ground states in moiré systems such as correlated insulators, unconventional superconductivity, strange metals, orbital magnetism and topologically nontrivial phases. These systems are clean and tuneable, where all phases can coexist in a single device, which opens up enormous possibilities to address key questions about the nature of correlation induced superconductivity and topology, and allows to create entirely novel quantum phases with enhanced interactions. In this talk we will introduce some of the main concepts underlying these systems, concentrating on magic angle twisted bilayer graphene (MATBG) and show how symmetry-broken states emerge at all integer electron fillings [1]. We further will discuss recent experiments including screened interactions [2], Chern insulators [4], magnetic Josephson junctions [4], quantum criticality [5], re-entrant correlated insulators at high magnetic fields [6] and discuss some of the avenues for novel quantum sensing applications [7].

References

[1] Nature, 574, 653 (2019).
[2] Nature, 583, 375–378 (2020).
[3] Nature Physics, 17, 710 (2021).
[4] arXiv:2110.01067 (2021).
[5] Nature Physics (2022).
[6] Phys. Rev. Lett. (2022).
[7] arXiv:2111.08735 (2021).

Valley-polarized Quantum Anomalous Hall effect in bilayer graphene

Jose H. Garcia
Marc Vila, Jose H Garcia, Stephan Roche
Catalan Institute of Nanoscience and Nanotechnology, Campus de la Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona
josehugo.garcia@icn2.cat

Realizations of some topological phases in two-dimensional systems rely on the challenge of jointly incorporating spin-orbit and magnetic exchange interactions. Here, we predict the formation and control of a fully valley-polarized quantum anomalous Hall effect in bilayer graphene, by separately imprinting spin-orbit and magnetic proximity effects in different layers. This results in varying spin splitting for the conduction and valence bands, which gives rise to a topological gap at a single Dirac cone. The topological phase can be controlled by a gate voltage and switched between valleys by reversing the sign of the exchange interaction. By performing quantum transport calculations in disordered systems, the chirality and resilience of the valley-polarized edge state are demonstrated. Our findings provide a promising route to engineer a topological phase that could enable low-power electronic devices and valleytronics applications as well as put forward layer-dependent proximity effects in bilayer graphene to create versatile topological states of matter.

References

[1] M Vila, Jose H. Garcia, and St Roche Phys. Rev. B **104**, L161113 (2021)

Figures

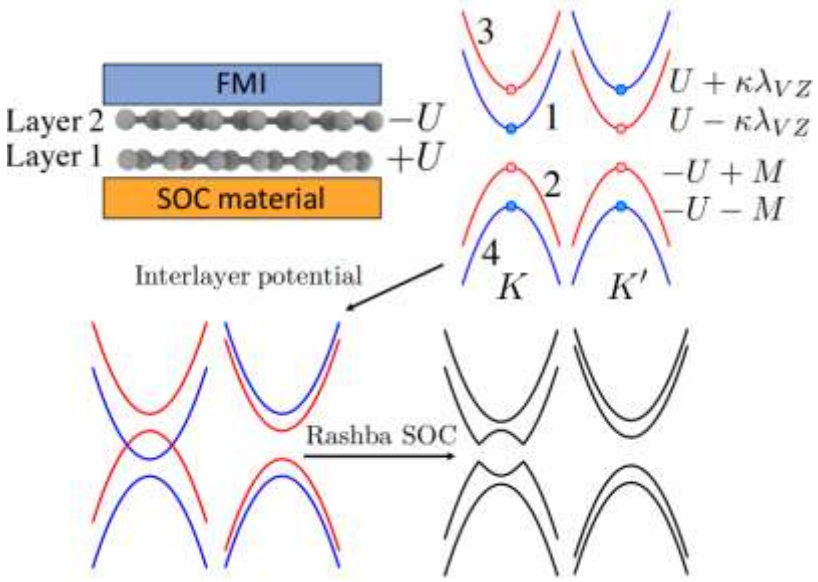


Figure 1: Top left: Van der Waals heterostructure comprised of a SOC material, bilayer graphene, and a ferromagnetic insulator. Top right and bottom: Mechanism of the valley-polarized quantum anomalous Hall effect. Red and blue colours depict up and down spins, respectively

Atomic lattice reconstruction in twisted transition metal dichalcogenides and arising interfacial ferroelectricity.

Roman Gorbachev
University of Manchester, Oxford Road, Manchester, UK
roman@manchester.ac.uk

Abstract

In this talk I will review our latest work on twisted TMDs bilayers and discuss atomic reconstruction that occurs when the twist angles are small. For small twist near the 2H stacking, stable 2H domains dominate, with nuclei of a second metastable MM phase. This appears as a kagome-like pattern at θ~1°, transitioning at θ→0 to a hexagonal array large 2H domains. The tunnelling measurements show that such reconstruction creates piezoelectric textures, opening a new avenue for engineering of 2D material properties.
For 3R stacking, a pattern of mirror reflected triangular 3R domains merges, featuring layer-polarized conduction band states caused by lack of both inversion and mirror symmetries. Surprisingly, the lack of inversion symmetry in 3R polytype leads to emergence of out-of-plane ferroelectricity due to layer-asymmetric interband hybridisation. The electrically-polarised domains can be switched by external electric field which opens a new pathway towards optoelectronic devices with memory effect.

References

[1] Weston et al. Nat. Nanotechnol. 2020, 15 (7), 592.
[2] Weston et al. Nat. Nanotechnol. 2022, 17 (4), 390.

Figures

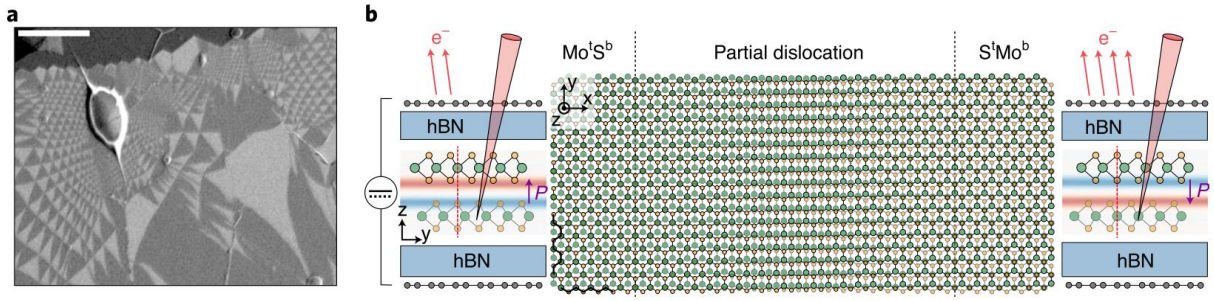


Figure 1: Ferroelectric domains in marginally twisted bilayer MoS_2. **a**, Example of BSECCI acquired on unencapsulated twisted bilayer MoS_2 placed onto a graphite substrate. Light and dark domain contrast corresponds to the two dominant stacking orders referred as Mo_tS_b and S_tMo_b. Scale bar, 1 μm. b, Centre: schematic demonstrating the transition from Mo_tS_b to S_tMo_b with perfectly stacked bilayer regions separated by a partial dislocation. Side panels: the cross-sectional alignment of the MoS_2 monolayers, viewed along the armchair direction, assembled within the double-gated device structure. Colour maps overlayed on top of the TMD atomic schematics show calculated charge density transferred between top and bottom layers.

Strange insulator in an extremely wide doping range in graphene

Zheng HAN
Institute of Opto-Electronics, Shanxi University, Taiyuan, China
Vitto.han@gmail.com

Abstract

It is a long standing prediction that correlated electron-hole states can occur in semiconductors with very small band gap or semimetals with very small band overlap, when cooled to a sufficiently low temperature, yielding a non-conducting Bose condensate. Such electron-hole paring degenerated quantum insulators are endowed with enriched intrinsic physics with Hamiltonians closely resembling that in superconductivity, and have attracted continuous attention since decades. However, owing to the dielectric screening and the recombination of electrons and holes, excitonic insulators remained largely unexplored in solids, especially in transport measurements.

In this talk, we will introduce our recent progresses in the experimental observation of an exotic insulator behavior: by bring bernal-stacked bilayer graphene into contact with a few-layered antiferromagnetic insulator CrOCl, the resulted vertical heterostructures can give rise to an extraordinarily robust ground state of exciton-enhanced insulator [1]. The consequential over 1 GOhms insulator can be readily killed by tuning the displacement field and effective doping, and the system recovers to a high mobility graphene with a sheet resistance of less than 100 Ohms. I-V curves as well as temperature- and magnetic field-dependences point such strange insulator to an excitonic-enhanced insulator behaviour, which is attributed to the subtle coupling of graphene-CrOCl interface. Such interfacial coupling can be a simple yet very powerful technique in effectively engineering the quantum electronic states.

References

[1] arXiv preprint arXiv:2110.02921.

How to use the polymer-derived ceramics route for the synthesis of boron nitride-based nanomaterials

Catherine Journet[1]
Camille Maestre[1,2], Yangdi Li[1,2], Boitumelo Matsoso[1], Wenjun Hao[1], Victor Vuillet-a-Ciles[1], Vincent Garnier[2], Philippe Steyer[2], Bérangère Toury[1], Catherine Marichy[1]
1 Laboratoire des Multimatériaux et Interfaces (LMI), UMR CNRS 5615, Univ. Lyon, Université Claude Bernard Lyon 1, F-69622 Villeurbanne, France
2 UCBL, CNRS, MATEIS, UMR 5510, Université de Lyon, INSA Lyon, 7 avenue Jean Capelle, Villeurbanne 69621 CEDEX, France
catherine.journet@univ-lyon1.fr

Hexagonal boron nitride (hBN) occupies a special place in the vast world of 2D materials, due to its excellent thermal, chemical, mechanical, and dielectric properties that make it a promising candidate for many revolutionary applications, especially for optoelectronic devices. However, it is now well established that the optical, electronic, and transport properties of these systems are highly dependent on the chemical purity and crystallinity of the hBN used, which in turn are highly dependent on the synthesis approach used.
For several years, we have been developing a polymer-derived ceramics (PDCs) synthesis route that allows the elaboration of ceramics with tailored textural and structural properties.[1] PDCs consists in synthesizing a molecular precursor and then polycondensing it into an inorganic polymer that can be shaped before ceramization. One of the main advantages is that from molecular or preceramic polymer precursors, it is possible to produce specific shapes, including fibers, films, or ceramic composites, which cannot be easily obtained by conventional powder technology.
Here, we demonstrate the value of the PDCs route for the synthesis of hBN.[2] Single crystal growth of hBN at relatively low temperature and atmospheric pressure is successfully achieved from a borazine precursor using the PDCs route alone.[3] Furthermore, by coupling PDCs with a sintering technique from the same preceramic polymer, it is possible to increase the crystal size to a few millimeters (Figure 1).[4] The resulting pure hBN single crystals can then be exfoliated into hBN nanosheets. Finally, by combining PDCs with atomic layer deposition (ALD), functional hBN nano-/heterostructures are successfully synthesized from highly structured sensitive templates, making this ALD process a promising alternative for the fabrication of functional hBN nanostructures.[5]

References

[1] S. Yuan, C. Journet, S. Linas, V. Garnier, P. Steyer, S. Benayoun, A. Brioude, B. Toury, Crystals, 6 (2016) 55
[2] 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
[3] B. J. Matsoso, V. Vuillet-A-Ciles, L. Bois, B. Toury, C. Journet, Nanomaterials, 10 (2020) 443
[4] C. Maestre, Y. Li, V. Garnier, P. Steyer, S. Roux, A. Plaud, A. Loiseau, J. Barjon, L. Ren, C. Robert, B. Han, X. Marie, C. Journet, B. Toury, 2D Materials, (2022), accepted
[5] W. Hao, C. Marichy, C. Journet, A. Brioude, Chemnanomat, 3 (2017) 656

Figures

Figure 1: Optical image of a few millimeters side hBN crystal

Properties of Electron-Beam-Modified Low-Dimensional Inorganic and Organic Materials

Ute Kaiser
Ulm University, Central Facility Materials Science Electron Microscopy, Albert Einstein Allee 11, 89081 Ulm, Germany
Ute.Kaiser@uni-ulm.de

Low-dimensional materials exhibit properties, which often differ strongly from those of the bulk counterparts and offer unique opportunities for new and miniaturized electronic and optical devices [1]. In situ electron microscopy allows to functionalize the thin material while imaging. Here we present recent results using our unique chromatic and spherical aberration-corrected SALVE instrument both in imaging and spectroscopy [2].

We first discuss the formation of defects in two-dimensional inorganic and organic crystals. For transition metal di-chalcogenides (TMDs) we show that the formation of vacancies is possible at electron voltages nearly half of the knock-on threshold and quantify the damage [3,4]. Further, we analyse in-situ structural and chemical modifications of different freestanding transition metal phosphorus tri-chalcogenides (TMPTs). The atomically resolved analysis of freestanding few-layer TMPTs is difficult, and rarely reported due to their susceptibility to oxidation. Here we present our work on the effect of electron irradiation in freestanding few-layer TMPTs at TEM acceleration voltages between 30 and 80 kV. Our first-principle calculations predict that the electron beam predominantly removes sulphur from the sample, which is confirmed by combined EELS and EDX experiments. In addition, we conduct in-situ experiments to study annealing and electron-beam-induced structure transformations of few-layer $MnPS_3$. We observe the formation of new phases with the net formula $MnS_{(1-x)}P_x$ and show that suitable dose rates allow their controlled growth embedded in the antiferromagnetic host. Complementary ab-initio calculations prove the stability of the new phases and predict their magnetic and electronic properties. As the TMPTs are often very oxygen-sensitive, they were prepared with the help of a newly-developed polymer-assisted sample preparation method [5].
We also present studies on the structure of two-dimensional polymer crystals and show that an accelerating voltage of 120kV is optimal to resolve the structure on the molecular level [6]. Furthermore, we present in-situ studies of a miniaturized electrochemical cell, where reversibly single-crystalline bilayer graphene is lithiated and delithiated in controlled manner using an electrochemical gate confined to a device protrusion [7]. Moreover, we report on the nucleation mechanism of the formed crystalline lithium phase, which we now understand on the level of the single atoms. We show that differentiating between the bond nature between two metal atoms is now possible [8].

References

[1] A. Hashemi et al., J. Phys. Chem. C, 121 (2017) 27207
[2] M. Linck, et al., Phys. Rev. Lett., 117 (2016) 076101
[3] S. Kretschmer, T. Lehnert et al., Nano Lett., 20 (2020), 2865
[4] T. Lehnert et al., ACS Appl. Nano Mater., 2 (2019) 3262
[5] J. Köster et al., Nanotechnology 32 (2021) 075704
[6] H. Qi et al., Science Advances 6 (2020) eabb5976
[7] M. Kühne, F. Börrnert et al., Nature 564 (2018) 234
[8] K. Cao et al., Science Advances 6 (2020) eaay5849

Moiré heterostructures: a condensed matter quantum simulator

Dante Kennes
RWTH Aachen University, Germany
dante.kennes@mpsd.mpg.de

We propose twisted van der Waals heterostructures as an efficient, reliable and scalable quantum platform that enables the seamless realization and control of a plethora of interacting quantum models in a solid state framework. These new materials hold great promise to realize novel and elusive states of matter in experiment. We survey these systems as platform to study strongly correlated physics and topology that is notoriously difficult to study computationally [1]. Among the features that make these materials a versatile toolbox are (i) tunability of properties via readily accessible external parameters (such as gating, straining, packing and twist angle), (ii) ability to realize and control a large number of fundamental many-body quantum models relevant in the field of condensed matter physics and beyond and (iii) state-of-the-art experimental readouts exist to directly map out their rich phase diagrams in and out of equilibrium. This general framework, besides unravelling new phases of matter, permits to identify their key microscopic ingredients and therefore to robustly realize and functionalize those new phases in other material systems, deepening our fundamental understanding and holding many promises for future technological applications. As examples we discuss our recent findings in twisted bilayer graphene, bilayer BN, double bilayer graphene, bilayer WSe2, bilayer MoS2, bilayer GeSe and generalizations to three dimensions [2]..

References

[1] Nature Physics 17, 155 (2021)
[2] Nature 572, 95-100 (2019), Nature Communications 11, 1124 (2020), Nature Materials 19, 861 (2020), Phys. Rev. B 102, 085109 (2020), Phys. Rev. B 103, 041103 (2021), arXiv:1911.00007 (PNAS in press), Nat Communications 12, 242 (2021), arXiv:2004.02964, , arXiv:2012.09649

Tuning the spin-orbit coupling in twisted graphene/TMDC heterostructures: spintronics meets twistronics

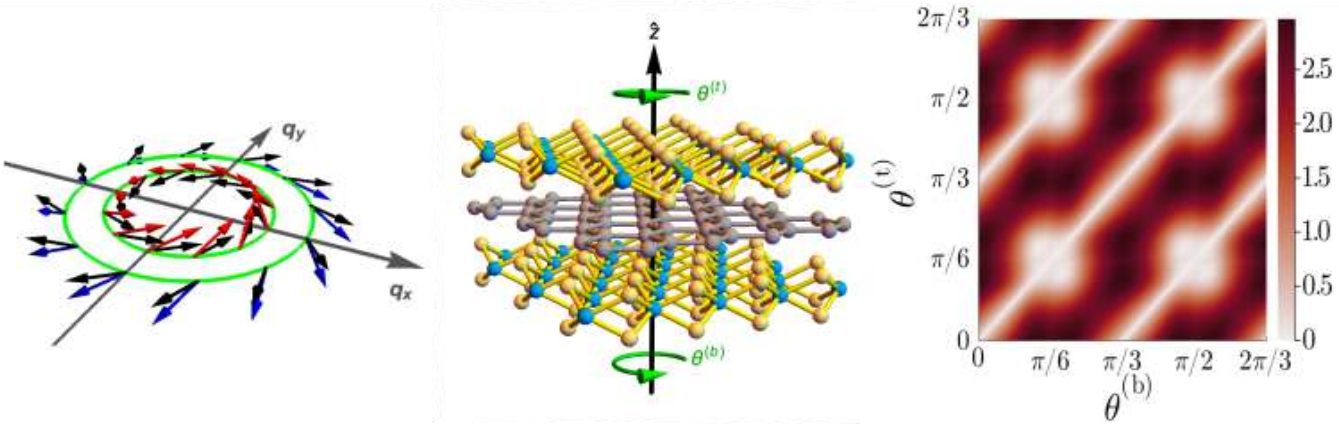
Andor Kormányos[1]
Csaba Péterfalvi[2], Alessandro David[3], Péter Rakyta[1], Guido Burkard[2]
[1]*Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary*
[2]*Department of Physics, University of Konstanz, D-78464 Konstanz, Germany*
[3]*Peter Grünberg Institute – Quantum Control (PGI-8), Forschungszentrum Jülich GmbH, Jülich, Germany*
andor.kormanyos@ttk.elte.hu

Multilayer stacks of two-dimensional materials have become an important platform for quantum simulators, which aim to explore a wide range of exciting quantum phenomena[1]. The proximity induced spin-orbit coupling (SOC) plays a pivotal role in many of these systems. We have shown[2] that the interlayer twist angle can be used to enhance the strength of the induced SOC in graphene/transition metal dichalcogenide (TMDC) bilayers. We have also found that the proximity induced Rashba SOC can be affected by quantum interference effects in twisted trilayers. We have calculated the quantum phase responsible for this effect in graphene/TMDC bilayers as a function of interlayer twist angle. We showed how this quantum phase affects the spin-polarization of the graphene bands and discuss its potential effect on spin-to-charge conversion measurements.

References

[1] D. M. Kennes et al, Nature Physics **17**, 155 (2021).
[2] A. David, P. Rakyta, A. Kormányos, G. Burkard, Phys. Rev. B **100**, 085412 (2019)
[3] Cs. G. Péterfalvi, A. David, P. Rakyta, G. Burkard, and A. Kormányos, arXiv:2111.02781 (accepted in Phys.Rev.Research)

Figures



An autonomous perovskite solar farm enabled by 2D materials

Emmanuel Kymakis
Department of Electrical & Computer Engineering, Hellenic Mediterranean University, Heraklion, Crete, Greece.
kymakis@hmu.gr

During the past decade, there was intensive research on the development of perovskite solar cells (PSCs), which have emerged as an alternative efficient energy harvester for both IoT devices and solar farms. The power conversion efficiency (PCE) of PSCs has rapidly increased and is now approaching the state- of-the-art PCE of 26.1%[1] obtained by crystalline-silicon PVs. However, this impressive PCE obtained on small-area cells and in laboratory conditions should be also valid to large-area PV panels in real outdoor conditions. Interface engineering, using solution processable 2D materials (e.g., graphene and transition metal dichalcogenides) is an effective approach to increase the readiness of this technology for manufacturing. The incorporation of the 2D materials improves the charge dynamics of the interfaces and most importantly protects the perovskite layer against diffusion of external agents, such as oxygen and moisture and the metal ion migration[2]. In this context, the Graphene Flagship partners University Rome Tor Vergata, BeDimensional S.p.A, Greatcell and Hellenic Mediterranean University demonstrated the validity of this technology through the entire value chain, from materials development, perovskite modules and panels fabrication and their integration in an autonomous solar farm, to outdoor field tests, and assessment of the real energy production output. The main validation of the proposed approach is the realization of an autonomous solar farm, consisting of 5m^2 perovskite PV panels in the HMU campus at Crete[3]. A continuous monitoring of the solar farm was performed through in-house developed maximum power point trackers, coupled with a correlation of the environmental conditions, recorded by a weather station, with the outdoor performance of farm. The assembled solar farm delivered peak power exceeding 260W, proving the scalability of the proposed technology. The energy production of the solar farm was monitored for 12 months, demonstrating a remarkable 20% reduction (T_{80}) of the PV performance over 8 months of operation. Moreover, the solar farm's electrical characteristics were monitored as a function of temperature and light intensity. The data analysis demonstrated that the perovskite panels enabled by 2D materials are promising for outdoor operation at elevated temperatures, such as in high-irradiance global locations.

References

[1] https://www.nrel.gov/pv/assets/images/efficiency-chart.png
[2] Bellani, et al. Chem. Soc. Rev. 50, 11870– 11965 (2021)
[3] S. Pescetelli, et al. Nature Energy (2022).

Figure 1: A photograph of the solar farm

Controlled covalent derivatization of graphene oxide for therapeutic applications

Cécilia Ménard-Moyon
CNRS, Immunology, Immunopathology and Therapeutic Chemistry, UPR 3572, University of Strasbourg, 67000 Strasbourg, France
c.menard@ibmc-cnrs.unistra.fr

The relatively low-cost production of graphene oxide (GO) and its dispersibility in various solvents, including water, combined with its tunable surface chemistry, make GO an attractive building block to design multifunctional materials. There are many applications for which it is fundamental to preserve the intrinsic properties of GO, for example in the biomedical field and for the development of fuel cells. As a consequence, the derivatization of GO to impart novel properties has to be well controlled and the characterization of the functionalized samples thoroughly done and unambiguous. Despite the great progress in the functionalization of GO, its chemistry is not always well controlled and not fully understood.[1]
In this context, I will explain some strategies for the controlled functionalization of GO through the selective derivatization of the epoxides and hydroxyl groups without alteration of its properties and with biomedical perspectives for drug release and cancer therapy.[2-3]

References

[1] Guo S, Garaj S, Bianco A, Ménard-Moyon C, Nat. Rev. Phys., 4 (2022) 247.
[2] Guo S, Nishina Y, Bianco A, Ménard-Moyon C, Angew. Chem. Int. Ed. Engl., 59 (2020) 1542.
[3] Guilbaud-Chéreau C, Dinesh B, Schurhammer R, Collin D, Bianco A, Ménard-Moyon C. ACS Appl Mater Interfaces, 11 (2019) 13147.

Ultrafast optical coherent control of a single-photon emitter in hBN

Steffen Michaelis de Vasconcellos[1]
Johann Preuß[1], Daniel Groll[2], Robert Schmidt[1], Thilo Hahn[2], Paweł Machnikowski[3], Tilmann Kuhn[2], Rudolf Bratschitsch[1], Daniel Wigger[3,4]
[1]*University of Münster, Institute of Physics and Center for Nanotechnology, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany*
[2]*University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany*
[3]*Wrocław University of Science and Technology, Department of Theoretical Physics, 50-370 Wrocław, Poland*
[4]*School of Physics, Trinity College Dublin, Dublin 2, Ireland*
michaelis@uni-muenster.de

The optical coherent manipulation of single solid-state quantum systems is a key challenge in the development of quantum communication devices and quantum computation. Recently, the family of solid-state quantum emitters was joined by single-photon sources in atomically thin transition metal dichalcogenides and other 2D van der Waals materials [1]. Among these, colour centres in hexagonal boron nitride (hBN) are attracting considerable attention due to their remarkable properties, including bright single-photon emission at room temperature, a wide spectral range, narrow emission lines, and an excellent tunability.
We demonstrate coherent state manipulation of a single hBN colour centre with ultrafast laser pulses using a double-pulse sequence, as schematically shown in Fig. 1 [2]. The coherence properties of the two-level system are detected by measuring the photoluminescence intensity, which is proportional to its occupancy, as a function of the pulse delay. Our experiments and simulations reveal the effects of different sources of spectral jitter on the ultrafast coherence dynamics. We also demonstrate that coherent control can not only be exerted resonantly on the optical transition but also phonon-assisted, which provides profound insight into the internal phonon quantum dynamics. In the case of optical phonons, we find that the increased decoherence rates are due to dephasing processes of the phonon states, partly due to their anharmonic decay. The dephasing induced by acoustic phonon generation manifests itself in a rapid decrease in the coherent control signal when propagating phonon wave packets are emitted. Our demonstration of phonon-assisted coherent control of single hBN colour centres is an important step towards hybrid quantum technologies that combine electronic and phononic excitations.

References

[1] S. Michaelis de Vasconcellos, D. Wigger, U. Wurstbauer, A.W. Holleitner, R. Bratschitsch, T. Kuhn, physica status solidi (b) 259, 2100566 (2022)
[2] J. A. Preuß, D. Groll, R. Schmidt, T. Hahn, P. Machnikowski, R. Bratschitsch, T. Kuhn, S. Michaelis de Vasconcellos, and D. Wigger, Optica 9, 522 (2022)

Figures

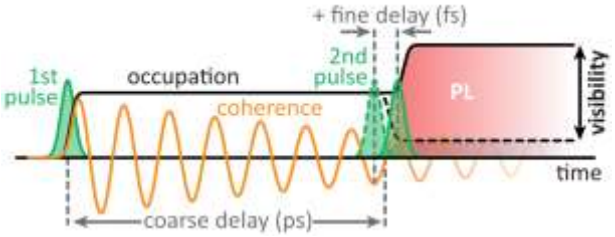


Figure 1: Double-pulse sequence of the ultrafast coherent control experiment. The initial phase of the quantum coherence is determined by the phase of the first laser pulse, while the timing of the second pulse affects the occupation of the quantum system, which is detected by measuring the photoluminescence intensity.

Structure, chemistry and electric field in epitaxially grown 2D layers investigated by 4D-STEM

Hanako Okuno[1]
Djordje Dosenovic[1], Kshipra Sharma[1], Yiran Lu[1], Martien den Hertog[2], Jean-Luc Rouviere[1], Céline Vergnaud[3], Matthieu Jamet[3], Alain Marty[3]
Univ. Grenoble Alpes, CEA-Grenoble, IRIG-MEM[1], IRIG-Spintec[3], 38054 Grenoble, France
Univ. Grenoble Alpes, CNRS-Institut Néel[2], 38054 Grenoble, France
Hanako.okuno@cea.fr

Epitaxial growth is a route to achieve highly crystalline continuous 2D layers. Molecular beam epitaxy (MBE) might lead to the formation of well-oriented large crystal with a great flexibility in the choice of the metals, allowing to realize van der Waals (vdW) heterostructures based on transition metal dichalcogenides (TMDs) with the desired configuration. In order to develop and control the synthesis of well-designed complex structures, multidimensional and multiscale structural analysis should be accessible in routine way. X-ray diffraction (XRD) gives a precise information on material quality regarding the crystallinity and the orientation distribution at mm scale, while scanning transmission electron microscopy (STEM) offers today the capability to study the detailled local atomic structures such as vacancies, grain boundaries as well as the associated chemical composition at atomic scale. However these techniques do not reveal complete material characteristiques because of the gap in scale between the information obtained by different techniques. Four dimensional (4D)-STEM is a new acquisition technique allowing to simultaneously record 2D images in real and recoprocal spaces [1]. Multiple information, from structure to electric field [2], at different scales can be reconstructed from signals appearing in diffraction pattern acquired at each pixel of the beam scan.

In this work, we demonstrate the use of 4D-STEM to study epitaxially grown 2D materials. Orientation and 1H-1T‘ phase maps in WSe_2 monolayers grown on vdW substrates are reconstructed at micron scale and directly correlated with both large scale XRD analysis and related atomic structures. In addition, the distribution of the charge density and the local electrostatic potential were also investigated at atomic scale by measuring the displacement of the centre of mass (CoM) of the transmitted beam. The results show the capacity to construct an overview of synthesized materials from mm scale down to atomic scale with information on structure, chemistry and electrostatic potential to study the growth mechanism and to explore the resulting physical properties.

References

[1] C. Ophus, Microscopy and Microanalysis, 25 (2019) 563
[2] J.A. Hachtel, J. C. Idrobo and M. Chi, Adv. Struct. Chem. Imag., 4:10 (2018)

Figures

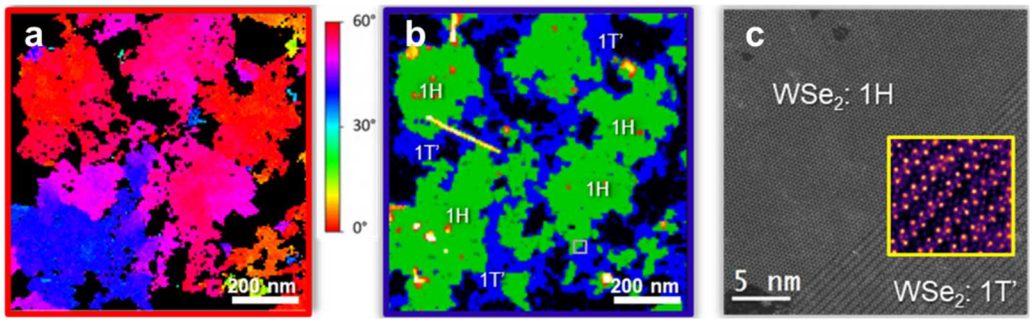


Figure 1: WSe_2 monolayer grown on mica substrate by MBE; (a) orientation and (b) phase maps reconstructed by 4D-STEM and (c) detailed atomic structure at interface between 1H and 1T' phases.

Graphene functionalization with molecular spacers for reversible storage of sodium and lithium ions

Jinhua Sun[1], Matthew Sadd[1], Philip Edenborg[1], Henrik Grönbeck[1], Peter Thiesen[2], Zhenyuan Xia[1], Vanesa Quintano[3], Ren Qiu[1], Aleksandar Matic[1], Vincenzo Palermo [1,3],*

[1] *Chalmers University of Technology, Göteborg, Sweden,*

[2] *Accurion GmbH, Stresemannstraße 30, Göttingen, Germany,*

[3] *Institute of Organic Synthesis and Photoreactivity (ISOF), National Research Council of Italy (CNR), Bologna, Italy.*

Vincenzo.palermo@isof.cnr.it

Sodium, in contrast with other group I and group II metals, cannot intercalate effectively in graphite. Fostering the sodium intercalation process would enable the use of this cheap, abundant element for applications in rechargeable batteries. Here, we report an artificial graphite-like anode for sodium ions storage, formed by stacked graphene sheets functionalized with an aminobenzene derivative only on one side, named as Janus graphene.[1] The asymmetric functionalization allows reversible intercalation of Na+ into such unique structure (Figure 1). This process can be easily monitored by operando Raman spectro-electrochemistry and visualized by imaging ellipsometry. The stacked Janus graphene with planar geometry has only one chemical group present, negligible local curvature, uniform inter-sheet pore size, controllable density of functional groups and minimal amount of edges. This material can store sodium ions differently from both graphite and stacked graphene films. Density Functional Theory (DFT) calculations demonstrate that Na^+ preferably occupies sites close to the $-NH_2$ group forming a synergic ionic bond to the graphene sheet, making the interaction process energetically favourable. Estimates based on electrochemical methods suggest a potential sodium storage as high as $C_{6.9}Na$, comparable to what is currently achieved in standard lithium ion batteries.

References

1. Real-time imaging of Na+ reversible intercalation in "Janus" graphene stacks for battery applications, **Science Advances**, (2021) 7, #eabf0812.

Figures

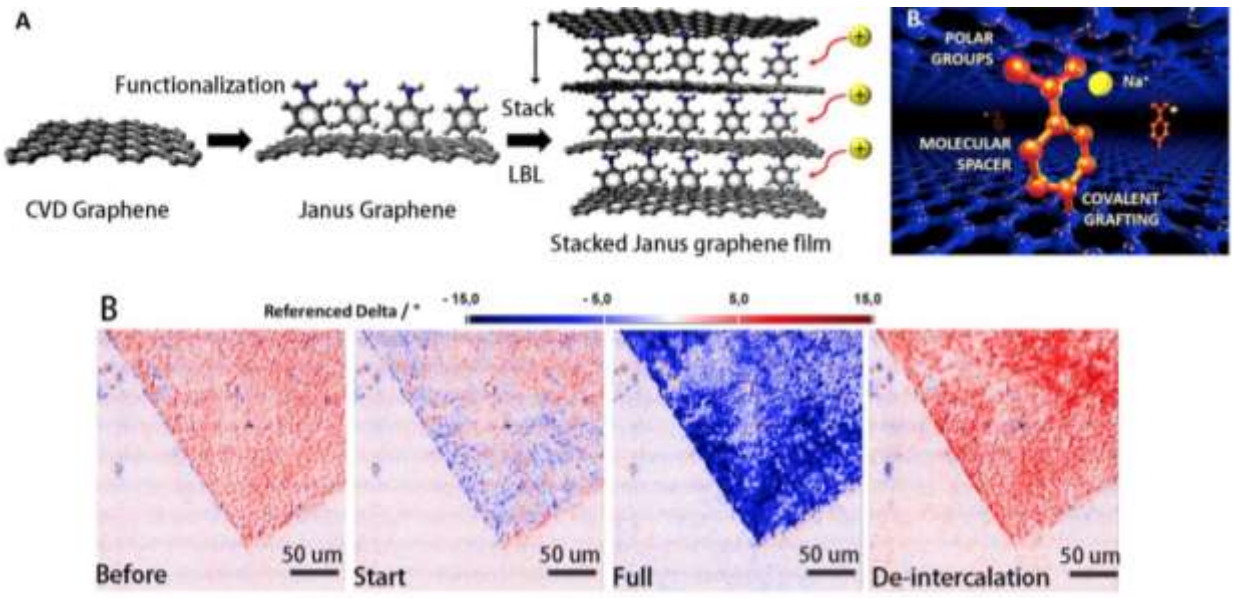


Figure 1: (A) Preparation of Janus graphene. (B) Ellipsometry imaging of sodium ions in/de-intercalation.

Engineering all interfaces in 2D transistors

Paolo Samorì
ISIS, Université de Strasbourg & CNRS, 8 alleé Gaspard Monge, 67000 Strasbourg, France
samori@unistra.fr

Abstract
The optimization of any electronic device requires the engineering of all interfaces to control and boost all fundamental physical processes governing the performance. The decoration of such interfaces with ad hoc molecules and assemblies thereof is a viable route to leverage the functional complexity of devices, enabling functional diversification by mastering a "more-than Moore" strategy. The structural perfection of two-dimensional materials represents a major advantage for such interface tailoring to create hybrid multifunctional structures with ad hoc characteristics for applications in (opto)electronics, sensing and energy. Molecules can be designed and synthesized to physisorb or chemisorb onto 2D materials in a controlled fashion, enabling functional diversification. [1]
In my lecture I will review our recent works on the interface engineering of 2D materials based field-effect transistors (FETs) providing specific example on:
(1) The integration of chemically functionalized electrodes in top-contact FETs based on MoS_2 by contact engineering through the dry transfer of SAMs pre-modified electrodes. Charge injection was optimized by using ad-hoc thiolated molecules with controlled dipole moments, thereby boosting the device performance. When asymmetrically functionalized electrodes were employed, Schottky diodes with a high rectification ratio could be realized. [2]
(2) The functionalization of the two surfaces of 2D semiconductors either in a symmetric[3] or asymmetric[4] fashion with molecular switches, to confer additional properties to WSe_2, thereby rendering 2D material-based transistors capable to respond up to four different independent external stimuli.
(3) The covalent functionalization of solution-processed TMDs (MoS_2, WS_2 and ReS_2) with bi-dentate semiconducting molecules enabled to simultaneously heal sulfur vacancies in metal disulfides and covalently bridge adjacent flakes, by promoting percolation pathways for charge transport, yielding a significant enhancement of the transistor characteristics.[5]
Our modular strategies relying on the combination of 2D material with molecules offer a simple route to generate multifunctional coatings, foams and nanocomposites with pre-programmed properties to address key global challenges in electronics, sensing and energy applications.

References

[1] Reviews on 2D materials + molecules for electronics: (i) M. Gobbi, E. Orgiu, P. Samorì, Adv. Mater. 2018, 30, 1706103. (ii) S. Bertolazzi, M. Gobbi, Y. Zhao, C. Backes, P. Samorì, Chem. Soc. Rev. 2018 47, 6845-6888. (iii) Y. Zhao, S. Ippolito, P. Samorì, Adv. Opt. Mater., 2019, 7, 1900286. (iv) Y. Zhao, M. Gobbi, L. Hueso, P. Samorì, Chem. Rev., 2022, 122, 50.
[2] B. Han, et al, Adv. Mater. 2022, 34, 2109445.
[3] (i) H. Qiu, et al., Adv. Mater. 2020, 32, 1907903. (ii) Y. Zhao, S. Bertolazzi, M. S. Maglione, C. Rovira, M. Mas-Torrent, P. Samorì, Adv. Mater. 2020, 32, 2000740.
[4] (i) H. Qiu, M. Herder, S. Hecht, P. Samorì, Adv. Funct. Mater., 2021 31, 2102721. (ii) H. Qiu, S. Ippolito, A. Galanti, Z. Liu, P. Samorì, ACS Nano 2021, 15, 10668.
[5] S. Ippolito, et al, Nat. Nanotech. 2021, 16, 592

From polycyclic aromatic hydrocarbons to nanopore - nanogap devices

Grégory F. Schneider
Leiden Institute of Chemistry
g.f.schneider@chem.leidenuniv.nl

Starting at the smallest scale, with polycyclic aromatic hydrocarbons, we investigate the conformational preference of propeller-shaped polycyclic aromatic hydrocarbons to design propellerene molecules as building blocks of millimeter to centimeter scale devices. We design and synthesize polyaromatic hydrocarbon based macromonomers capable of self-assembling into 2D materials, which we integrate in fuel cells, electrolyzers, electro-osmosis and desalination devices.

Zooming out a little bit more, we use as-prepared membranes like graphene to tailor nanopores tiny and functional enough to – we hope – only allow the passage of a proton. We are currently looking into time-dependent diazonium solution treatment to obtain leak-tight graphene selective ion channels. At the device level, we use chemistry to tailor graphene devices. We designed graphene field-effect transistors that can electrically probe the molecular state of spin crossover crystals using chemo-electrical gating. As an electrode, we use graphene as a model carbon-based electrode and systematically introduce nitrogen and oxygen dopants, together with vacancy defects, to study ORR. The latter work not only indicates a non-negligible contribution of oxygen and especially oxygenated vacancy defects for the catalytic activity of nitrogen-doped graphene, but also provides important insights into the fundamental understanding of activity-structure correlations for tailoring the catalytic performance of carbon-based, most particularly graphene-based electrode materials.

Importantly, graphene edges offer interesting chemical opportunities for sensing. The inability to systematically characterize covalently functionalized graphene edges however, could still potentially limit the use of graphene in nanogap constructs for single molecule detection and recognition. We develop now parallel routes for edge functionalization that will allow the in situ spectroscopic characterization of edge functionality.

On the other side of the spectrum, our knowledge of graphene handling and graphene transfer allows now a high-yield graphene liquid cell fabrication, which will enable – we believe – the progression of the liquid phase electron microscopy field with 2D materials.

Chemistry has a lot to bring to the research field of graphene and 2D materials in general, from the smallest molecular scale to the device level: graphene instrisic's wetting properties in water, edge reactivity in devices, chemical routes for the alignment of tunneling junction in nanoporous nanofluidic devices for single molecule detection, graphene devices in water, on ice and on hydrogels, 2D functional membranes, to name a few.

Thermal transport in 2D materials and their heterostructures

Marianna Sledzinska
X. Peng, A. Arrighi, E. Chavez Angel, A. El-Sachat, F. Alzina and C.M. Sotomayor Torres
Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain
marianna.sledzinska@icn2.cat

In-plane, phonon thermal conductivity (κ) in 2D materials spans over wide range, from very high in graphene (2000 W/mK) and hBN (700-450 W/mK) to below 100 W/mK in transition metal dichalcogenides (TMDs. For instance, molybdenum disulfide (MoS2), one of the most representative TMD exhibits the thickness dependent κ which increases from ~25 W/mK to ~ 100 W/mK with the thickness increasing from single layer to bulk. Therefore, 2D materials offer an interesting platform to study thermal transport in the nanoscale. The current understanding of thermal transport by phonons will be reviewed considering a few exemplary cases.
I will discuss the case of few-layer, single crystal MoS_2 and $SnSe_2$ membranes in which the sample preparation is crucial to eliminate effects of imperfections and contamination focusing on the thickness dependence of κ [1, 2]. Two-laser Raman scattering thermometry (2LRT) was used for determining κ, combined with real time measurements of the absorbed laser power.
In the second part of the talk, I will discuss various strategies on tuning the thermal transport in 2D materials, such as creation of heterostructures using the example of MoS_2/hBN [1]. Furthermore, I will explain the effects of phonon scattering on the defects, grain boundaries and intentionally nanopatterned 2D materials [3].
Finally, on the methodological part, the sources of errors in the determination of thermal properties and outstanding questions concerning phonon transport in TMDCs will be discussed with view to find reliable figures of merits for a future benchmarking.

References

[1] A. Arrighi et al., 2D Mater. 9 (2022) 015005
[2] P. Xiao et al., Nano Lett. 21 (2021) 9172−9179
[3] P. Xiao et al., submitted Authors, Journal, Issue (Year) page

Figures

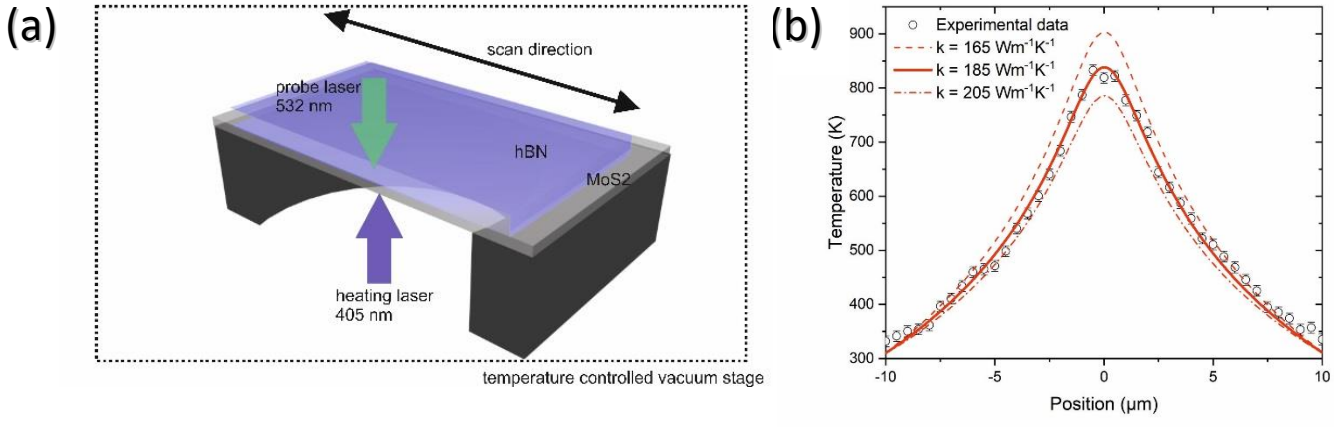


Figure 1: (a) Schematics of 2LRT measurements on MoS_2/hBN heterostructure (b) temperature distribution for absorbed heating laser power P_{abs} = 7.078 mW

Spin and Valley Blockade and Leakage Current in Graphene Quantum Dots

Chuyao Tong[1]
Annika Kurzmann[1], Rebekka Garreis[1], Wei Wister Huang[1], Samuel Jele[1], Marius Eich[1], Lev Ginzburg[1], Christopher Mittag[1], Kenji Watanabe[2], Takashi Taniguchi[2], Klaus Ensslin[1] and Thomas Ihn[1]
[1] *Solid State Physics Laboratory, ETH Zurich, CH-8093 Zurich, Switzerland*
[2] *National Institute for Material Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
ctong@phys.ethz.ch

The Pauli blockade effect in coupled double quantum dots is the foundation of successful characterization and manipulation of spin qubits [1,2]. Pauli spin blockade is well established for systems where the single-dot two-particle ground state is a spin-singlet [1,2,3]. In our bilayer graphene quantum dots, however, the additional valley degree of freedom provides us with a spin-triplet-valley-singlet single-dot two-particle ground state [4,5,6], altering the canonical picture where Pauli spin blockade shows up at alternating even-odd triple-points, to one that is more complex with a four-by-four grid [7]. With good understanding and control [3,4,5] of our few-carrier spin and valley states by gate voltages and magnetic field, we study at different magnetic fields the type of Pauli blockade (valley, spin, or mixed) at electron numbers between zero and four, and the relevant blocked transitions involved. At triple points where we observe Pauli spin blockade at zero magnetic field, we study the dependence of spin blockade leakage current on magnetic field. We gain insight into spin-mixing mechanisms which lift the spin-blockade, in particular into hyperfine interaction and spin-orbit interaction effects in bilayer graphene quantum dots [7].

References

[1] K. Ono, D. 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. C. Johnson, J. R. Petta, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Phys. Rev. B, 72 (2005) 165308.
[4] A. Kurzmann, M. Eich, H. Overweg, M. Mangold, F. Herman, P. Rickhaus, R. Pisoni, Y. Lee, R. Garreis, C. Tong, K. Watanabe, T. Taniguchi, K. Ensslin, and T. Ihn, Phys. Rev. Lett., 123 (2019) 026803.
[5] C. Tong, R. Garreis, A. Knothe, M. Eich, A. Sacchi, K. Watanabe, T. Taniguchi, V. Fal'ko, T. Ihn, K. Ensslin, A. Kurzmann, Nano Lett., 21 (2021) 1068–1073.
[6] C. Tong, A. Kurzmann, R. Garreis, W. W. Huang, S. Jele, M. Eich, L. Ginzburg, C. Mittag, K. Watanabe, T. Taniguchi, K. Ensslin, and T. Ihn, Phys. Rev. Lett. 128, (2022) 067702.
[7] C. Tong, et al. In preparation (2022).

Figures

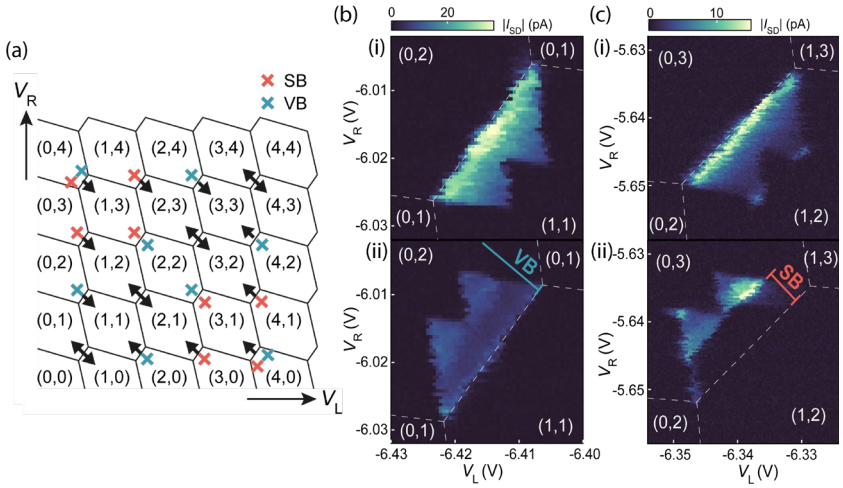


Figure 1: (a) Schematic charge-stability diagram for bilayer graphene double quantum dots at zero magnetic field, where blue and red crosses at triple points label valley and spin blocked transitions. (b, and c) Finite-bias triangles at zero magnetic field with (i) positive, and (ii) negative source–drain bias V_{SD}, around triple points with carrier occupancy (b): (0,2)↔(1,1) showing valley blockade, and (c): (0,3)↔(1,2) showing spin blockade.

Recent Progress Towards Wafer-scale Graphene MEMS

Aravind Vijayaraghavan
Katherine Smith, Daniel Melendrez Armada, Rory Phillips, Christian Berger
University of Manchester, Oxford Road, Manchester, UK
aravind@manchester.ac.uk

In this talk, I will chart the progress we have made towards wafer-scale and commercial fabrication of graphene-based MEMS devices and the challenges that still lie ahead.

The major breakthrough that enables this is the development of the graphene-polymer heterostructure (GPH) membrane [1-3], which overcomes the challenges associated with defects and contamination intrinsic to CVD graphene growth and transfer. GPH membranes were shown to result in 100% yield of intact suspended graphene drums and high-performance pressure sensors that can operate in both suspended and 'touch' mode.

Recently, we have undertaken the modelling of such GPH membranes by solving the Föppl–von Kármán (FvK) equations using an object-oriented, multi-physics finite-element library [4]. This is required because GPH membranes can not be modelled simply by the traditional assumptions of 'purely out-of-plane bending' or 'purely in-plane stretching'.

I will then talk about the integration of the GPH membrane with a commercial MEMS fabrication process known as PiezoMUMPS [5], resulting in high-performance graphene capacitive pressure sensors and resonators, where all but the final step of the graphene transfer is fabricated in a commercial MEMS fab. I will discuss the final missing piece of the puzzle, a wafer-scale implementation of the 'strained transfer' technique, which will enable GPH MEMS devices to become a commercial reality.

References

[1] C. Berger, Nanoscale, vol. 9, no. 44, pp. 17439, 2017.
[2] C. N. Berger, Nanoscale, vol. 8, no. 41, pp. 17928, 2016.
[3] C. Berger, *2D Mater.*, vol. 5, no. 1, 2018.
[4] K. Smith et al, Submitted, 2022
[5] K. Smith et al, Submitted, 2022

Figures

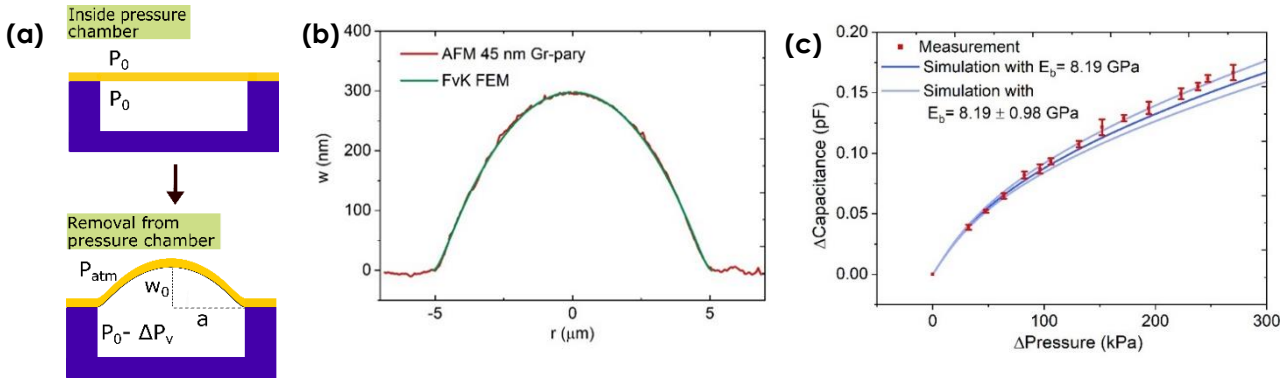


Figure 1: (a) 2-d schematic cross-section depicting the micro-blister inflation testing procedure with a single cavity and actuating membrane with significant parameters labelled. **(b)** 2-d topographical line profile of inflated 45 nm thick GPH micro-blister pressurized to ΔP= 116 kPa, compared to the FEM solution to FvK equations **(c)** Change in device capacitance against change in external pressure compared to that predicted by FEM simulation.

Band dispersions and interlayer interactions in 2D heterostructures revealed by angle resolved photoemission spectroscopy

Neil R. Wilson,[1]
Abigail J. Graham,[1] James Nunn,[1] Natalie C. Teutsch,1 P.V. Nguyen,2, Nicholas Hine,1 Alexei Barinov,3 Xiaodong Xu,2 and David H. Cobden[2]
[1] Department of Physics, University of Warwick, Coventry, CV4 7AL, U.K., [2] Department of Physics, University of Washington, Seattle, WA, USA, [3] Elettra – Sincrotrone Trieste, S.C.p.A, Basovizza (TS), 34149, Italy, [4] Department of Materials Science and Engineering, University of Washington, Seattle, WA, USA.
Neil.Wilson@warwick.ac.uk

We report band structure measurements of heterostructures of 2D materials, using angle-resolved photoemission spectroscopy with submicrometre spatial-resolution (nanoARPES), with a focus on heterostructures that include graphene and the MoWSeS group of semiconducting transition metal dichalcogenides (MX_2, where M = Mo / W and X = S / Se). We show that nanoARPES can directly reveal layer-dependent valence band dispersions in similar heterostructures to those used for optical and transport studies, measure interlayer hybridisation effects, and directly correlate valence band alignments to the binding energies of interlayer excitons for twisted MX_2 heterobilayers [1]. By fabricating samples in a field-effect transistor geometry, with flakes partially capped by graphene and supported by a hexagonal boron nitride on graphite back gate, we can electrostatically dope during ARPES measurements [2], populating the conduction band minimum in semiconducting samples. In this way, beyond the valence band parameters usually accessible by ARPES, the conduction band edge can be determined and inter- and intra-layer band gaps measured as a function of carrier concentration. Field-dependent band alignments between layers can also be probed [3]. In addition, twist-dependent effects interlayer interaction effects, such as moiré-induced replica bands, can be directly measured.

References

[1] Wilson, N. R.; Nguyen, P. V.; Seyler, K.; Rivera, P.; Marsden, A. J.; Laker, Z. P. L.; Constantinescu, G. C.; Kandyba, V.; Barinov, A.; Hine, N. D. M.; Xu, X.; Cobden, D. H. Sci. Adv. 2017, 3 (2), e1601832. https://doi.org/10.1126/sciadv.1601832.
[2] Nguyen, P. V.; Teutsch, N. C.; Wilson, N. R. N. P. N. R.; Kahn, J.; Xia, X.; Graham, A. J.; Kandyba, V.; Giampietri, A.; Barinov, A.; Constantinescu, G. C.; Yeung, N.; Hine, N. D. M.; Xu, X.; Cobden, D. H.; Wilson, N. R. Nature 2019, 572 (7768), 220–223. https://doi.org/10.1038/s41586-019-1402-1.
[3] Nguyen, P. V.; Teutsch, N. C.; Wilson, N. P.; Kahn, J.; Xia, X.; Graham, A. J.; Kandyba, V.; Barinov, A.; Xu, X.; Cobden, D. H.; Wilson, N. R. Nano Lett. 2021, 21 (24), 10532–10537. https://doi.org/10.1021/acs.nanolett.1c04172.

Figures

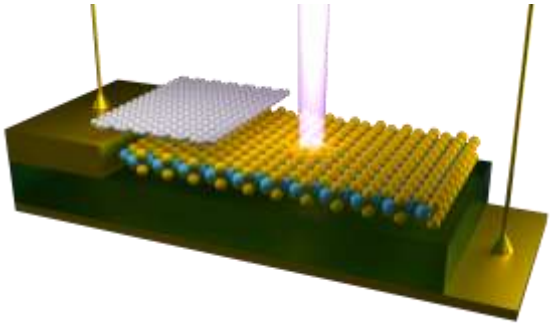


Figure 1: Illustration of 2D heterostructure under inverstigation by nanoARPES

Graphene-based Wireless Interconnects for Next-Generation Computing Systems

Sergi Abadal
Universitat Politècnica de Catalunya, 08034 Barcelona, Spain
abadal@ac.upc.edu

Computing systems are ubiquitous in our daily life and have transformed the way we learn, work, or communicate with each other, to the point that progress is intimately tied to the improvements brought by new generations of the processors that lie at the heart of these systems. However, a common trait of current computing systems is that their internal data communication has become a fundamental bottleneck, rendering traditional interconnects insufficient and threatening to halt progress unless fast and versatile communication alternatives are developed [1-2]. In this context, graphene offers a set of very interesting properties for the creation of miniaturized and tunable antennas [3] and Radio Frequency (RF) circuits, which are proposed as key enablers of a novel approach: wireless chip-scale interconnects [1, 4]. In this talk, recent progress in the design of versatile integrated graphene antennas in the Terahertz band (0.1-1 THz) will be reviewed, stressing the capacity of achieving joint frequency-beam reconfigurability with a very small form factor. The potential impact of such a novel wireless strategy on the microprocessor industry will be illustrated through the analysis of (i) the opportunities that this new paradigm opens at the computer architecture level, and (ii) the technological challenges that need to be overcome along the way.

References

[1] S. Abadal *et al.*, IEEE Wireless Communications Magazine (2022).
[2] S. Rodrigo *et al.*, IEEE Micro, 5 (2021) 48-56.
[3] S. E. Hosseininejad, IEEE Transactions on Nanotechnology, 1 (2019) 734-746.
[4] M. Imani, S. Abadal, P. Del Hougne, Advanced Science (2022).

Figures

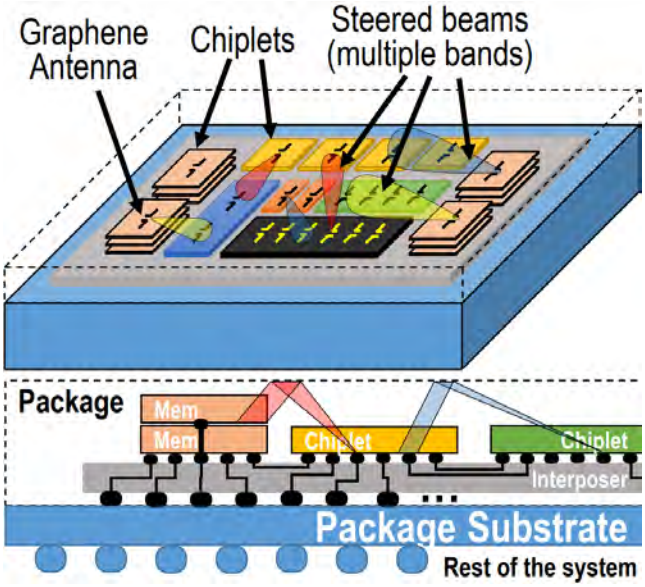


Figure 1: Schematic diagram of a multi-chip computer architecture and whose interconnect fabric is composed of a wired network within the computing package augmented with graphene-based agile wireless links.

Scalable Optoelectronic Devices Based on Two-Dimensional Transition Metal Dichalcogenides

Gerd Bacher[1]
Yannick Beckmann[1], Dominik Andrzejewski[1], Henrik Myja[1], Ulrike Hutten[1], Annika Grundmann[2], Songyao Tang[2], Clifford McAleese[3], Xiaochen Wang[3], Ben Conran[3], Sergej Pasko[4], Simonas Krotkus[4], Holger Kalisch[2], Michael Heuken[2,4], Andrei Vescan[2], Tilmar Kümmell[1]
[1]Werkstoffe der Elektrotechnik and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany
[2]Compound Semiconductor Technology, RWTH Aachen University, 52074 Aachen, Germany
[3]AIXTRON Ltd., Cambridge CB24 4FQ, United Kingdom
[4]AIXTRON SE, 52134 Herzogenrath, Germany
gerd.bacher@uni-due.de

Two-dimensional (2D) transition metal dichalcogenides (TMDCs) exhibit efficient light absorption and light emission combined with sub-nm thickness and are thus attractive for optoelectronic devices on rigid, curved or flexible substrates. While first proof-of-concept devices relied on mechanically exfoliated 2D TMDCs, the transfer to real-world applications is currently in the focus of research activities requiring both scalable materials and scalable device architectures. Here, we report on our recent efforts on the development of scalable concepts for both, light emitting and light sensing devices based on 2D TMDCs.

Wafer-scale films of TMDC monolayers [1] and TMDC heterostructures [2] have been grown in an AIXTRON MOCVD reactor and were integrated into optoelectronic devices with different architectures. First, a vertical p-i-n architecture was chosen for fabricating light emitting devices. Hereby, WS_2 monolayers were embedded between inorganic and organic support layers at the cathode and anode side, respectively. Large-area electroluminescence has been achieved with turn-on voltages as low as 2.5 V on rigid [3] as well as flexible [4] substrates. This concept has been extended by replacing WS_2 with a directly grown type II WS_2-MoS_2 heterostructure to realize a self-powered p-i-n photodetector that exhibits an on-off ratio of 10^5 and an EQE of 17 %.

Second, a lateral device architecture with an interdigital contact mesh was developed for assembling large-area photosensors. The direct growth of a heterostructure comprising WS_2 and MoS_2 monolayers enables device fabrication without involving any transfer process. We demonstrate an enhancement of the responsivity by more than 5 orders of magnitude as compared to a single layer device, which we attribute to an efficient separation of optically generated electron-hole pairs at the WS_2-MoS_2 heterointerface [5]. In photosensors that combine a MOCVD-grown WS_2 monolayer as light sensitizer with CVD-grown graphene as a highly conductive channel, we have been able to shed light on the widely varying values of responsivity reported in literature for such devices. We demonstrate that adsorbate desorption can mask the intrinsic photoresponse in 2D heterostructure photodetectors. By using a multicolor optical pump – electrical probe technique, we disentangle both effects and extract the intrinsic photoresponse [6].

References

[1] A. Grundmann et al., MRS Advances 4 (2019) 593
[2] A. Grundmann et al., MRS Advances 5 (2020) 1625
[3] D. Andrzejewski et al., ACS Photonics 6 (2019) 1832
[4] D. Andrzejewski et al., Adv. Opt. Mat. 8 (2020) 2000694
[5] U. Hutten et al., 2D Materials 8 (2021) 045015
[6] Y. Beckmann et al., submitted

Characterization of 2D materials growth

Dr. Marcello Binetti
Dr. Eugen Speiser
LayTec AG, Seesener Str. 10-13, 10719 Berlin, Germany
marcello.binetti@laytec.de

Ben Conran, Dr. Clifford McAleese, Dr. Xiaochen Wang
AIXTRON Ltd, Buckingway Business Park, Anderson Road, Swavesey, Cambridge CB24 4FQ, UK

Graphene and other 2D materials opened exciting new device and materials possibilities. Thermal chemical vapor deposition (CVD) is among the most promising methods to synthesize 2D materials[1], that are characterized with several powerful (but time consuming) ex-situ techniques like Raman spectroscopy, atomic force microscopy, etc. LayTec's in-situ metrology systems EpiCurve TT enable close control of key deposition parameters like wafer temperature and surface coverage. Therefore, they can accelerate the research on 2D materials and the scale-up of the related industrial production processes. In the following, we will present some results on the analysis of in-situ reflectance, temperature and wafer bow data as measured with an EpiCurve TT during the deposition of Graphene in an AIXTRON reactor. Moreover, we will discuss the advantages of a mapping station combining very accurate Raman spectroscopy [2] with white light reflectance (WLR) measurements, for a fast analysis of wide area samples.

References

[1] Xin Jiat Lee et al., J Taiwan Inst Chem Eng, Volume 98 (2019) 163-180
[2] W.-J. Zhao et al., J. Am. Chem. Soc., 133 (2011) 5941-5946

Figures

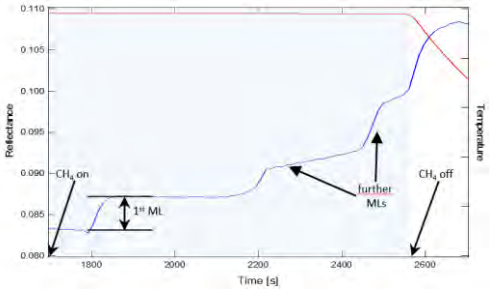
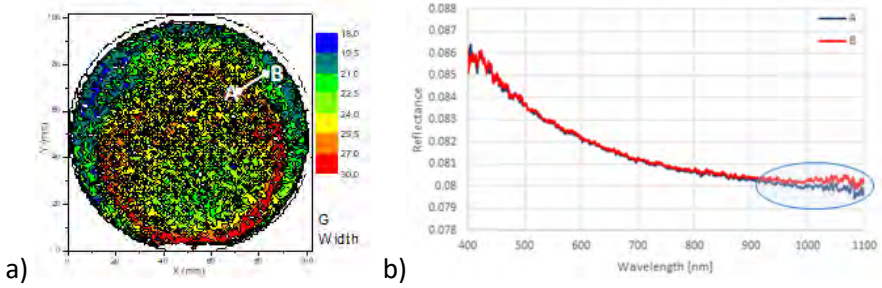


Figure 1: 405nm Reflectance measured in-situ, during the deposition of 3ML of graphene on sapphire allows direct determination of the graphene coverage



a) b)

Figure 2: 1 ML graphene on a 100mm sapphire wafer. Comparison between width of Raman G peak (a) indicating the strain of the layer, and WLR at two position A and B with different strain (b): the NIR portion of the spectra correlates with the strain state of the layer.

Can terahertz spectroscopy become the gold standard of 2D quality control?

Peter Bøggild[1]
Peter Uhd-Jepsen[2]
[1]*DTU Physics and* [2]*DTU Fotonik, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark*
Contact: pbog@dtu.dk

Over the past decade, we demonstrated terahertz spectroscopy to be an efficient tool for fast, non-destructive electrical characterisation of graphene on various substrates [1-4], including silicon, sapphire and polymers. Key parameters such as conductivity, carrier density, carrier mobility and uniformity can be extracted across wafer-scale graphene, and a metrology standard for THz-TDS of graphene was published recently through the International Electrotechnical Commission [3]. Several important questions arise: can THz-QC be applied to roll-2-roll production systems? How reliable and robust is THz-QC, and does it work equally well on all substrates? Will THz-QC be useful for TMDs? For process development? What can we learn about the uniformity and grain structure of 2D films? In this talk I will briefly overview the state-of-the-art and recent progress in THz-based quality control (THz-QC) and address possibilities, problems and open questions related to this emerging technology, and show preliminary results on R2R inline THz-QC, large-scale mapping of TMD films and graphene micro- and nanoribbon gratings.

References

[1] P. Bøggild et al, 2D Materials 4 (2017) 042003
[2] P. W. Whelan et al, 2D Materials 8 (2021) 022003
[3] J. Buron et al, Nano Letters, 12 10 (2012) 5074
[4] J. Buron et al, Nano Letters , 14 (2014) 6348
[5] P. U. Jepsen et al, "Graphene-based material – sheet resistance : terahertz time-domain spectroscopy", IEC TS 62607-6-10:2021 (2021)

Figures

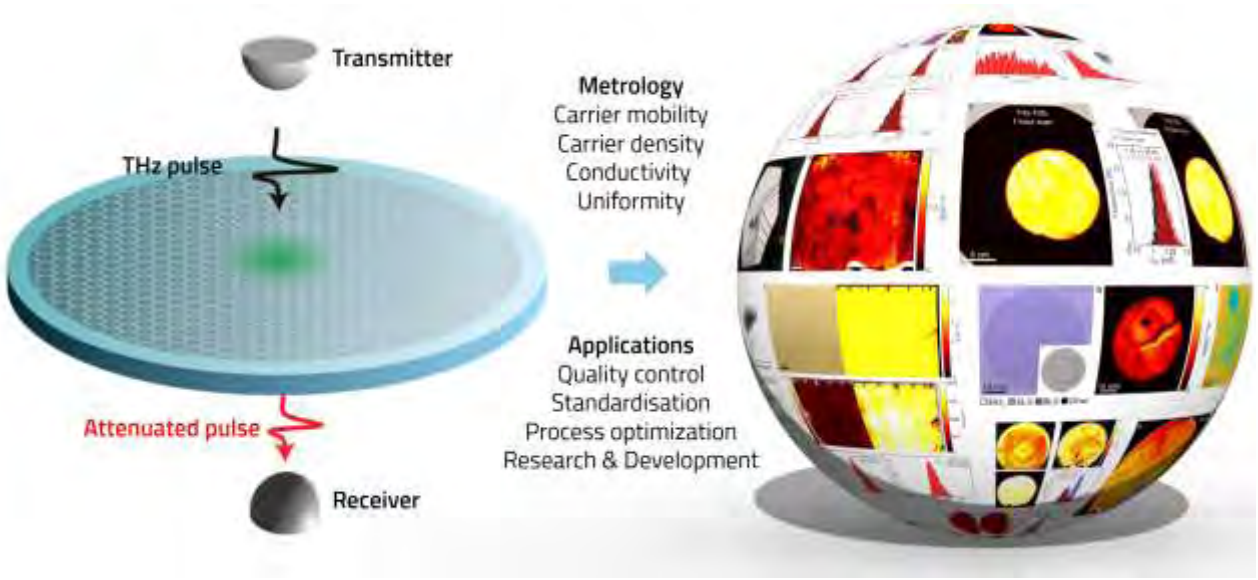


Figure 1: THz time-domain spectroscopy of 2D materials can be used to extract a number of critically important electrical and structural parameters without physical contact or damage, and is a candidate for quality control in 2D large-scale manufacturing.

Industrial production of high-quality 2D crystals for energy applications

Francesco Bonaccorso[a,b]
[a] *BeDimensional S.p.A., Via Lungotorrente Secca 30R, Genova, 16163, Italy*
[b] *Istituto Italiano di Tecnologia, Via Morego 30, Genova, 16163, Italy*

f.bonaccorso@bedimensional.it

In this presentation we will provide an overview of the strategy of BeDimensional in the development of industrial-scale, reliable, inexpensive production processes of graphene and related two-dimensional materials (GRMs).[1-3] This is a key requirement for their widespread use in several application areas,[1-8] providing a balance between ease of fabrication and final product quality. In this context, we will show the effectiveness of the production of GRMs by wet-jet milling [3] and the route towards future Industrial scale up, maintaining the high-quality production ruled by the ISO standard.
Afterward, we will provide a brief overview on some key applications of the as-produced GRMs, with particular focus on the energy sector. In this context, the production of GRMs in liquid phase by wet-jet milling [2,3] represents a simple and cost-effective pathway towards the development of GRMs-based energy devices, presenting huge integration flexibility compared to other production methods. We will provide an insight into some application areas such as anticorrosion coatings and energy conversion and storage devices. [4,8-16]

References

[1] F. Bonaccorso, et. al., *Adv. Mater*. 28, 6136-6166 (2016).
[2] F. Bonaccorso, et al., *Materials Today*, 15, 564-589, (2012).
[3] A. E. Del Rio Castillo et. al., *Mater. Horiz*. 5, 890 (2018).
[4] E. Pomerantseva, F. Bonaccorso, et al., *Science* 366 (6468) eaan8285 (2019).
[5] G. Iannaccone F. Bonaccorso, et al., *Nature Nanotech* 13, 183, (2018).
[6] A. C. Ferrari, F. Bonaccorso, *et al.*, *Nanoscale*, 7, 4598-4810 (2015).
[7] F. Bonaccorso, et. al., *Nature Photonics* 4, 611-622, (2010).
[8] F. Bonaccorso, et. al., *Science*, 347, 1246501 (2015).
[9] L. Najafi et al., *Advanced Energy Materials* 8 (16), 1703212 (2018).
[10] E. Lamanna et al., *Joule* 4, 865-881 (2020).
[11] S. Bellani, et al., Chem. Soc. Rev. 50, 11870-11965 (2021).
[12] M. Garakani, et al. *Energy Storage Materials 34, 1-11* (2020).
[13] S. Bellani, et al. *Nano Lett*. 18, 7155-7164 (2018).
[14] A. E. Del Rio Castillo, et al., Chem. Mater. 30, 506-516 (2018).
[15] S. Bellani, et al. *Nanoscale Horizons* 4, 1077 (2019).
[16] L. Najafi, et al. *ACS Nano 16, (1), 351–367* (2022).

"This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement GrapheneCore3 - 881603"

Exotic properties of 2D materials: physics and real expectations for applications

Paolo Bondavalli
Thales Research and Technology, 1,Av Fresnel, Palaiseau, France
Paolo.bondavalli@thalesgroup.com

Abstract

The recent discoveries of exotic properties of 2D materials have opened the horizons for potential new applications that can finally project us in the Beyond CMOS realm. Indeed, 2D materials when discovered have been implemented in Moore's approach as in case of 2D used for transistors. This is not the right approach in order to achieve real advances in physics and in defining the implementation of the new roadmaps for new devices based on innovative concepts. In this contribution, we will analyse the main phenomena recently discovered such as magic angle, valleytronics and 2D topological insulators in order to understand which are the potential applications of these devices. We will analyse in a completely objective way which are the main potential implementations of these phenomena. We will perform a roadmap identifying the major turning point in each case. This analysis will allow to have a precise idea of what could be only a hype phenomenon and what could be a real game changer for specific applications.

References

[1] 2D Materials: And Their Exotic Properties (De Gruyter Stem) Planned Publication: July 4, 2022, ISBN: 9783110656329

Industrial applications of Monolayer Graphene on polymer

Vincent Bouchiat
Grapheal, 25 avenue des Martyrs, 38042 Grenoble Cedex 09
vbouchiat@grapheal.fr

After a more than a decade and tens of thousands of publications, graphene produced by chemical vapour deposition on copper foils still remain at the sweet spot regarding cost , speed and quality for large scale production of monolayers on insulators. I will briefly recall the principle of these techniques and then present the use of this process for the industrial production of medical-grade films . In particular I will be insisting on the possibility to combine therapeutics (biostimulation, healing) and diagnostics (biosensing) features in the same device.
I will also present more recent works on the realization of in vitro diagnostics based on the same material. we are developing a concept of an electronic strip based on a new material for medicine, graphene, whose maturity finally allows its introduction at the industrial scale. The implementation of synthesis techniques of this material from microelectronics allows to produce it in mass at low cost using clean-room free processes based on printed electronics. These sensors are connected and powered by a simple smartphone link. They can be easily coupled with a digital monitoring solution via the smartphone that will improve the diagnosis in the field and the monitoring of chronic diseases. I will detail the functioning of the testNpass™, for the detection of the SARS-CoV-2 virus, in particular the process of conversion of the biochemical signal into an electrical signal. Finally, I will show that a myriad of other use cases of this technology exists beyond the Covid crisis.

References

[1] https://www.grapheal.com
[2] Flyer available at https://tinyurl.com/2s46bd6w
[3] Flyer available at https://tinyurl.com/4fm4ck39

Figures

Figure 1: WoundLAB™ , a platform for wound management and healing monitoring

Figure 2: TestNpass™, a secure & biometric antigen biosensor generating a tamperproof digital sanitary certificate.

Theory and optimization of graphene photothermoelectric detectors

Aron W. Cummings
Aleandro Antidormi
Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain
aron.cummings@icn2.cat

This talk is part of the info session for the ULISSES project, which aims to develop a cheap, compact, efficient, and low-power multi-gas sensor. Here I will discuss the design and optimization of the photodetector component of the gas sensor, which is based on the photothermoelectric effect (PTE) in graphene [1-4]. There are many design parameters impacting the performance of this detector, including the light profile, the device geometry, and the material quality.

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. 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 [5].

References

[1] X Cai et al., Nat Nanotechnol 9, 814 (2014)
[2] S Schuler et al., Nano Lett 16, 7107 (2016)
[3] S Castilla et al., Nano Lett 19, 2765 (2019)
[4] J Muench et al., Nano Lett 19, 7632 (2019)
[5] A Antidormi and AW Cummings, Phys Rev Appl 15, 054049 (2021)

Figures

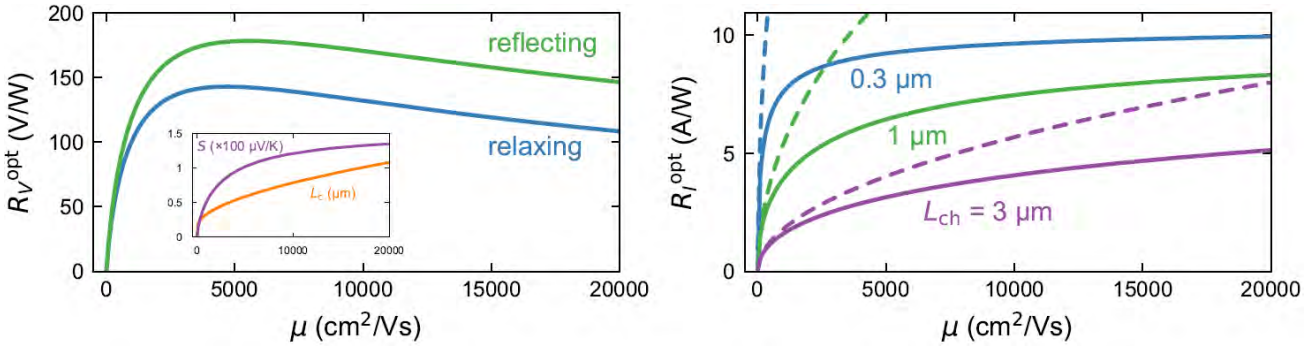


Figure 1: Optimal photovoltage (left) and photocurrent (right) as a function of graphene carrier mobility. In both cases, the photoresponse saturates for a mobility around 5000 cm2/Vs.

Customer-oriented development of graphene materials for commercial applications

Alessandro Dani
LayerOne AS, Oksenøyveien 10, 1366 Lysaker, Norway
alessandro.dani@layeronematerials.com

Graphene, and graphene-based material, have been considered wonder materials. Thanks to their incredible properties they could theoretically be utilized in a multitude of applications, ranging from composites to electronics. Still, many years went by since the first graphene synthesis in 2004, and yet, these materials are not integral part of our lives, they are not included in almost any product that surrounds us. The commercial use of graphene materials is still limited to few applications in niche products. Are we in the bottom part of the hype cycle, the so called "Trough of Disillusionment"? If this is the case, how can we get out of this rut?

Our perspective is that the graphene industry is currently facing a chicken-egg situation. Graphene materials are too expensive; even their amazing properties are not good enough to offset the extra costs. This leads to a low market demand for graphene materials. A low market demand makes it difficult to exploit economy of scale to drive down the cost of the material to an acceptable level.

How can we overcome this impasse? Our strategy is to put deep technical expertise at the service of customer-oriented development of new products. All while making sure to access the capital to scale-up the business.

To develop technical expertise, we put effort on upstream R&D aimed to reach technical breakthroughs and to develop transformative innovations, which create graphene materials that could serve as a base for new products.[1] To make sure our R&D efforts are focused on generating value for the customers, we listen closely to their needs and we create custom made graphene materials that are designed to suit their processes and to improve their products.[2]

Industrial collaborations between graphene manufacturers and the companies that make use of it, are crucial to open the way to the commercial application of graphene materials and to their industrialization. In this way the end users, meaning all of us, will get the full advantages of the use of "the wonder material" in our lives.

References

[1] Ahmad Umar, Ceramics International, (2022) (doi.org/10.1016/j.ceramint.2022.05.371)
[2] María Cámara-Torres, Nanoscale, 13 (2021), 14382

Direct growth of PtSe2 for integration of photonic devices

Georg S. Duesberg
Institute of Physics, EIT 2, Faculty of Electrical Engineering and Information Technology, Institute of Physics, Universität of the Bundeswehr Munich &
SENS Research Center
Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany
georg.duesberg@unibw.de

Two-dimensional materials such as transition metal dichalcogenides (TMDs) are intensively investigated because of their potential applications in future electronics. Thickness dependent electronic and optical properties such metal-to-semiconductor transitions, high mobilities, and low temperature synthesis have moved the group 10 (Pt/Pd) TMDs or Nobel Metal Dichalcogenides (NMDs) to the center of attention. These layered materials have shown high potential for NEMS, optoelectronic devices and chemical sensors.
The low temperature synthesis of various polycrystalline TMDs is presented in this talk. [1] The composition and morphology of the grown films are investigated by several characterization techniques including Raman spectroscopy, SPM and X-ray photoelectron spectroscopy. Challenges in the understanding of the structure-property relationship of polycrystalline TMD films are discussed. The effects of growth parameters and underlying substrates on the film properties are investigated, to gain further understanding of the films. [2] The low temperature synthesis allows the back end of line (BEOL) integration compatible with silicon technology. [3] In this regard, examples for high performance chemical sensors, [1] IR-photodetectors[4] and MEMS[5] devices with PtSe2 will be presented

References

[1] Yim et al. ACS Nano, 10 (10), 9550 2016.
[2] Lukas et al., Advanced Functional Materials 31 (35), 2102929 2021
[3] Prechtl et al. Advanced Functional Materials 31 (46), 2103936 2021
[4] Yim, et al. Nano Letters, 3 (18), 1794 2018
[5] Wagner et al. Nano Letters, 8 (6), 3738 2018

Low temperature 2D growth and its need for the IC industry

Salim El Kazzi[1,2*], Lum Ya Woon[2], Vejay Girija Jagadeesan[1,2], Ivan Erofeev[2], Saumitra Vajandar[2], Thomas Osipowicz[2], Sergej Pasko[3], Simonas Krotkus[3], Wang Xiaochen[4], Ben Coran[4], Oliver Whear[4] and Utkur Mirsaidov[1,2]

[1]*NUS-AMAT Advanced Materials Corporate Lab, 5 Engineering Drive 1, 117608 Singapore*

[2]*Department of Physics, National University of Singapore, 2 Science Drive 3, 117551 Singapore*

[3] *AIXTRON SE, Dornkaulstr. 2, Herzogenrath, 52134 Germany*

[4] *AIXTRON Ltd, Anderson Road, Buckingway Business Park, Cambridge CB24 4FQ, UK*

*dbssali@nus.edu.sg

The increasing demand for 2D materials in the IC industry is highlighting the need for wafer-scale and fab-compatible techniques to synthesize 2D materials like graphene, h-BN and transition metal dichalcogenides. Most of recent studies indicate that high-temperature growth processes are needed to produce large 2D grains and thus better device performance [1]. The main integration scheme is nowadays the 2D growth on foreign substrates (like sapphire, metal foils, and etc) and an additional transfer step to integrate the 2D layer on a Si-compatible substrate. However, this integration scheme can cause technological limitations for some of the FAB production processes, especially if 2D would be integrated on non-planar structures (like trenches, nanowires, etc…). Furthermore, the high temperature growth of some 2D materials seems to induce more vacancy defects than low temperature processes, which, in turn, deteriorates the intrinsic properties of the material [2].

In this work, we give an overview of main CMOS applications where 2D materials are expected to play an important role. In the first part, we will describe in more details the use of 2D materials as Cu-diffusion barriers in future BEOL interconnects. Then, we highlight the barrier efficiency of our wafer-scale WS_2 grown by MOCVD. We demonstrate that crystalline 2D barrier layers can also be used as liner replacements in order to improve the metal conductivity in scaled trenches. In a second part, we will discuss the synthesis of freestanding amorphous 2D layers. We will conclude by highlighting the impact of molecular beam deposition conditions on the quality of amorphous 2D transition metal dichalcogenides.

Our results shed more light on low-temperature 2D growth and its impact on different optoelectronic applications. This is expected to play a pivotal role in pushing forward the roadmap of 2D integration into Si-CMOS technology.

References

[1] S. H. *Choi et al.*, Nature communications (2022) 13:1484

[2] E. Mitterreiter *et al.*, Nature communications (2021) 12 3822

Graphene Standardization – Status update and future

Norbert Fabricius
Werner Bergholz, Gerd Weking
ISC - International Standards Consulting GmbH & Co. KG, Verdistr. 15A, 30989 Gehrden, Germany
isc-office@isc-team-eu

During the autumn 2012 meeting of IEC/TC 113 in Milpitas (CA) the potential of graphene for electrotechnical products and systems was discussed in detail for the first time under the aspect of electrotechnical standardization. The starting point of the discussion was, of course, the extraordinary electrical properties of the material. However, the materials available on the market under the trade name graphene often had little to nothing to do with real graphene. It was therefore clear from the beginning that the availability of technical specifications and standardized measurement procedures for the properties (Key Control Characteristics, KCCs) specified therein is an indispensable prerequisite for the technical use of graphene. In addition to direct electrical properties, such as electrical conductivity, the list of KCCs to be specified also includes structural, chemical, and mechanical properties, as these significantly determine the performance of the electrotechnical end products.

Ten years later, after a decade of intensive research and development, graphene is increasingly finding its way into the industrial production of new and/or improved products. This process is supported by the development of standards demanded by the industry. This lecture will report on the current status of graphene standardization:

Where do we stand? Where will the focus for standardization activities be in the coming years?

In any case, the need to develop new standards remains high and participation in standardization is becoming increasingly important for the competitive situation of companies.

Stefan Gomes da Costa
Jan Englert, Thomas Dieing, and Ute Schmidt
WITec GmbH, Lise-Meitner Str. 6, Ulm, Germany (www.witec.de)
Stefan.Gomesdacosta@witec.de

The characterization of 2D materials such as graphene or transition metal dichalogenides (TMDs) often require more than a single characterization technique to gather comprehensive information in order to understand and predict their behavior for specific applications. Graphene[1] and TMDs[2] have a layered structure in common, with significantly changes their properties when compared to in the bulk making them very attractive materials for electronic designs. The optimization of electronic device performance is strongly tied to the structure, degree of crystallinity and exciton dynamics of 2D materials. The scope of this contribution is to provide insight into how a combination of spectroscopic (Raman/Photoluminescence) and microscopy techniques (confocal/AFM/SEM) contribute to an ample characterization of such 2D materials.
Raman spectroscopy and more importantly still, Raman imaging proved to be of great value due to clearly different spectra obtained from single, double, triple and multi-layered 2D materials. Furthermore, Raman imaging is by now routinely used to determine strain, doping type and level, stacking, chirality and disorder in graphene. All these information can be extracted from Raman spectroscopy and imaging can well be complemented with other techniques such as various forms of atomic force microscopy (AFM), Scanning Nearfield Optical Microscopy (SNOM), Current sensing, scanning electron microscopy (SEM) or measurements at low temperatures (<10K) and under high magnetic fields (up to 9T).
The two dimensional forms of TMD materials are also often characterized using the same experimental methods. Fig. 1 shows an example of a correlative Raman-SEM measurement of CVD grown MoS_2. For this group of 2D materials the information obtained through the combination of the techniques is even more valuable since the transition of indirect to direct semiconductor when going to a single layer gives rise to pronounced photoluminescence (PL)[3], which can easily be measured with exceptionally high resolution using SNOM-PL.
In this contribution we illustrate the benefit of correlating the above mentioned techniques spatially applying confocal Raman imaging in order to deepen the understanding of the samples under investigation.Abstract (Century Gothic 11)

References

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V.Grigorieva and A. A. Firsov, Science 306 (2004) 666
[2] M. Xu, T. Liang, M. Shi and H. Chen, Chem. Rev. 113 (2013) 3766
[3] A. Steinhoff, J.-H. Kim, F. Jahnke, M. Rösner, D.-S. Kim, C. Lee, G. H. Han, M. S. Jeong, T. O. Wehling and C. Gies, Nano Lett. 15 (2015) 6841

Figures

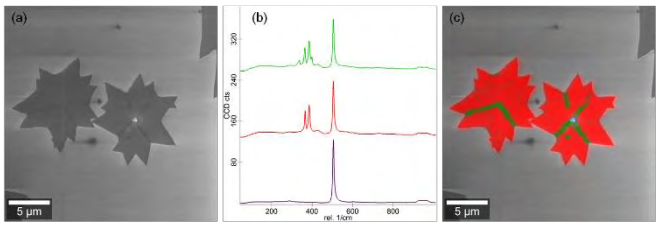


Figure 1: SEM-Raman imaging of CVD grown MoS2 on a Si-substrate: (a) SEM image, (b) Raman spectra evaluated from the 2D spectral array of a Raman image, and (c) RISE image, a combination of SEM and Raman image of the same sample area. The colors in the RISE image match the colors of the Raman spectra.

Enabling a world of enhanced perception

Stijn Goossens
Qurv Technologies S.L., Carrer d'Esteve Terrades 1, 08860 Castelldefels (Barcelona), Spain
stijn.goossens@qurv.tech

Qurv develops wide-spectrum image sensor technologies and integrated solutions to enable next-gen computer vision applications, addressing the expanding needs of an autonomous and intelligent new world. Qurv's technology leverages current CMOS scalable manufacturing and quantum materials to unlock new levels of performance, reliability and function in XR devices, service robots and automotive.

Qurv image sensors based on CMOS compatible quantum materials such as 2D materials and colloidal quantum dots are sensitive to visible (Vis), near-infrared (NIR) and short-wave infrared (SWIR) light: from 300 nm up to 2 µm and in the near future beyond 2 µm. [1,2] Sensitivity in the range beyond silicon CMOS imager sensitivity (>1 µm wavelength) provides for dramatically reduced sunlight interference and eye safe LIDAR operation. Furthermore, sensitivity in the SWIR range can enable true night vision, all weather vision and molecular vision.

References

[1] Akinwande, D., Goossens S., *et al.* Graphene and two-dimensional materials for silicon technology. *Nature* vol. 573 507–518 (2019).
[2] Goossens, S. *et al.* Broadband image sensor array based on graphene-CMOS integration. *Nat. Photonics* (2017)

Figures

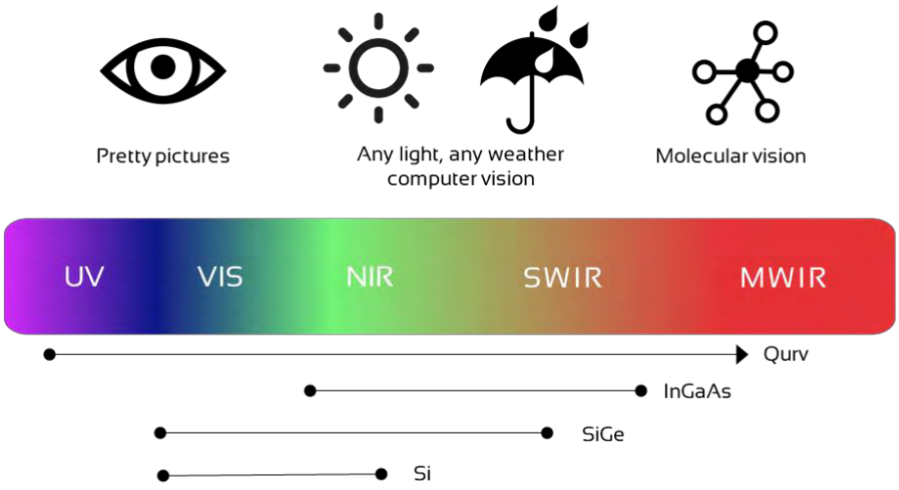


Figure 1: *The accessible electromagnetic spectrum with different imaging technologies and their respective spectral range. The icons illustrate the advantages for different types of use cases enabled by the different ranges of the spectrum.*

Limitations and opportunities of metal-organic chemical vapor deposition of MoS_2 and WS_2

Benjamin Groven
Yuanyuan Shi, Henry Medina Silva, Vladislav Voronenkov[1], Dries Vranckx, Raf Rennen, Wim Huysecom, Jarne De Boeck, Brecht De Vos, Sebastiaan Nijs, Sreetama Banerjee, Quentin Smets, Tom Schram, Xiangyu Wu, Dennis Lin, Inge Asselberghs, Stefan De Gendt[1], Pierre Morin
imec, Kapeldreef 75, Leuven, Belgium; [1]KU Leuven, Celestijnenlaan 200F, Leuven, Belgium
Benjamin.Groven@imec.be

Group-VI transition metal dichalcogenides (MX_2), such as molybdenum- and tungsten disulfide (MoS_2, WS_2), emerge as two-dimensional (2D) semiconductors that can complement workhorse silicon as channel material in ultra-scaled nanoelectronic devices [1,2]. Manufacturable approaches to deposit highly crystalline MX_2 layers, tailor the layer number down to the atomic level, and remain compatible with temperature sensitive structures, are essential to unlock the desired material functionality. However, fundamental understanding is lacking on how to design Fab-compatible chemical deposition processes for 2D MX_2, such as chemical vapor deposition (CVD). This presentation focuses on metal-organic (MO-)CVD from metal hexacarbonyl and dihydrogen sulfide precursors using industry-standard, customized 200 mm and 300 mm epitaxial reactors. Based on a qualitative growth model, we review the limitations and opportunities of MX_2 MOCVD, such as poor diffusional transport of adsorbed surface species and undesired metal co-deposition (Figure 1). We describe how the MX_2 growth behavior depends on the starting surface by comparing the nucleation and growth evolution on an amorphous (e.g., SiO_2) and single crystalline (e.g., sapphire) substrate using complementary microscopy and spectrometry techniques [3]. From that insight, we reveal how these limitations can be overcome, yielding microcrystalline MoS_2 monolayers on sapphire with median mobilities at 30 cm^2/Vs and drive currents up to 420 µA/µm [4].

References

[1] Q. Smets et al., IEDM, 23.2. 1-23.2. 4 (2019)
[2] D. Lin et al., Symposium on VLSI Technology, 1-2 (2021)
[3] Y. Shi et al., ACS Nano, 15 (2021) 9482-9494
[4] Wu et al., IEDM, 7.4.1-7.4.4 (2021)

Figures

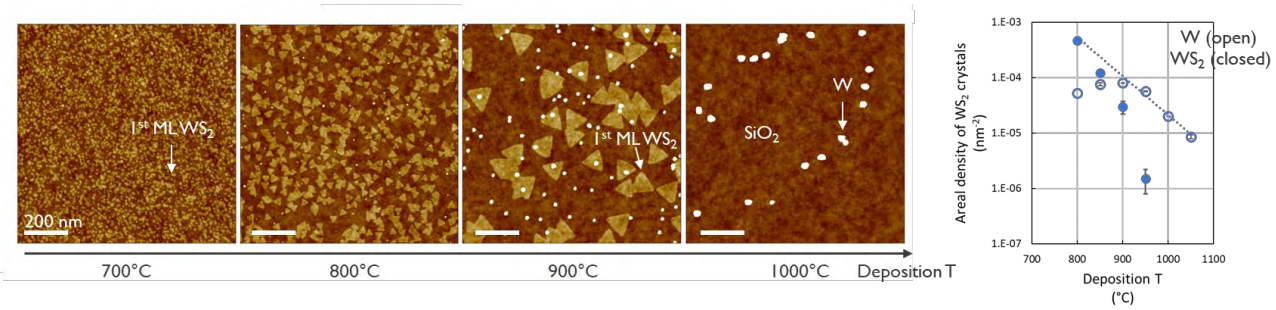


Figure 1: Growth evolution of WS_2 MOCVD on amorphous SiO_2 starting surface as a function of deposition temperature. W and WS_2 are simultaneously deposited. The areal density of WS_2 crystals decreases with deposition temperature but remains high at technologically relevant deposition temperatures introducing grain boundaries when neighbouring crystals coalesce.

Integrated optical gas sensors based on silicon photonics and 2D materials

Kristinn B. Gylfason
Pen-Sheng Lin, Arne Quellmalz, Po-Han Huang, Gaehun Jo, Frank Niklaus
KTH Royal Institute of Technology, Malvinas väg 10, Stockholm, Sweden
Nour Negm[†,‡], Shayan Parhizkar[†,‡], Stephan Suckow[†], Anna Lena Giesecke[†], Max C. Lemme[†,‡]
[†]*AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen, Germany*
[‡]*Chair of Electronic Dev., RWTH Aachen University, Otto-Blumenthal-Str. 25, 52074Aachen, Germany*
Sarah Zayouna, Eleonora De Luca, Stephan Schröder, Floria Ottonello-Briano
SenseAir AB, Stationsgatan 12, Delsbo, Sweden
gylfason@kth.se

Abstract

Optical spectroscopy is among the most important chemical analysis techniques, due to its high specificity and long-term stability. For spectroscopic analysis of gas compositions, the mid infrared (mid-IR) region is particularly important, owing to the rovibrational resonances in that spectral range. Hence, there is great interest in miniaturizing and reducing the power consumption of optical spectroscopic sensors, but until recently the mid-IR range has been out of reach. Within the European projects ULISSES and AEOLUS, we are working on miniaturization of mid-IR optical gas sensors, by combining silicon photonics and 2D materials. We discuss our work on integrated optical waveguides [1,2], emitters [3] and detectors, as well as wafer-level packaging of sensors [4], and demonstrate spectroscopic sensing of carbon dioxide (CO_2) using an integrated silicon waveguide at the strong absorption peak at 4.23 µm wavelength.
This work has received funding from the European Union through H2020 Industrial Leadership 101017186 (AEOLUS), H2020 780283 (MORPHIC), H2020 825272 (ULISSES),

References

[1] F. Ottonello-Briano, C. Errando-Herranz, H. Rödjegård, H. Martin, H. Sohlström, and K. B. Gylfason, Opt. Lett., 45, (2020), doi: 10.1364/OL.45.000109.
[2] P-S. Lin, A. Quellmalz1, P-H. Huang, S. Parhizkar, N. Negm, S. Suckow, F. Ottonello-Briano, M. C. Lemme, F. Niklaus, and K. B. Gylfason, Proc. CLEO (May 2022).
[3] N. Negm, S. Zayouna, S. Parhizkar, P-S Lin., P-H Huang., S. Suckow, S. Schröder, E. De Luca, F. Ottonello Briano, A. Quellmalz, F. Niklaus, K. B. Gylfason, M. C. Lemme, Proc. Device Research Conference (DRC) (June 2022).
[4] G. Jo et al., Photonics Research, 10, (2022), doi: 10.1364/PRJ.441215.

Figures

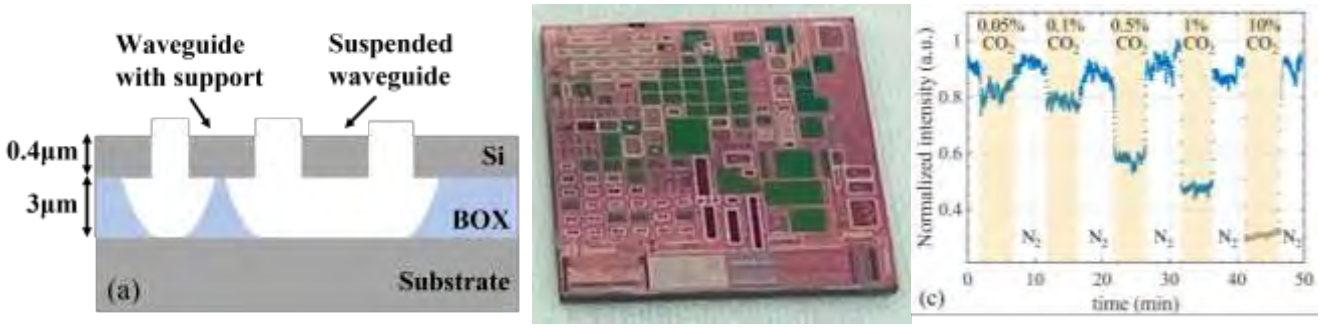


Figure 1: (a) Illustration of the waveguide cross-section. (b) Photonic chip with wafer-level sealed vacuum cavities [4]. (c) Sensing of five CO_2 concentrations with a 7 cm long waveguide. The signal at 10% CO_2 drops out of the sensing range [2].

Raman Characterization of 2D Materials

Oliver Hartwig[1]
Max Prechtl[1], Rita Tilmann[1], Sebastian Lukas[2], Arne Quellmalz[3], Corinna Weiß[4], Kristinn B. Gylfason[3], Max C. Lemme[2,5], Frank Niklaus[3], Andreas Hirsch[4], Georg S. Duesberg[1]
1 Institute of Physics, EIT 2, Faculty of Electrical Engineering and Information Technology University of the Bundeswehr Munich & SENS Research Center Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany
2 RWTH Aachen University Otto-Blumenthal-Str. 2, 52074 Aachen, Germany
3 Division of Micro and Nanosystems, School of Electrical Engineering and Computer Science, KTH Royal Institute of Technology, Stockholm, Sweden
4 Chair of Organic Chemistry II Friedrich-Alexander Universität (FAU) Erlangen-Nürnberg Erlangen 91058, Germany
5 AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen, Germany
georg.duesberg@unibw.de

In recent years there has been increased interest in exploiting the remarkable properties of 2D materials for novel electronic devices. The synthesis of 2D materials is still under development and is always in need of quality control. Post-growth processing often includes lithography and transfer techniques allowing the integration of 2D materials on full wafer scale. Raman spectroscopy provides a fast and contactless method for accessing material quality and homogeneity. With this it enables monitoring of the device fabrication helping to find ways preserving material integrity while undergoing several processing steps.
Raman spectroscopy performed as imaging provides material data distributed over the materials surface. Homogeneity, composition, and location of structural defects can be identified. With high lateral and vertical resolution in the sub-µm range, even 3D-data of materials stacks can be extracted.
Raman imaging was successfully employed in the characterization of heterostructures of large-scale MoS_2 and graphene on silicon wafers, fabricated by wafer bonding [1].
Also, functionalization of 2D materials can be evaluated by Raman spectroscopy. The arrangement of perylenes on thin MoS_2 and graphene films was analysed. Preferred accumulation of the molecules to the 2D materials rather than the SiO_2 substrate was observed [2].
Direct post-growth analysis after synthesis of 2D materials such as of TAC-grown $PtSe_2$ is performed to gauge material quality. The Raman mode width of the grown materials can be used as quality metric and was correlated to electrical properties such as field-effect mobility and sheet resistance [3].
This work has received funding from the German Ministry of Education and Research (BMBF) under grant agreement 16ES1121 (ForMikro-NobleNEMS) and from the European Union's Horizon 2020 research and innovation programme under grant agreements 829035 (QUEFORMAL), 825272 (ULISSES), 881603 (Graphene Flagship Core 3), and 881603 (GREAT).

References

[1] A. Quellmalz et al., Nat. Commun., 1 (2021) 1–11
[2] R. Tilmann et al., Adv. Electron. Mater., 7, (2021) 31–33
[3] [1] S. Lukas et al., Adv. Funct. Mater., 35 (2021) 2102929

Figures

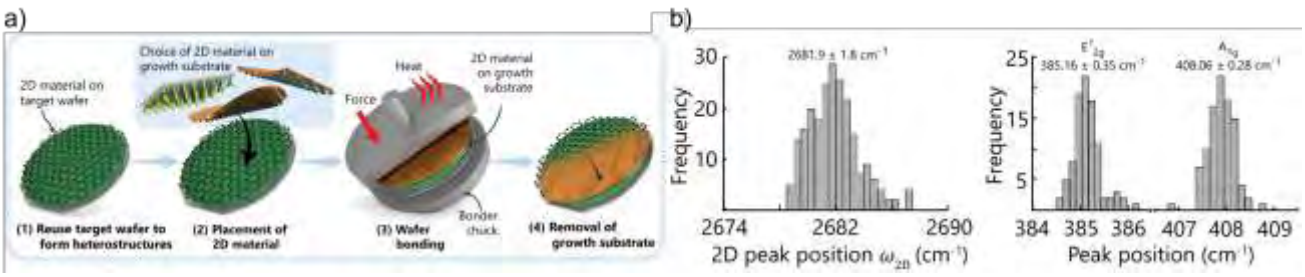


Figure 1: a) Formation of 2D material heterostructures by wafer-bonding. b) Raman characterization of the formed MoS_2/graphene heterostructure by statistical analysis of imaging data.

NanoFrazor Technology: Enabling Unique 2D Material Device Fabrication

N. Hendricks
M. Käppeli, J. Vergés, J. Chaaban, and E. Çağin
Process and Applications Lab., Heidelberg Instruments Nano, Bändliweg 30, 8048 Zürich, Switzerland
nicholas.hendricks@himt.ch

2D materials are enabling exciting new electrical and optical devices. To realize the true potential of such novel materials, nanofabrication techniques and processes must advance equally. One nanofabrication technique that is gaining interest in the 2D material community, both academically and industrially, is that of thermal scanning probe lithography (t-SPL) facilitated by the NanoFrazor technology [1]. As a direct-write nanolithography technique, t-SPL generates patterns by scanning a cantilever with an ultrasharp tip (radius <10nm) over a sample surface to induce local changes with a thermal stimulus (via an integrated heating element), all without the need for energetic particles. Integrated within the cantilever is a thermal topography sensor that allows for real time surface topography measurements that enables closed-loop grayscale patterning (with 1nm vertical accuracy [2]) and marker-less overlay to generate patterns on 2D materials (with <5nm precision [3]) without the aid of alignment markers.

Within this presentation, the background and workings of t-SPL will be briefly introduced and nanostructuring on 2D materials will be discussed along with electrical and optical device performance for 2D material-based devices fabricated with t-SPL.

References

[1] Howell et al., Microsystems & Nanoengineering, 6 (2020) 21
[2] Kulmala et al., Proc. SPIE 10584, Novel Patterning Technologies 2018, 1058412 (2018)
[3] Rawlings et al., IEEE Transactions on Nanotechnology, 6 (2014) 1204
[4] Zheng et al., Nature Electronics, 2 (2019) 17

Figures

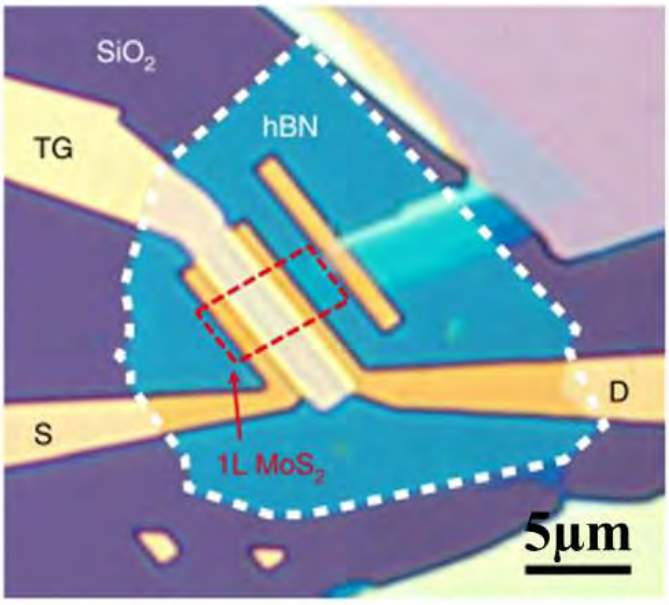


Figure 1: Optical microscope image of single layer molybdenum disulfide (MoS_2) with h-BN dielectric. Source (S), drain (D), and top-gate (TG) electrodes were patterned with t-SPL. [4]

Scalable Two-Dimensional Semiconductors for Electronics and Photonics

Deep Jariwala
University of Pennsylvania, Philadelphia, PA, USA
dmj@seas.upenn.edu

Abstract

The isolation of a growing number of two-dimensional (2D) materials has inspired worldwide efforts to integrate distinct 2D materials into van der Waals (vdW) heterostructures. While a tremendous amount of research activity has occurred in assembling disparate 2D materials into "all-2D" van der Waals heterostructures and making outstanding progress on fundamental studies, practical applications of 2D materials will require a broader integration strategy. I will present our ongoing and recent work on integration of 2D materials with 3D electronic materials to realize logic switches and memory devices with novel functionality that can potentially augment the performance and functionality of Silicon technology. First, I will present our recent work on gate-tunable diode[1] and tunnel junction devices[2] based on integration of 2D chalcogenides with Si and GaN. Following this I will present our recent work on non-volatile memories based on Ferroelectric Field Effect Transistors (FE-FETs) made using a heterostructure of MoS_2/AlScN[3, 4] and I also will present our work on Ferroelectric Diode devices also based on thin AlScN.[5]

Next, I will present our work on light-trapping in excitonic systems[6] namely, 2D chalcogenides and halide perovskites. I will present the effect of nano-structuring on hybridization between excitons, plasmons and cavity photons.[7] I will extend this concept to artificial superlattice of 2D excitonic materials[8] as well as natural superlattices in the form of 2D halide perovskites[9] and demonstration of hybrid exciton-polariton emission at room temperatures.[10] If time permits, I will discuss our recent results on light trapping and giant linear dichroism in 2D antiferromagnetic semiconductors.[11] I will end by giving a broad perspective on future opportunities of 2D and other low-dimensional materials in basic science and applied microelectronics technology.

References

1. Miao, J.; et al. Jariwala, D., *Nano Letters* **2020,** *20* (4), 2907-2915.
2. Miao, J.; et al.Jariwala, D., *arXiv preprint arXiv:2111.06396* **2021**.
3. Liu, X.; et. al. Jariwala, D., *Nano Letters* **2021,** *21* (9), 3753-3761.
4. Kim, K.-H.; et al. Jariwala, D., *arXiv preprint arXiv:2201.02153* **2022**.
5. Liu, X.; et al. Jariwala, D., *Applied Physics Letters* **2021,** *118* (20), 202901.
6. Anantharaman, S. B.; Jo, K.; Jariwala, D., *ACS Nano* **2021**.
7. Zhang, H.; et al. Jariwala, D., *Nature Communications* **2020,** *11* (1), 3552.
8. Kumar, P.; et al. Jariwala, D., *Nature nanotechnology* **2022,** *17* 182–189.
9. Song, B.; et al. Jariwala, D., *ACS Materials Letters* **2021,** *3* (1), 148-159.
10. Anantharaman, S. B.; et al. Jariwala, D., *Nano Letters* **2021,** *21* (14), 6245-6252.
11. Zhang, H.; et al. Jariwala, D., *Nature Photonics* **2022,** *16*, 311-317.

From labs to pilot lines: Graphene and related materials device fabrication solutions

Dr Harm Knoops
Oxford Instruments Plasma Technology, North End, Yatton, Bristol, UK
Harm.knoops@oxinst.com

Extensive efforts in the research and development of graphene-based technologies over the last 15 years has resulted in steady increase in technology readiness. Today, we see an emergence in efforts for development of graphene-based applications (such as modulators, detectors, gas and biosensors) at scale. For successful scaling up of prototypical applications demonstrated to date, robust technologies, and processes for large area device fabrication are required.

Traditionally, plasma-based processing has been thought of as too harsh to achieve high-quality graphene devices, as any ion/radical interaction with the graphene surface can result in physical damage to the 2D hexagonal structure. In contrast pure thermal deposition of dielectrics suffer from lower film quality and nucleation challenges. In this work, we show that remote plasma techniques enable the deposition of high-quality thin layers of Al_2O_3 on single layer graphene using either transferred hBN or an in-situ deposited seed layer, with negligible damage. Furthermore, utilising plasma enhanced techniques broadens graphene applications to thermally sensitive substrates/devices expanding the range of potential applications for graphene based electrical devices.

In this talk I will first give an overview of lab & fab technologies developed at Oxford Instruments and collaboration partners towards growth of Graphene, other layered materials and heterostructures by CVD and ALD followed by our developments in technology for device fabrication processes such as dielectric deposition by ALD and device pattern etching by RIE and ALE.

Advanced data encryption using two-dimensional materials

Mario Lanza
Physical Science and Engineering Division, King Abdullah University of Science and Technology
Mario.lanza@kaust.edu.sa

Advanced data encryption requires the use of true random number generators (TRNG) to produce unpredictable sequences of bits. TRNG circuits with high degree of randomness and low power consumption may be fabricated by using the random telegraph noise (RTN) current signals produced by polarized metal/insulator/metal (MIM) devices as entropy source. However, the RTN signals produced by MIM devices made of traditional insulators, i.e. transition metal oxides like HfO_2 and Al_2O_3, are not enough stable due to the formation and lateral expansion of defect clusters, resulting in undesired current fluctuations and the disappearance of the RTN effect. In this talk I will present the fabrication of highly stable TRNG circuits with low power consumption, high degree of randomness (even for a long string of 224-1 bits) and high throughput of 1 Mbit/s by using MIM devices made of multilayer hexagonal boron nitride (h-BN); we also demonstrate their application to produce one time passwords ideal for the internet-of-everything. The superior stability of the h-BN based TRNG is related to the presence of few-atoms-wide defects embedded within the layered and crystalline structure of the h-BN stack, which produces a confinement effect that avoids their lateral expansion and results in stable operation.

References

[1] C. Wen et al. Advanced Materials, 33, 2100185 (2021)
[2] Shaochuan Chen et al. Nature Electronics 3, 638-645 (2020)
[3] Yuanyuan Shi et al. Nature Electronics 1, 458–465 (2018)
[4] Fei Hui et al. Nature Electronics, 2, 221-229 (2019)
[5] Mario Lanza et al. Nature Communications, 11, 5689 (2020)

Figures

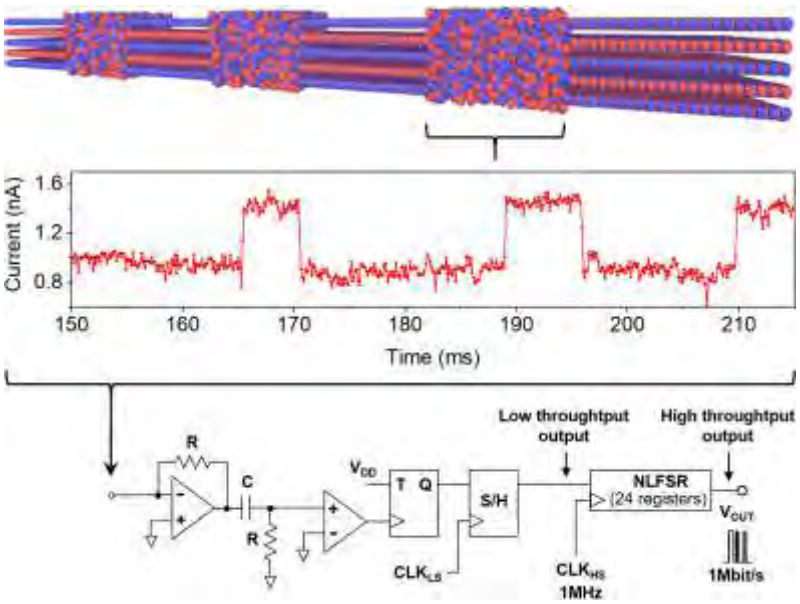


Figure 1: Top-view SEM image of a portion of a 100 x 100 crossbar array of Au/h-BN/Au memristors, each of them with a size of 320 x 400 nm. This is the 2D materials based electronic circuit with a highest number of electronic devices and with a highest integration density ever reported to date.

Development of graphene-based devices in 200 mm wafer scale

R. Lukose[1]
M. Lisker[1,2], M. Lukosius[1], A. Mai[1,2]
[1]*IHP- Leibniz Institut für innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany*
[2]Technische Hochschule Wildau, *Hochschulring 1, 15745 Wildau, Germany*
lukose@ihp-microelectronics.com

Abstract

Graphene processing and integration in standard pilot line of silicon technology, would be a direct way allowing transfer of graphene from the laboratory-scale towards fabrication of graphene-based devices. At this point, various technological challenges, such as growth and transfer, as well as standard integration steps used in CMOS technologies have to be solved.
In this talk the main processing steps of graphene in 200 mm pilot line will be presented. The advantage of graphene growth on epitaxial germanium will be underlined in respect to quality and cross-contamination issues in comparison to graphene grown on Cu. Additionally, the transfer, patterning and contacting approaches will be discussed. Finally, examples of fabricated graphene-based devices will be presented including graphene-based capacitors and electro-optic modulators.

Figures

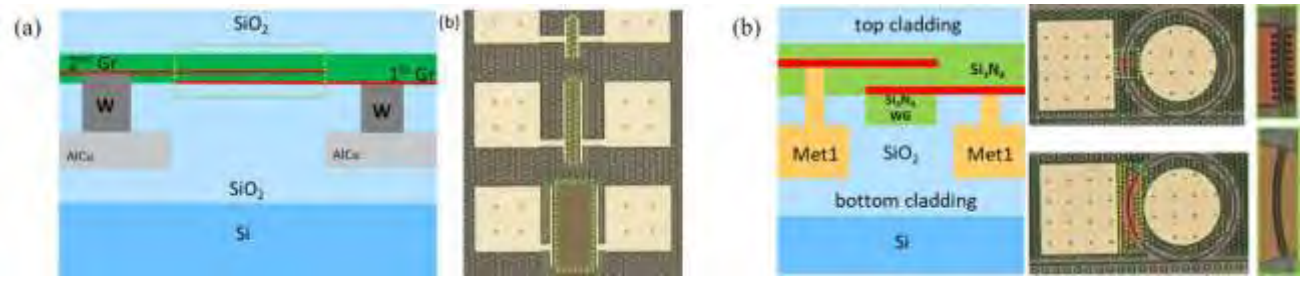


Figure 1: Schematic representations and micrographs of (a) graphene-based capacitor, (b) dual-layer graphene ring e/o modulator.

Atomic Layer Deposition of Large-Area Polycrystalline Transition Metal Dichalcogenides at 100 °C

Miika Mattinen
Marcel Verheijen, Erwin Kessels, Ageeth Bol
Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands
m.j.mattinen@tue.nl

Synthesis of high-quality, large-area transition metal dichalcogenide (TMDC) films under industrially relevant conditions is a considerable challenge. This is especially true for applications based on plastic substrates, such as flexible electronics.[1] Atomic layer deposition (ALD) is an industry-approved gas phase thin film deposition method based on self-limiting surface reactions of alternately pulsed precursors that can be used for low-temperature deposition of TMDCs.[2,3]

We have deposited polycrystalline MoS_2, TiS_2, and WS_2 films of accurately controlled thickness using plasma-enhanced ALD (PEALD). Deposition at record-low temperatures down to 100 °C is enabled by highly reactive, plasma-generated radicals as well as tailoring of plasma chemistry by addition of H_2 into the plasma feed gas. The latter is a crucial factor in controlling the stoichiometry and consequently crystallinity of the deposited films (Figure 1a,b). At 100 °C, MoS_2 films can be directly deposited on plastic substrates, such as poly(ethylene terephthalate) (PET, Figure 1c) as well as Si wafers (Figure 1d). In addition to detailed characterization of film growth, morphology, crystallinity, and composition, electrical properties of MoS_2 films deposited at 100 °C have been studied.

References

[1] Yao and Gang, *J. Appl. Phys.*, 127 (2020) 030902
[2] Mattinen et al., *Adv. Mater. Interfaces.*, 8 (2021) 2001677
[3] Kim et al., *Adv. Mater.*, 33 (2021) 2005907

Figures

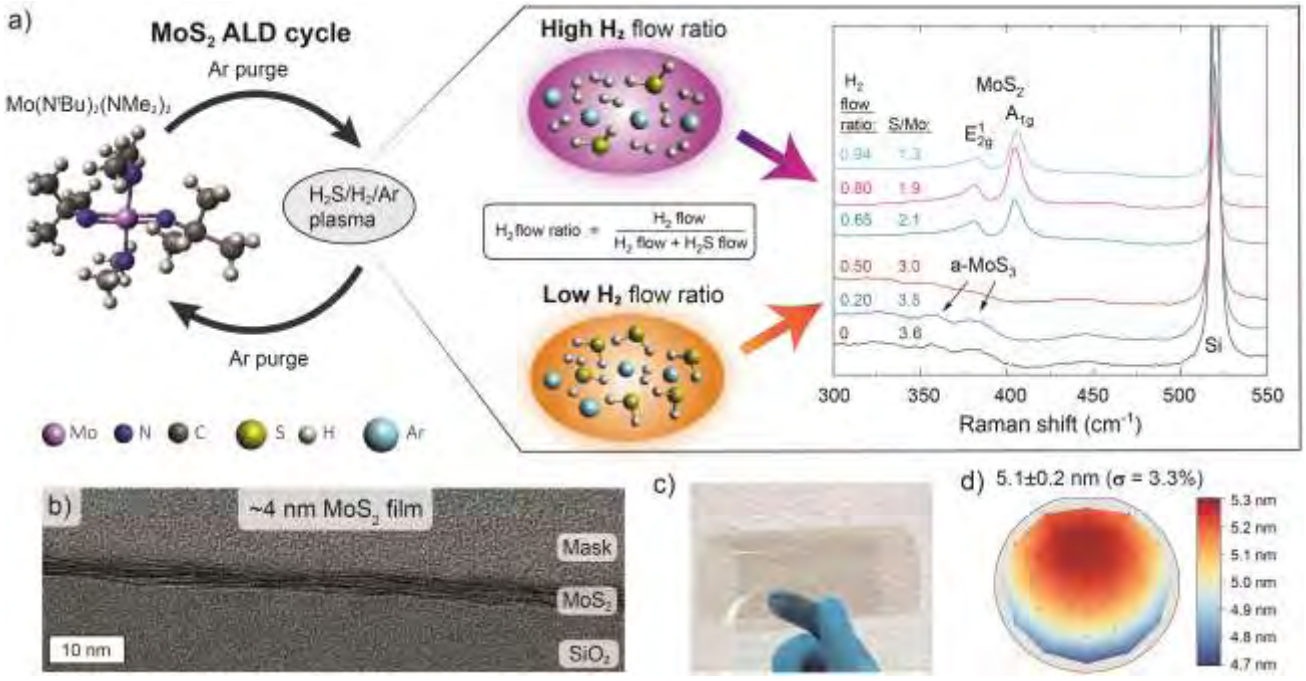


Figure 1: a) Schematic of the PEALD process and the effect of H_2 flow ratio in controlling crystallinity (Raman spectra) and stoichiometry (XPS) at 150 °C. b) Cross-sectional TEM image, c) photograph of ~5 nm MoS_2 on PET (15×15 cm), and d) thickness map on 4" SiO_2/Si wafer of 100 °C MoS_2 films.

Graphene-based biosensors for diagnostics

Arben Merkoçi
Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain.
ICREA - Institucio Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain
arben.merkoci@icn2.ca

Graphene has shown to be an interesting material for building advantageous biosensors with interest for diagnostics. Between the various forms of graphene graphene oxide (GO) and graphene quantum dots (GQDs) display valuable characteristics with interest for biosensing platforms and even smart devices such as nano/micromotors for various applications. We focus on both optical and electrical-based biosensing applications in which exfoliated graphene is involved. Our various applications of graphene include a) GO – based microarray & laterals flow technologies taking advantages of high quenching efficiency of GO. A "turn ON by a pathogen" device will be shown as a highly sensitive detection system using plastics or paper/nanopaper substrates; b) GQDs–based sensors for contaminants detection based on the use of multifunctional composite materials that enable rapid, simple and sensitive platforms in connection to smartphone; c) electroluminescent-based approaches d) A water activated GO transfer technology combined with laser scribing for fast patterning of a touch sensitive device with interest for electronic devices including sensing as well as for a cost-efficient nanomotor building technology for several applications.
This work is supported by EU (Graphene Flagship), CERCA Programme / Generalitat de Catalunya.

Graphene for NEMS Devices

Frank Niklaus
Division of Micro and Nanosystems, KTH Royal Institute of Technology
Malvinas väg 10, Stockholm, Sweden
E-mail: frank@kth.se ; *Phone:* +46 76 216 73 49

Abstract

Graphene has exiting potential in nanoelectromechanical system (NEMS) applications due to its ultimate thinness in combination with its mechanical stability and interesting electrical properties. In this presentation we will discuss the potential of using suspended graphene structures in NEMS sensors and provide an overview of graphene NEMS sensors demonstrated in literature, including different types of graphene pressure sensors, resonators, and accelerometers [1-4]. We discuss suitable transduction mechanisms that are relevant for use in NEMS sensors, including piezoresistive and resonant transduction. We also discuss key graphene integration and fabrication technologies for graphene NEMS sensors that are compatible with standard CMOS integrated circuit wafers and with the existing semiconductor manufacturing infrastructure [5]. In summary, graphene has great potential as structural and transducer material in NEMS sensors featuring ultra-small size and competitive sensitivities.

References

[1] M. C. Lemme et al., "Nanoelectromechanical Sensors Based on Suspended 2D Materials," *Research*, vol. 2020, pp. 1–25, 2020, doi: 10.34133/2020/8748602.
[2] A. D. Smith et al., "Electromechanical Piezoresistive Sensing in Suspended Graphene Membranes," *Nano Lett.*, vol. 13, no. 7, pp. 3237–3242, 2013, doi: 10.1021/nl401352k.
[3] X. Fan et al., "Graphene ribbons with suspended masses as transducers in ultra-small nanoelectromechanical accelerometers," Nat. Electron., vol. 2, pp. 394–404, 2019.
[4] X. Fan et al., "Suspended Graphene Membranes with Attached Silicon Proof Masses as Piezoresistive Nanoelectromechanical Systems Accelerometers" *Nano Lett.*, vol.19, 2019.
[5] A. Quellmalz et al., "Large-area integration of two-dimensional materials and their heterostructures by wafer bonding," *Nat. Commun.*, vol. 12, no. 1, 2021.

Figures

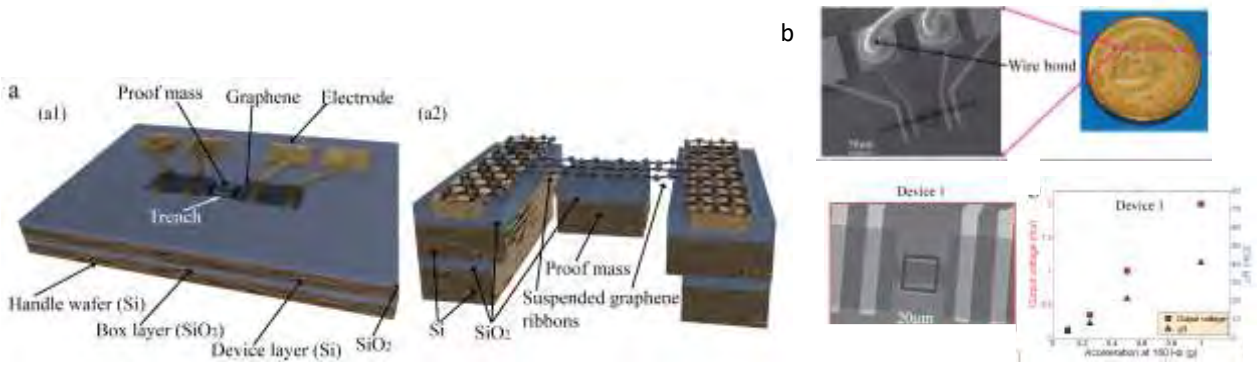


Figure 1. A graphene NEMS accelerometer. (a) Schematic of the graphene ribbon accelerometer. (b) SEM and optical images of graphene accelerometer and the output signal of a graphene ribbon accelerometer. [3]

Advancing 2D Monolayer CMOS Through Contact, Channel and Interface Engineering

Kevin P. O'Brien
Chelsey D Dorow, Ashish Penumatcha, Kirby Maxey, Ande Kitamura, Susu Lee, Carl H. Naylor, C. Rogan, D. Adams, T. Tronic, T. Zhong, A. Oni, A. Sen Gupta, R. Bristol, S. Clendenning, M. Metz, U. Avci
Components Research, Intel Corporation, Hillsboro, OR 97214, USA.
kevin.p.obrien@intel.com

Abstract
2D CMOS transistors fabricated with transition metal dichalcogenide (TMD) materials are a potential replacement for silicon transistors at sub-12 nm channel length [L_G].[1],[2],[3]. Here we present progress towards the ultimate goal and outline critical research needs. We share a design choice that theoretically beats Silicon and saves significant switching energy. We demonstrate record NMOS contacts using a high melting point metal, down to 146 Ω–μm contact resistance (R_C). We present the best PMOS performance on a grown monolayer WSe2 film with 100 μA/μm Ion and low sub-threshold swing (SS) using a Ruthenium contact metal, showing record PMOS contact resistance, RC = 2.7 kΩ-μm. We present 300 mm wafer growth options of 4 different 2D TMD films: MoS2, WS2, WSe2, MoSe2 grown at BEOL temperatures. Finally, we benchmark our results against leading TMD devices, while arguing for more directed research in the pmos device area.

References

[1] K.P. O'Brien, C.D. Dorow et al, IEDM 2021
[2] C.D. Dorow, K.P. O'Brien et al VLSI 2021
[3] K. Maxey et al VLSI 2022

Epitaxial Growth of Transition Metal Dichalcogenide Monolayers for Large Area Device Applications

Joan M. Redwing
Haoyue Zhu, Nadire Nayir, Tanushree Choudhury, Nicholas Trainor, Thomas V. McKnight, Sai Bachu, Benjamin Huet, Nasim Alem, Vincent Crespi, Adri C.T. van Duin
The Pennsylvania State University, University Park, PA USA
jmr31@psu.edu

Abstract

Wafer-scale epitaxial growth of semiconducting transition metal dichalcogenide (TMD) monolayers such as MoS_2, WS_2 and WSe_2 is of significant interest for device applications to circumvent size limitations associated with the use of exfoliated flakes. Epitaxy is required to achieve single crystal films over large areas via coalescence of TMD domains. Our research has focused on epitaxial growth of 2D semiconducting TMDs on c-plane sapphire substrates using metalorganic chemical vapor deposition (MOCVD). Steps on the miscut sapphire surface serve as preferential sites for nucleation and can be used to induce a preferred crystallographic direction to the TMD domains which enables a reduction in inversion domain boundaries in coalesced films. The step-directed growth is dependent on the surface termination of the sapphire which can be altered through pre-growth annealing in H_2 and chalcogen-rich environments. Uniform growth of TMD monolayers with significantly reduced inversion domains is demonstrated on 2" diameter c-plane sapphire substrates enabling large area transfer of monolayers for characterization and device fabrication and testing. Applications for wafer-scale TMD monolayers in nanoelectronics, sensing and photonics will be discussed.

Figures

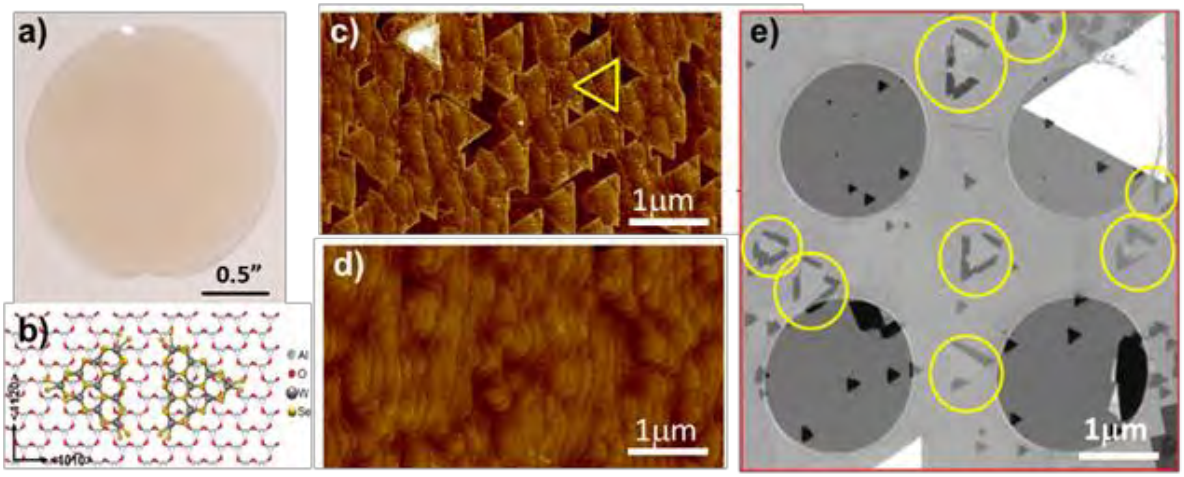


Figure 1: a) WSe_2 monolayer grown by MOCVD on 2" c-plane sapphire; b) Schematic illustration of 0° and 60° oriented WSe_2 domains on (0001) sapphire; c) Partially coalesced WSe_2 on sapphire showing dominant 0° orientation (illustrated by yellow triangle); d) Fully coalesced WSe_2 monolayer; e) Composite dark-field TEM image of WSe_2 monolayer after layer transfer from sapphire growth substrate showing uniform contrast single crystal region. Inversion domain boundaries (yellow circles) exhibit preferential etching. Small pinholes and tears are also present which result from layer transfer. (White triangles are bilayer domain and circular features are artifacts from holes in the TEM grid.)

The Experimental Graphene Pilot Line at AMO

Gordon Rinke
Zhenxing Wang, Herbert Kleinjans, Max Lemme
AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen Germany
rinke@amo.de

Devices based on graphene have attracted a lot of attention due to its extraordinary electronic, optical and sensing properties and consequently its effect on the device performance. [1, 2] However, the fabrication on large scale and thus the availability as well as the introduction into the market remains challenging. With the mission to efficiently close the gap between university research and industrial application, AMO provides as one of the partners in the European 2D Experimental Pilot Line (2D-EPL) project multi project wafer (MPW) runs. The establishment of a route for 2D material integration on large scale and the access to this technology for interested customer is the aim here. In this talk, I will give an insight to the facilities at AMO and some application examples together with hint to next MPW runs within the 2D-EPL project as well as our tailored graphene foundry services.

Acknowledgement: "This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 2D-EPL (952792) and GrapheneCore3 (881603)."

References

[1] D. Neumaier, S. Pindl, M. C. Lemme, Nature Materials, 18 (2019) 525.
[2] M. C. Lemme, et al. Nature Communications, 13 (2022) 1392.

Figures

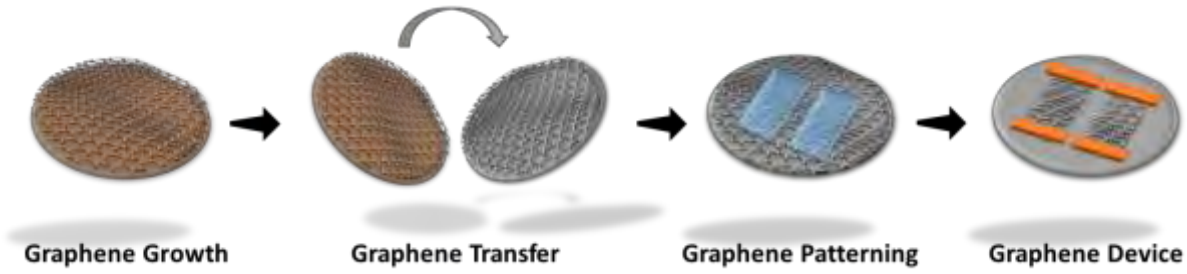


Figure 1: Graphene Pilot Line Fabrication Steps

High-resolution Terahertz near-field inspection for 2D-materials

Simon Sawallich
Alexander Michalski, Michael Nagel
Protemics GmbH, Aachen, Germany
sawallich@protemics.com

For the production and transfer of graphene layers, a variety of tools and techniques are available. Some of them allow high material quality and exact tailoring of specific properties. Non-destructive quality inspection of the produced material is therefore essential for graphene manufacturers to comply with standards – and for device manufacturers to assure high fabrication yields. A highly versatile approach for the non-destructive, quantitative characterization of conductive thin-films, including 2D-materials such as graphene, is based on terahertz (THz) time-domain spectroscopy (TDS) transmission measurements [1].
The application of near-field techniques further increases the potential due to an improved spatial resolution that enables the detection of micron-scale defects and local inhomogeneities in charge-carrier properties of the material. The key-enabling technology for high-resolution THz imaging are photoconductive THz near-field microprobes [2]. Applied for THz transmission measurements at graphene, the outcomes include spatially resolved conductivity and mobility information. Exemplary results are plotted in figure 1: a) shows the THz near-field microprobe in the imaging setup. b) and c) display the obtained THz time-domain and spectral data that allow the extraction of frequency-resolved charge carrier properties. Conductivity results for a 4" graphene layer on a 6" silicon substrate wafer are plotted in fig.1 d) and e), enabling the identification of large-scale inhomogeneities as well as ruptures and microscopic cracks that were introduced during a transfer step.
Recently, we applied high-resolution THz near-field transceiver probe-tips for the inspection of graphene-layers in reflection-mode (instead of transmission-measurements). By taking advantage of the additional interface-selectivity, we can now directly discern substrate- from top-layer inhomogeneity, which is important for the reliable 2D-layer characterization on inhomogeneous substrates.
Graphene manufacturers and researchers can directly benefit from recent developments by the integration of TeraSpike microprobe detectors into existing THz-TDS setups, by the acquisition of complete THz near-field imaging systems or by custom inspection runs in our characterization systems. We gratefully acknowledge funding by the German BMBF in the framework of the GIMMIK project 03XP0210.

References

[1] I. P. Bøggild, D. M. A. Mackenzie, P. R. Whelan, D. H. Petersen, J. D. Buron, A. Zurutuza, J. Gallop, L. Hao and P. U. Jepsen, 2D Materials, 2017, vol. 4, no. 4, p. 042003
[2] M. Wächter, M. Nagel and H. Kurz, Applied Physics Letters 2009, vol. 95, no. 4, 041112

Figures

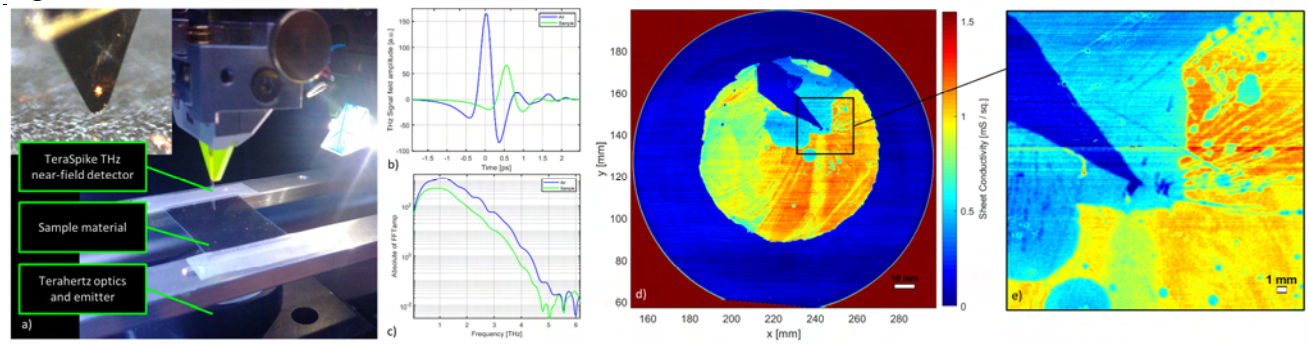


Figure 1: Terahertz near-field setup (a) together with typical THz transients (b) and spectral data (c). Results of conductivity measurements for a 4" graphene layer on a 6" silicon substrate (d and e).

Mapping strain fields in graphene by Raman spectroscopy

Christoph Stampfer[1,2]
[1]*JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany*
[2]*Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany*
stampfer@physik.rwth-aachen.de

Graphene is often portrayed as the "ultimate conductor", thanks to its flexibility and to its excellent conductivity. However, it has been shown that the electrical and the structural quality of graphene are intimately connected, and that nanoscale lattice deformations or local strain fields caused by surface corrugations are a major factor that limits the mobility of electrons in graphene [1]. The flatness of the graphene sheet is therefore a key control characteristic for the fabrication of high-quality graphene layers for electronic devices – and the possibility of measuring it with a simple and fast method is a major technological advantage.
We show that confocal Raman spectroscopy mapping allows to obtain unambiguous information on the amount of nanometer-scale strain variations in a graphene sheet, i.e. on its flatness [2, 3] and allows to map strain fields in graphene. Finally, we will present graphene-based electromechanical systems where the strain-fields can be tuned in-situ [4].

References

[1] N. J. G. Couto, D. Costanzo, S. Engels, D.-K. Ki, K. Watanabe, T. Taniguchi, C. Stampfer, F. Guinea, A. F. Morpurgo, Phys. Rev. X 4, 041019 (2014).
[2] C. Neumann, S. Reichardt, P. Venezuela, M. Drögeler, L. Banszerus, M. Schmitz, K. Watanabe, T. Taniguchi, F. Mauri, B. Beschoten, S. V. Rotkin, and C. Stampfer, Nature Communications 6, 8429 (2015).
[3] IEC TS 62607-6-6 "Nanomanufacturing – Key control characteristics – Part 6-6: Graphene – Strain uniformity: Raman spectroscoopy" https://webstore.iec.ch/publication/34162.
[4] M. Goldsche, J. Sonntag, T. Khodkov, G. Verbiest, S. Reichardt, C. Neumann, T. Ouaj, N. von den Driesch, D. Buca, and C. Stampfer, Nano Lett. 18, 1707 (2018)

Figures

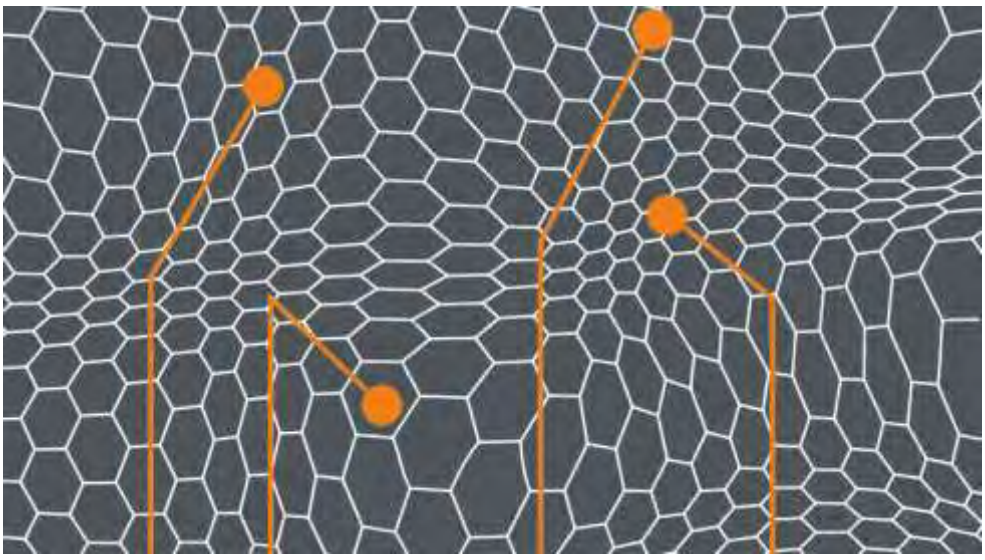


Figure 1: Schematic representation of what corrugations and strain fluctuation might look like in graphene.

2D-material based photodetectors for mid-IR sensing

Stephan Suckow[†]
Shayan Parhizkar[†,‡], Anna Lena Giesecke[†], Sebastian Lukas[‡], Nour Negm[†,‡], Max C. Lemme[†,‡]
[†]*AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen, Germany*
[‡]*Chair of Electronic Dev., RWTH Aachen University, Otto-Blumenthal-Str. 25, 52074Aachen, Germany*
Daniel Schall
Black Semiconductor GmbH, Schloss-Rahe-Strasse 15, 52072 Aachen
Maximilian Prechtl, Oliver Hartwig, Georg S. Duesberg,
Institute of Physics, EIT 2, Faculty of Electrical Engineering and Information Technology, University of the Bundeswehr Munich & SENS Research Center, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany
Sophia Wahl, Matthias Wuttig,
Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany
Arne Quellmalz, Kristinn Gylfason
KTH Royal Institute of Technology, Malvinas väg 10, Stockholm, Sweden
suckow@amo.de

Abstract
Optical spectroscopy is among the most important chemical analysis techniques, due to its high specificity and long-term stability. For spectroscopic analysis of gas compositions, the mid infrared (mid-IR) region is particularly important, owing to the rovibrational resonances in that spectral range. In our European projects ULISSES and AEOLUS we are working on the miniaturization of such gas sensors. One of their key components are mid-IR photodetectors (PDs) suitable for on-chip integration. Starting from our pioneering work on graphene PDs [1,2] we discuss evolving these devices into mid-IR PDs, leading to $PtSe_2$ based PDs where the active material can be grown directly on the waveguide [3,4].
This work has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreements 825272 (ULISSES), 101017186 (AEOLUS) and 881603 (Graphene Flagship Core 3), as well as the German Ministry of Education and Research (BMBF) under grant agreement 16ES1121 (ForMikro-NobleNEMS).

References
[1] D. Schall et al., ACS Photonics 1 (2014), 781 – 784. DOI: 10.1021/ph5001605
[2] D. Schall et al., *Optical Fiber Communications Conference (OFC)* 2018, 1-3
[3] M. Prechtl et. al, Adv Funct Materials 31 (2021) 2103936
[4] S. Parhizkar et al., *ACS Photonics* 9 (2022), 859-867. DOI: 10.1021/acsphotonics.1c01517

Figures

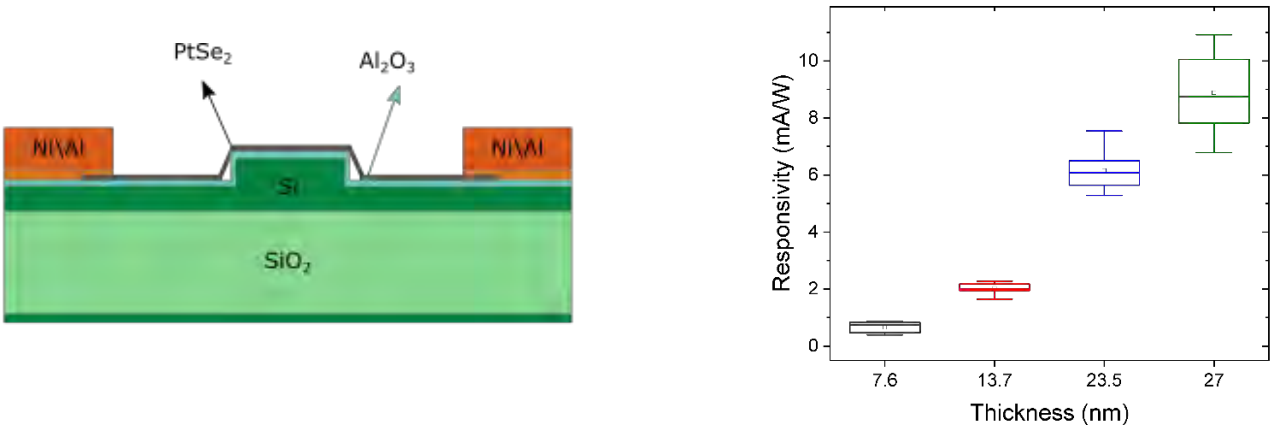


Figure 1: (left) Schematic cross section of mid-IR PDs based on the 2D material $PtSe_2$ and silicon waveguides [3]. (right) Box plot of photodetector responsivities for different thicknesses of $PtSe_2$ photodetectors measured at 4.5 V applied bias and 1550 nm wavelength [3].

Direct Correlative Nanoscopy Imaging of 2D materials

Agnès Tempez[1], Ophélie Lancry[1], Andrey Krayev[2], Marc Chaigneau[1]
[1]HORIBA France, Palaiseau, France [2]HORIBA Instruments Incorporated, Novato, USA
marc.chaigneau@horiba.com

2D transition metal dichalcogenides (TMDCs) materials are considered of very high potential semiconductors for future nanosized electronic and optoelectronic devices. An information-rich nanoscale characterization technique is required to qualify these materials and assist in the deployment of 2D material-based applications.
Scanning Probe Microscopy (SPM) is a powerful technique to image physical properties of 2D materials, such as topography, surface potential or other electrical properties. Combining SPM and Raman in a single instrumentation is extremely powerful as it makes imaging of both chemical and physical properties possible. As Raman is diffraction limited, only plasmon enhanced Raman and photoluminescence spectroscopies yield correlated electrical and chemical information down to the nanoscale.

In this talk, we will report on Tip-Enhanced Photoluminescence (TEPL) and Tip-Enhanced Raman spectroscopy (TERS) data obtained on single crystal TMDC flakes directly grown on SiO_2/Si. TEPL and TERS images will be correlated with contact potential difference and capacitance maps as results of Kelvin force probe microscopy acquisition.
Beside these semiconductor/dielectric (SiO_2) interfaces, probing TMDC/metal interfaces is also essential to integrate TMDCs in 2D or 3D complex structures of devices. We will show results from WS_2 on silver and WSe_2 and MoS_2 on gold. Such transferred surfaces exhibit nanoscale inhomogeneities observed in correlated CPD and Raman maps.
Finally, TEPL together with AFM topography data on a lateral single layer $WS_2/WS_xSe_{1-x}/WSe_2$ heterostructure grown on SiO_2/Si will be presented: nanoscale PL response variations are observed beyond the smooth nano-resolution topography.

References

[1] Nature Communications 9, 2891 (2018)
[2] The journal of physical chemistry letters, 11(15), 6112 (2020)
[3] Nature Nanotechnology 15, 854–86 (2020)
[4] Chem. Commun. 57, 6895 (2021)
[5] J. Phys. Chem. C 125, 48, 26883–26891(2021)
[6] J. Phys. Chem. Lett. 2022, 13, XXX, 5854–5859(2022)

Figures

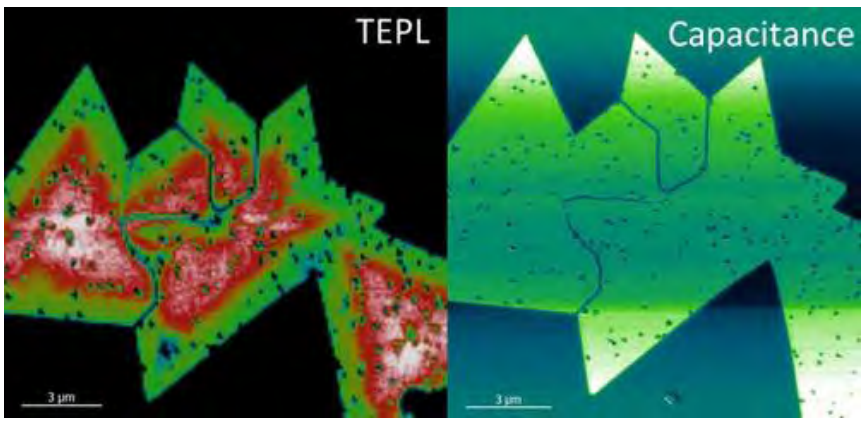


Figure 1: Correlated Tip-enhanced Photoluminescence and Capacitance measurements on WSe_2 flakes.

New insights into graphene-based materials using spectroscopic and operando imaging ellipsometry

Peter H. Thiesen
Shun Okano
Accurion GmbH, Stresemannstrasse 30, Göttingen, Germany
pt@accurion.com

Imaging Ellipsometry has been used for many years in the research on two-dimensional materials due to its outstanding thin-film sensitivity and microscopic lateral resolution. Many studies have been actively carried out for 2D materials produced by the exfoliation method [1],[2],[3],[4]. These applications typically require microscopic resolution, as the flakes are too small to be measured with conventional ellipsometers, even when microprobes are applied. To measure the optical constants and thickness of individual exfoliated flakes, spectroscopic IE was applied. Because of the high lateral resolution, not only the optical properties of exfoliated materials, but also the microscopic in-plane homogeneity of those flakes can be characterized. For CVD-grown graphene, Imaging Ellipsometry enables the visualization of the inhomogeneity as well as gain boundaries of polycrystalline CVD graphene. Especially the Ellipsometric Contrast Micrography mode is a fast, noncontact, wafer-Scale, atomic layer Resolved Imaging technique for Two-Dimensional Materials [6]

Operando imaging ellipsometry has been applied for in-situ measurements of multi-layer graphene as an electrode for rechargeable batteries [] modulation of the optical properties of graphene by back-gating [2]. This is because the back-gating changes the charge carrier density in graphene, which in turn affects the dielectric function.

To round off the lecture, new applications from the everyday laboratory work of the Accurion Application Lab and new technical developments will be presented.

References

[1] U. Wurstbauer et al., Appl. Phys. Lett. 97 (2010), 231901.
[2] A. Matković et al., Journal of Applied Physics 112 (2012), 123523
[3] S. Funke et al., J. Phys.: Condens. Matter 28 (2016) 385301
[4] G.A. Ermolaev et al., Nat Commun 12 (2021), 854.
[5] P. Braeuninger-Weimer et al.,ACS Nano 12, (2018) 8555–8563
[6] J. Sun et al. (2021) Sci. Adv. 7, (2021) eabf0812
[7] S. Okano et. al., Adv. Opt. Matt. 8 (2020) 2000861

Figures

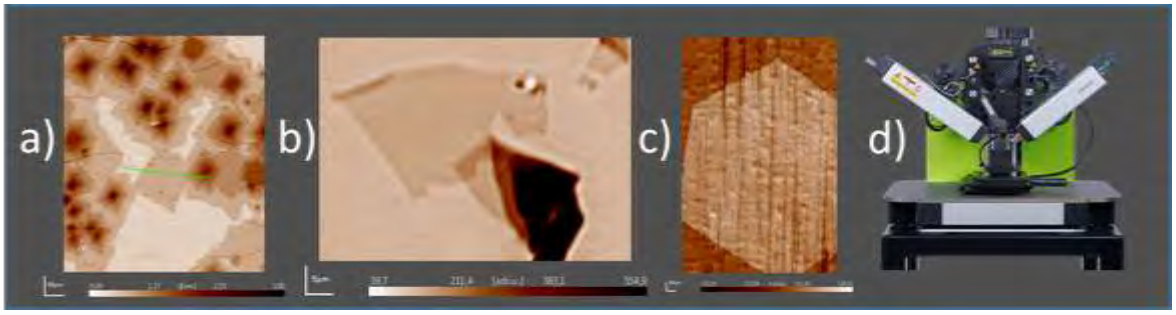


Figure 1: Thickness map of CVD graphene (a), ECM of MoS2/WSe2 heterostructure (b) Delta map of graphene on copper (c) measured with an imaging ellipsometry (d).

Delivering a commercially viable graphene electronic device

John Tingay
Paragraf Limited, 7-8 West Newlands, Somersham, Cambridgeshire, England, PE28 3EB, UK
j.tingay@paragraf.com

Graphene has been shown to provide a material platform for a wide range of electronic devices at a Laboratory scale across a diverse range of applications. Realisation of these structures at an industrial has been limited by a scalable route to production, a method giving process control and fitting with the economic models already prevalent in the semiconductor industry.

Paragraf was formed to commercialise the invention of a transfer and catalyst free method of graphene production invented in the Materials Science department at the University of Cambridge, The aim was to use this technology to develop and bring to market a range of electronic devices and explore the fundamental application of graphene and other 2D materials to the challenges of future semiconductor devices.

The first product to Market from Paragraf is a graphene based Hall sensor. The excellent mechanical and electrical properties of graphene, which make it highly suitable for use in Hall sensors have been theorised and realised in academic literature. [2] Paragraf have developed a commercially scalable device, producing robust, highly sensitive Hall sensors opening new sensing applications.

In order to achieve the level of production control expected by the industry not only does the graphene deposition have to be repeatable but all the subsequent steps have to be well qualified and understood. Exploiting the properties of graphene

This talk will discuss the challenges of bringing a graphene device to market, production requirements, the benefits of graphene and interaction with existing semiconductor supply chain.

References

[1] Thomas, S. "A method of producing a two-dimensional material", WO2017029470
[2] Song, G. et al. "Operation of graphene magnetic field sensors near the charge neutrality point." Communications Physics 2.1 (2019): 1-8.

Scalable production and integration of graphene

Richard van Rijn
Applied Nanolayers (ANL), Delft, The Netherlands
info@appliednanolayers.com

Applied Nanolayers BV (ANL) has spent the last years developing solutions for graphene production and integration, such as wafer scale growth processes and tools and wafer-to-wafer transfer processes and tools, combined with wafer scale quality analysis, and wafer scale device fabrication. We now offer a foundry service to integrate these materials on existing semiconductor technology to precisely those customers who wish to bring their graphene application to a higher TRL. This allows SME's as well as larger companies to develop their intended 2D material device applications without having to invest upfront in expensive production infrastructure.

ANL has its own 200 mm automated CVD platform to enable the consistent growth of high-quality graphene. For the transfer ANL has developed a unique wafer-to-wafer transfer technique with dry graphene transfer. This transfer method is more reliable and easier to automate than liquid based transfer methods. It also provides better control over stress, strain and wrinkles in the graphene layer, which results in more uniform final device performance.

Next to its foundry service ANL has also developed a graphene Application Development Kit (ADK). This enables ANL's customers to execute fast prototyping using ANL's graphene and use a manual dry bond. This method provides the best possible results, only to be topped by ANL's automated transfer. The ADK can be used at wafer level, but it can also be cut in pieces and transferred to individual chips or other small size applications.

Figures

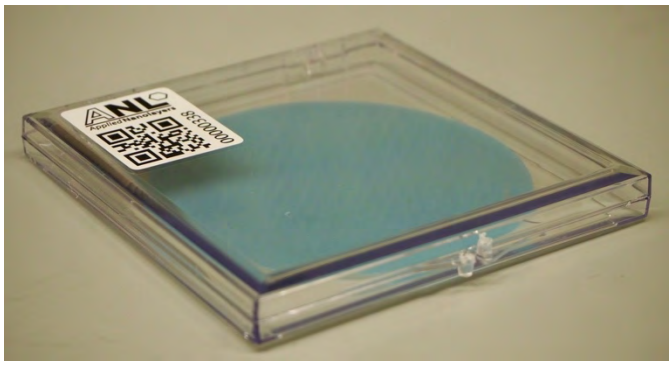


Figure 1: Picture of Graphene Application Development Kit

This project has received funding from the European Union's Horizon 2020 research and innovation programme Graphene Flagship under grant agreement No 881273

2D/3D Heterostructure Diodes for High Performance Electronics and Optoelectronics

Zhenxing Wang
AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen Germany
wang@amo.de

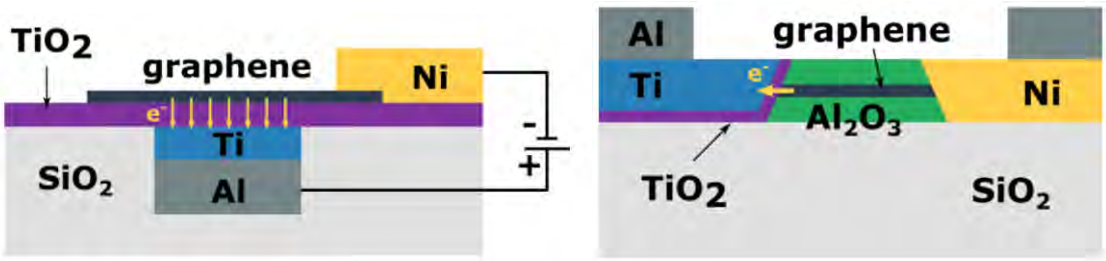
Abstract

Diodes made of heterostructures of the 2D material graphene and conventional 3D materials will be reviewed in this talk, with several applications in high frequency electronics and optoelectronics highlighted. In particular, advantages of metal–insulator–graphene (MIG) diodes over conventional metal–insulator–metal diodes are discussed with respect to relevant figures-of-merit.[1] The MIG concept is extended to 1D diodes, with a demonstration in energy harvesting application.[2,3] Several experimentally implemented radio frequency circuit applications with MIG diodes as active elements are presented.[4] Furthermore, graphene-silicon Schottky diodes as well as MIG diodes are reviewed on their potential for photodetection.[5,6] Here, graphene-based diodes have the potential to outperform conventional photodetectors in several key figures-of-merit, such as overall responsivity or dark current levels. Obviously, advantages in some areas may come at the cost of disadvantages in others, so that 2D/3D diodes need to be tailored in application-specific ways.

References

[1] M. Shaygan et al. Nanoscale, 9 (2017) 11944.
[2] Z. Wang et al. ACS Appl. Electron. Mater., 1 (2019) 945.
[3] A. Hemmetter et al. ACS Appl. Electron. Mater., 3 (2021) 3747.
[4] M. Saeed et al. Adv. Mater., (2022). doi: 10.1002/adma.202108473
[5] D. De Fazio et al. ACS Nano, 14 (2020) 11897.
[6] S. Riazimehr et al. ACS Photonics, 6 (2019) 107.
[7] Z. Wang et al. Adv. Electron. Mater., 7 (2021) 2001210.

Figures



(a) (b)

Figure 1: Structure of MIG diodes. (a) 2-dimensional MIG diode, (b) 1-dimensional MIG diode. [7]

AEOLUS, leveraging integrated photonics for a miniaturised, cloud connected multi-gas sensor for air quality measurements

Charalampos Zervos
Giannis Poulopoulos, George Syriopoulos, Dimitris Apostolopoulos, Hercules Avramopoulos
Photonics Communication Research Laboratory, National Technical University of Athens, 9 Heroon Polytechniou, Athens, Greece
hzervos@mail.ntua.gr

The quality of the air we breathe is a vital asset affecting human health and well-being, as well as environmental resources such as water, soil and forests. The increasing awareness on air pollution's socioeconomic impacts has significantly promoted initiatives at an international, national and regional level, aiming at legally binding deals for containing greenhouse gases and other harmful trace gases threatening human health. Inherent to any policy for air pollution reduction is a mechanism for monitoring, reporting and evaluation of the measures taken. Currently, air pollution is measured regularly at selected locations, mainly at the largest sources of pollution and in city centres. Accurate air quality monitors are costly and bulky; therefore the number of air pollution stations is limited and assessing the spatial distribution of pollutants, dispersion models are used; however, their accuracy is restricted by virtue of variable traffic distribution as well as micro-meteorological effects of urban geometry such as street canyons. Deploying a dense pollution monitoring network, working in tandem with dispersion models to provide real-time mapping of the spatial and temporal variations of urban air quality with high precision, enabling assessment of exposure at a localized/personal level is needed, especially in view of environmental challenges. The demand for 'smart', networked and truly affordable gas sensors will only grow.
Within this premise, we will present AEOLUS, a Horizon 2020 European Innovation Action project, which aims to being together key technologies to develop an affordable multi gas photonic sensors that is cloud connected, assisted with Big Data analytics deployed in a smart sensing platform. AEOLUS is using MID-IR Absorption Spectroscopy based on Nondispersive infrared (NDIR) techniques with high degree if on-chip integration. AEOLUS goals include the use of low-cost and wafer scale manufacturing and packaging methods to promote the affordability, while leveraging an envisaged proliferation of the sensor in an Internet of Things environment feeding data in artificial intelligence algorithms. More specifically, AEOLUS will capitalise on well-established Silicon (Si) platform, develop low cost and miniaturized, allowing for high integration sensing elements with enhanced performance, investigate the leveraging of CMOS compatible Germanium on Insulator processes and extend detection range up to ~10 μm, use wafer level processes to considerable minimize the sensor's cost and footprint, demonstrate a system on chip integrated photonic sensor for multiple gases, use well established embedding PCB technologies for miniaturisation, develop and validate machine learning models that will provide emerging patterns, accurate chemometric analysis and predictions.
This work has received funding from the European Union's Horizon 2020 innovation programme under grant agreement No. 101017186 (AEOLUS).

Graphene manufacturing and integration at wafer scale

Amaia Zurutuza
Graphenea Semiconductor, Paseo Mikeletegi 83, Donostia-San Sebastian, Spain
a.zurutuza@graphenea.com

Over the past years, extensive efforts have been placed in the research and development of graphene-based applications, as a consequence, certain applications have experienced an increase in the technology readiness level. However, in order to get closer to the market, reliable and reproducible processes at wafer scale are needed. At present, the most mature catalyst technology relies on copper foils, where graphene at 200mm wafer scales can be obtained. Graphene transfer has also evolved from the so-called wet transfer to the more scalable semi-dry transfer where standard semiconductor industry equipment such as wafer bonders can be employed. Finally, device fabrication at relevant wafer scales is critical for a successful market uptake.

Depending on the application, the substrate might require planarization for reliable graphene transfer as in the case of waveguide containing substrates. During this talk, I will cover the transfer of graphene on waveguide containing wafers relevant for optical gas sensor applications as well as the latest progress on graphene transfer [1]. In addition, graphene integration in sensors will also be covered [2-4].

References

[1] S. Papazoglou, D. Kaltsas, A. Logotheti, A. Pesquera, A. Zurutuza, L. Tsetseris and I. Zergioti, 2D Mater., 8 (2021) 045017.
[2] N. Tran, I. Fakih, O. Durnan, A. Hu, A. Aygar, I. Napal, A. Centeno, A. Zurutuza, B. Reulet, and T. Szkopek, Nanotechnology, 32 (2021) 045502.
[3] I. Fakih, O. Durnan, F. Mahvash, I. Napal, A. Centeno, A. Zurutuza, V. Yargeau, and T. Szkopek, Nature Commun., 11 (2020) 3226.
[4] I. Fakih, A. Centeno, A. Zurutuza, B. Ghaddab, M. Siaj, and T. Szkopek, Sens. Actuators B Chem., 291 (2019) 89.

Electrostatic Control of the Threshold Voltage in Graphene-GaAs Field-Effect Transistors for Digital Logic Applications

Luca Anzi[1]
Artur Tuktamyshev[2], Alexey Fedorov[3], Amaia Zurutuza[4], Stefano Sanguinetti[2], and Roman Sordan[1]
[1] *L-NESS, Department of Physiscs, Politecnico di Milano, Polo di Como, Via Anzani 42, 22100 Como, Italy*
[2] *Department of Material Science, Università di Milano Bicocca, Via Cozzi 53, 20125 Milano, Italy*
[3] *CNR-IFN and L-NESS, Department of Physics, Politecnico di Milano, Via Anzani 42, 22100 Como, Italy*
[4] *Graphenea, Avenida de Tolosa 76, 20018 Donostia/San Sebastián, Spain*

luca.anzi@polimi.it

The threshold voltage (V_{th}) of a field-effect transistor (FET) impacts its power consumption and switching speed. The undesired shift of V_{th} limits the minimum power supply voltage in digital circuits, which leads to increased static power dissipation. In conventional FETs, V_{th} cannot easily be adjusted because it is set by the work function of the metal gate. In metal-semiconductor FETs (MESFETs), V_{th} is additionally constrained by the semiconductor work function and channel thickness. All these parameters are chosen during fabrication and set V_{th} at a fixed value.

GaAs MESFETs are used in high-speed integrated circuits (ICs) because of the high carrier mobility in their semiconductor channels [1]. To limit the gate leakage current, the gate forward bias voltage should be smaller than the turn-on voltage of the gate Schottky diode. As a result, it is challenging to fabricate ICs in which MESFETs are biased by a positive gate voltage, which is required in digital logic gates.

In this talk, we will introduce a GaAs-based MESFET in which the metal gate was replaced by a monolayer graphene gate (Figure 1a). Graphene forms a Schottky junction with GaAs [2], which was used to control the conductivity of the transistor channel. An additional Al/AlO_x control gate stack was fabricated on top of the graphene gate (Figure 1b). The control gate was used to adjust the work function of the graphene gate by shifting its Fermi level. This resulted in the modulation of the graphene-GaAs Schottky barrier height (SBH) and, therefore, the modulation of the threshold voltage of the FET. Such effect has been used in the past to realize graphene barristors [3] and vertical heterostructures [4].

We exploited the modulation of the SBH to realize GaAs FETs in which V_{th} was changed from -0.8 to 0.6 V by changing the control gate voltage (V_{GC}) from 0 to 1.8 V. The transfer characteristics of such GaAs FET are shown in Figure 2. The increase of V_{th} increases the cut-in voltage of the gate Schottky diode and, therefore, allows the use of the FETs under larger gate voltages without increasing the gate leakage current.

To demonstrate the operation of the fabricated FETs, we realized digital logic gates with a positive switching threshold, which is a fundamental requirement for the realization of more complex logic circuits.

References

[1] Voinigescu S., Cambridge University Press: Cambridge, 2013.
[2] Tongay S. et al., Physical Review X 2012, 2, 011002.
[3] Yang H. et al., Science 336.6085 (2012), 1140-1143.
[4] Sata Y. et al., Japanese Journal of Applied Physics 54.4S (2015), 04DJ04.

Figures

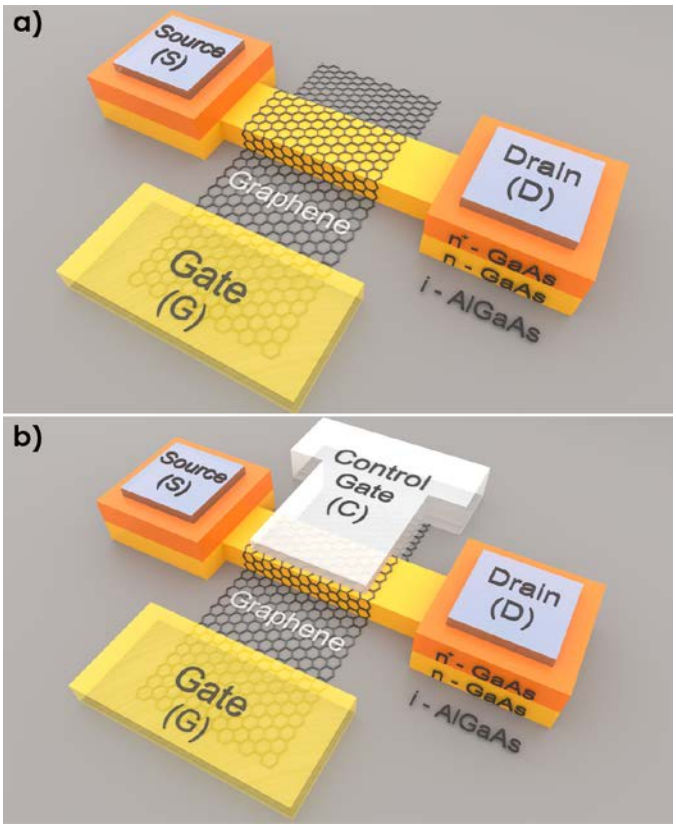


Figure 1: GaAs FETs with a graphene gate. (a) Schematic of a single-gate graphene-GaAs FET on an insulating AlGaAs substrate. The graphene gate is deposited on top of an n-GaAs layer with a donor concentration of 10^{17} cm^{-3} and connected externally by an Au gate pad (G). The graphene gate controls the conductivity of the GaAs channel, modulating the current flow between source (S) and drain (D). (b) Schematic of a dual-gate graphene-GaAs FET. The additional control gate (C) controls the graphene Fermi level and, therefore, Schottky barrier height (which affects the modulation of the current in the transistor channel).

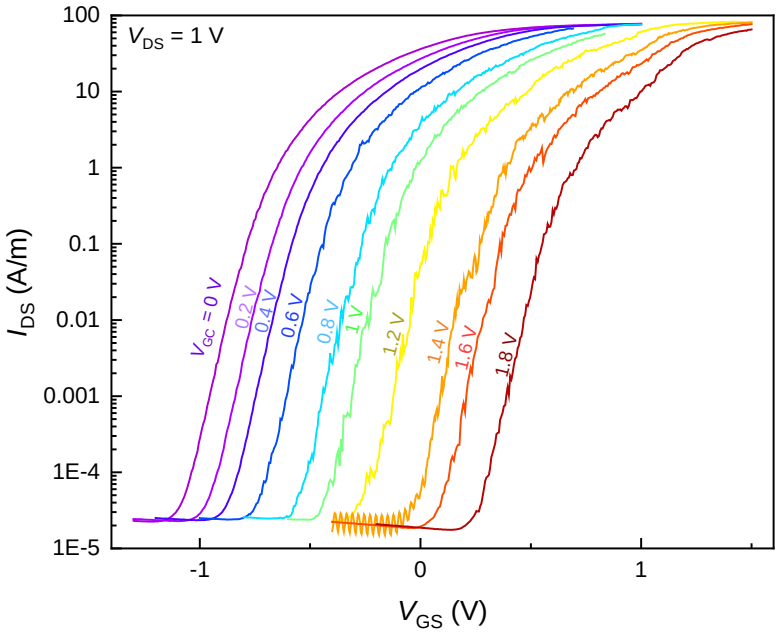


Figure 2: Transfer characteristics of a dual-gate graphene-GaAs FET where the drain current I_{DS} (normalized by the channel width) is measured as a function of V_{GS} at different V_{GC}. Increasing V_{GC} from 0 V to 1.8 V shifts the curves and V_{th} to more positive V_{GS}.

Electrical detection of high quality 2D polaritonic nanoresonators

Sebastián Castilla[1]
Hitesh Agarwal[1], David Alcaraz[1], Yuliy Bludov[2], Ioannis Vangelidis[3], Adrià Grabulosa[1], Matteo Ceccanti[1], Iacopo Torre[1], Hanan Herzig-Sheinfux[1], Elefteris Lidorikis[1], Nuno Peres[2], Frank Koppens[1]
1 ICFO, Av Carl Friederich Gauss 3 - Castelldefels (Barcelona), Spain
2 Universidade do Minho, Portugal, 3 University of Ioannina, Greece
sebastian.castilla@icfo.eu

Polaritons are coupled excitations of incident light with charged particles (plasmons polaritons) or lattice vibrations (phonon polaritons). In particular, for two dimensional (2D) materials their properties become even more intriguing in several aspects such as extreme light confinement and long lifetimes. Hence, they lead to a myriad of applications such as gas and molecular sensors, enhancing photodetection and quantum computing.

In this talk, we initially show efficient coupling between plasmonic nanoantennas with hyperbolic phonon-polaritons (HPPs) in hBN for highly concentrate mid-infrared light into a graphene pn-junction in order to overcome its small absorption and photoactive area [1]. We guide these HPPs with constructive interferences towards the photodetector active area. This room temperature ultrafast infrared photodetector exceeds any commercial technology. It has a response time of <15 ns (setup limited), while at the same time showing excellent sensitivity: we extracted a noise-equivalent-power (NEP) down to 82 pW/√Hz at 6 μm (50 THz). [1]

Then, we show a novel concept of 2D polaritonic nanoresonators that consist on merging into one single platform the polaritonic material and the detector as shown in Figure 1 [2]. We obtain a highly compact device since we get rid of the need of an external detector for performing infrared spectroscopy. We show high Q factors (>200) and confinement record of these nanoresonators. [2] We geometrically and electrically tune these nanoresonators to change their spectral photoresponse. Due to this, we are able to identify different interactions such as the hybridization between graphene plasmons with the HPPs, modification of the HPPs waveguide modes and the interplay between the different graphene plasmons (acoustic and optical).

Finally, we investigate the photoresponse of these 2D polaritonic nanoresonators as a function of the temperature, reaching values down to 30 K. [3] The devices show higher values of photocurrent due to the interplay of the contributions of the photothermoelectric effect and longer lifetimes of the polartionic resonators. We determine that the Q factor values increase significantly at these lower temperatures and the results are supported by theoretical simulations.

References

[1] S. Castilla, I. Vangelidis, VV. Pusapati, et al. Plasmonic antenna coupling to hyperbolic phonon-polaritons for sensitive and fast mid-infrared photodetection with graphene. Nature Communications, 11, 4872 (2020)
[2] S. Castilla, et al. To be submitted (2022)
[3] S. Castilla, et al. In preparation (2022)

Figures

Figure 1: Schematic of the 2D polaritonic nanoresonator that show the field intensity of the propagating mode.

Inkjet-printed low-dimensional materials-based complementary electronic circuits on paper

Elisabetta Dimaggio[1]
Irene Brunetti[1], Lorenzo Pimpolari[1], Silvia Conti[1], Robyn Worsley[2], Subimal Majee[2], Dmitry K. Polyushkin[3], Matthias Paur[3], Giovanni Pennelli[1], Giuseppe Iannaccone[1], Massimo Macucci[1], Francesco Pieri1, Thomas Mueller[3], Cinzia Casiraghi[2], Gianluca Fiori[1]
[1]*Dipartimento di Ingegneria dell'Informazione, University of Pisa, Pisa, Italy*
[2]*Department of Chemistry, University of Manchester, Manchester, UK*
[3]*Institute of Photonics (TU Wien), Vienna, Austria*
elisabetta.dimaggio@unipi.it

At the dawn of the flexible and wearable electronics age, the seek for new materials enabling the integration of complementary metal-oxide-semiconductor (CMOS) technology on flexible substrates finds in low-dimensional materials (either 1D or 2D) extraordinary candidates. Together with their excellent electrical and mechanical properties, low-dimensional materials are solution processable and suitable to be cost-effectively deposited using high-throughput techniques, compatible with direct printing on different flexible substrates [1]. Here, we report an inkjet-printed CMOS-like technology on paper, combining *n*-type MoS_2-based and *p*-type carbon nanotubes (CNTs)-based field effect transistors (FETs) with hBN dielectric (Figure 1a). Both types of printed transistors exhibit good performances in terms of mobility (in the order of 10 cm^2/Vs) and ON/OFF current ratio (> 10^3), and their characteristics can be matched adjusting the channel dimensions (Figures 1b, c) [2]. The proposed devices have been successfully used to design and fabricate some fundamental CMOS building block, such as low-voltage inverters (Figure 2a), NOR gates (Figure 2b) and D-latches (Figure 2c), showing a path for the fabrication of efficient CMOS circuits for cost-effective applications.

References

[1] F. Bonaccorso et al., Advanced Materials vol. 28 (2016), 6136-6166
[2] I. Brunetti et al., npj 2D Materials and Applications vol. 5, (2021), 85.

Figures

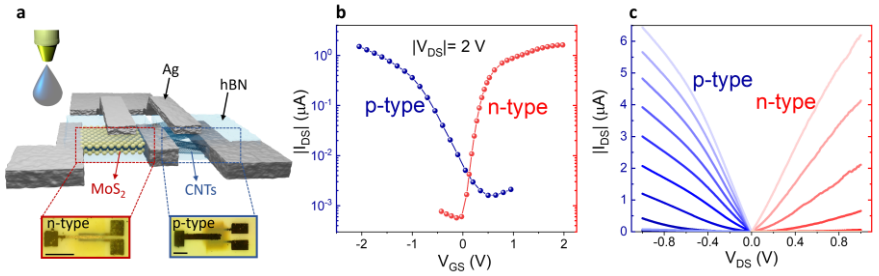


Figure 1: a) Sketch of the proposed CMOS-like circuit, together with the input (b) and output (c) characteristics of a p-type and a n-type FET.

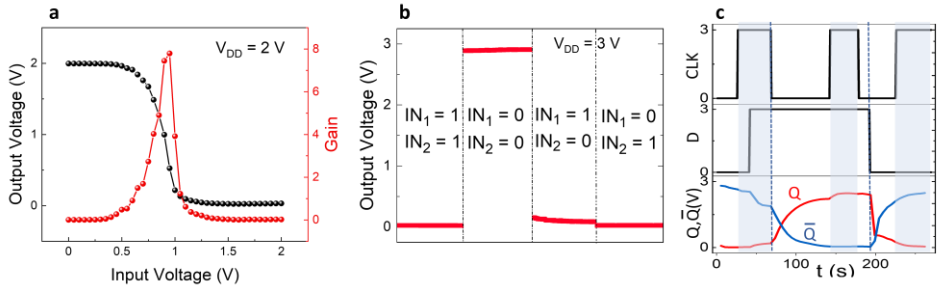


Figure 2: a) Input-Output characteristic (left axis) and voltage gain (right axis) of an inverter. b) Output voltage of a NOR gate as a function of the input states. c) Time evolution of the output, Q and /Q, as a function of the input signal, D, and clock, CLK.

Visible-frequency graphene plasmons

Gergely Dobrik
Péter Nemes-Incze, Bruno Majérus, Péter Süle, Péter Vancsó, Gábor Piszter, Miklós Menyhárd, Benjámin Kalas, Péter Petrik, Luc Henrard, Levente Tapasztó
Institute of Technical Physics and Materials Science, Centre for Energy Research, H-1121 Budapest, Konkoly-Thege ut 29-33, Hungary
dobrik.gergely@ek-cer.hu

Abstract

The nanoscale confinement of its charge carriers is an effective approach for engineering the properties of graphene[1,2]. We demonstrate that amplifying the random nanoscale corrugation of graphene, create an edge-free lateral confinement in ultra-small (sub-5nm) areas[3]. This soft confinement allows the low-loss lateral ultra-confinement of graphene plasmons, scaling up their resonance frequency from the native terahertz to the commercially relevant visible range[4]. Visible frequency graphene plasmons enable at least three orders of magnitude stronger Raman enhancements than previously achieved with graphene, allowing the detection of molecules from femtomolar solutions or ambient air with high selectivity. SERS substrates based on nanocorrugated graphene offer a series of practical advantages over conventional nanoparticle films[5], such as much simpler and cheaper fabrication, better reproducibility and highly improved environmental stability of up to several months. Moreover, nanocorrugated graphene sheets also support propagating visible plasmon modes, as revealed by scanning near-field optical microscopy observation of their interference patterns[6,7,8] (Fig.1).

References

[1] Han, M. Y. et al., Phys. Rev. Lett. 98 (2007) 206805
[2] Abajo, F. J. G. et al., ACS Photonics 1 (2014) 135–152
[3] Dobrik, G. et al., Nat. Nanotechnol. 17 (2022) 61–66
[4] Tongrattanasiri, S. at al., ACS Nano 6 (2012) 1766–1775
[5] Grigorenko, A. N. et al., Nat. Photonics 6 (2012) 749–758
[6] Chen, J. et al., Nature 487 (2012) 77–81
[7] Fei, Z. et al., Nature 487 (2012) 82–85
[8] Stockman, M. I. et al., Phys. Rev. Lett. 87 (2001) 167401

Figures

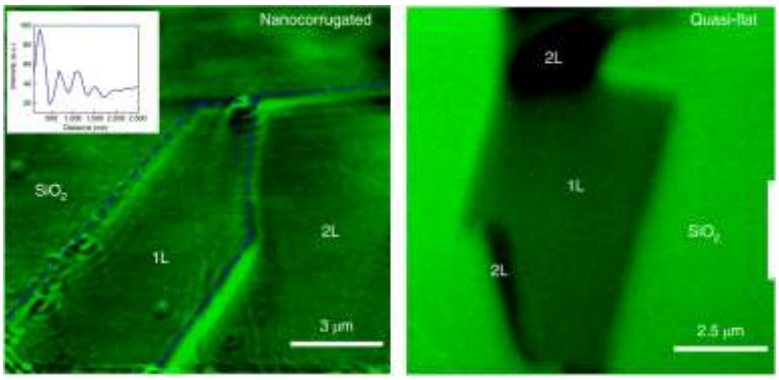


Figure 1: [Left], SNOM image (wavelength λ = 488 nm) of nanocorrugated graphene revealing clear interference maxima and oscillations in the proximity of edges (marked by dashed lines) and defects. The inset shows a line cut perpendicular to the graphene edge. 1L represents the single layer and 2L the bilayer graphene areas on the SNOM images. [Right], SNOM image of quasi-flat graphene recorded under the same conditions, showing no interference patterns

2D framework material films via interfacial synthesis

Renhao Dong
Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany

renhao.dong@tu-dresden.de

In our work, we have employed interfacial chemistry toward the precision synthesis of 2D framework materials (2DFMs) with diverse structures and functions. For instance, we demonstrated the synthesis of 2D conjugated metal-organic framework (2D c-MOF) at the air-water or liquid-liquid interfaces. The 2D c-MOFs feature with stacked layers and possess unique electronic properties, such as full π delocalization, narrowed band gaps and high conductivity, which render 2D c-MOFs as advanced electronic materials. One representative iron-bis(dithiolene) 2D MOF exhibited as a p-type semiconductor with a band-like transport and high mobility of ~220 cm^2/Vs.[1] Owing to their conductivity, the 2D c-MOFs have shown potential for transistors, photodetectors, sensing, magnetics, and energy storage and conversion.[2] In addition, we have also synthesized highly crystalline 2D polymers on the water surface. For instance, we have employed a surfactant-monolayer-assisted interfacial synthesis (SMAIS) method to prepare 2D polymers, like 2D polyimides, 2D polyimines and boronate ester 2D polymers, which exhibit few-layers and micrometer-sized single-crystalline domains, which have been utilized as active layers for optoelectronics and memory devices.[3,4] In our latest work, we have developed charged 2D polymer single crystals through an irreversible Katritzky reaction under pH control, which could act as an anion-selective membrane for osmotic energy generation, offering a high chloride ion selectivity.[5]

References

[1] Nat. Mater. 17 (2018) 1027-1032.
[2] Chem. Soc. Rev. 50 (2021) 2764-2793.
[3] Angew. Chem. Int. Ed. 59 (2020) 8218-8224.
[4] Angew. Chem. Int. Ed. 60 (2021) 13859-13864.
[5] Nat. Synth. 1 (2022) 69-76.

Figures

Twist-tunable polaritonic nanoresonators

A. I. F. Tresguerres-Mata[2†*]
O. G. Matveeva[1†], R. V. Kirtaev[1], K. V. Voronin[1], J. Taboada-Gutiérrez[2,3], C. Lanza-García[2], J. Duan[2,3], J. Martín-Sánchez[2,3], V. S. Volkov[1,4], P. Alonso-González[2,3*], A. Y. Nikitin[5,6*].
[1]*Center for Photonics and 2D Materials, Moscow Institute of Physics and Technology, Dolgoprudny 141700, Russia.*
[2]*Department of Physics, University of Oviedo 33006, Spain.*
[3]*Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo), El Entrego 33940, Spain.*
[4]*GrapheneTek Skolkovo Innovation Center, Moscow 143026, Russia.*
[5]*Donostia International Physics Center (DIPC), Donostia/San Sebastián 20018, Spain.*
[6]*IKERBASQUE, Basque Foundation for Science, Bilbao 48013, Spain.*
*anaiftresguerresmata@uniovi.es; pabloalonso@uniovi.es; alexey@dipc.org
† *These authors contributed equally to this work.*

Optical nanoresonators are fundamental building blocks in a number of nanotechnology applications (e.g. in spectroscopy) due to their ability to efficiently confine light at the nanoscale. Recently, nanoresonators based on the excitation of phonon polaritons (PhPs) – light coupled to lattice vibrations – in polar crystals (e.g. SiC or h-BN) have attracted much attention due to their strong field confinement, high-quality factors, and potential to enhance the photonic density of states at mid-infrared (IR) frequencies [1]. Here, we go one step further by introducing PhPs nanoresonators that not only exhibit these extraordinary properties but also incorporate a new degree of freedom: twist tuning, i.e. the possibility to be spectrally controlled by a simple rotation (Fig. 1a). To that end, we both take advantage of the low-loss-in-plane hyperbolic propagation of PhPs in the van der Waals crystal α-MoO_3 [2], and realize a dielectric engineering of a pristine α-MoO_3 slab placed on top of a metal ribbon grating, which preserves the high quality of the polaritonic resonances. By simply rotating the α-MoO_3 slab in the plane (from 0 to 45°), we demonstrate by far- and near-field measurements that the narrow polaritonic resonances (with quality factors Q up to 200) can be tuned in a broad range (up to 32cm^{-1}, i.e. up to ~6 times its full width at half maximum, FWHM~5 cm^{-1}) (Fig 1b). Our results open the door to the development of tunable low-loss nanotechnologies at IR frequencies with application in sensing, emission, or photodetection.

References

[1] Li, Peining. *et al.*, Science, 359 (2018) 892-896.
[2] Ma, W. *et al.*, Nature, 562 (2018) 557-562.

Figures

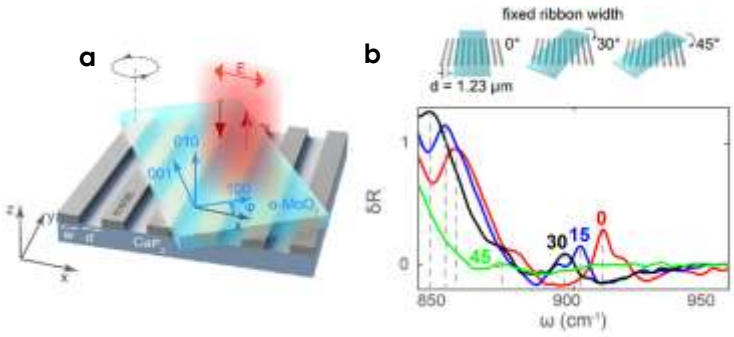


Figure 1: PhPs nanoresonators in α-MoO_3 defined by placing a pristine α-MoO_3 slab on top of metal ribbons. **a.** Schematics of the studied structure that allows defining the nanoresonators by ''dielectric engineering'' and controlling them by a twist angle, φ. **b.** Measured relative reflection spectra, δR for twist angles φ =0,15,30 and 45°.

Giant effective Zeeman splitting in a monolayer semiconductor realised by spin selective strong light-matter coupling

D. J. Gillard
T.P. Lyons, C. Leblanc, J. Puebla, D.D. Solnyshkov, L. Klompmaker, I.A. Akimov, C. Louca, P. Muduli, A. Genco, M. Bayer, Y. Otani, G. Malpuech, and A.I. Tartakovskii
Department of Physics and Astronomy, The University of Sheffield, Sheffield, S3 7RH, UK
d.j.gillard@sheffield.ac.uk

Strong coupling between light and fundamental excitations of a two-dimensional electron gas (2DEG) are of foundational importance to both pure physics and to the understanding and development of future photonic nano-technologies [1-7]. Here we study the relationship between spin polarisation of a 2DEG in a monolayer semiconductor, $MoSe_2$, and light-matter interactions modified by a zero-dimensional optical microcavity. We find robust spin-susceptibility of the 2DEG to simultaneously enhance and supress trion-polartion formation in opposite photon helicities. This leads to the observation of a giant effective Zeeman splitting by over five times. Going further, we observe robust effective optical non-linearity arising from the highly non-linear behaviour of the valley-specific strong light-matter coupling regime, and allowing all-optical tuning of the polaritonic Zeeman splitting from 4 to more than 10 meV.

References

[1]: Smolka, S. et al. *Science* **346** (2014). [2]: Efimkin, D. K. & MacDonald, A. H. *PRB* **95** (2017). [3]: Back, P. et al. *PRL* **118** (2017). [4]: Sidler, M. et al. *Nat. Physics* **13** (2017). [5]: Tan, L. B. et al. *PRX* **10** (2020). [6]: Klein, J. et al. *PRR* **3** (2021). [7]: Roch, J. G. et al. *Nat. Nano.* **14** (2019).

Figures

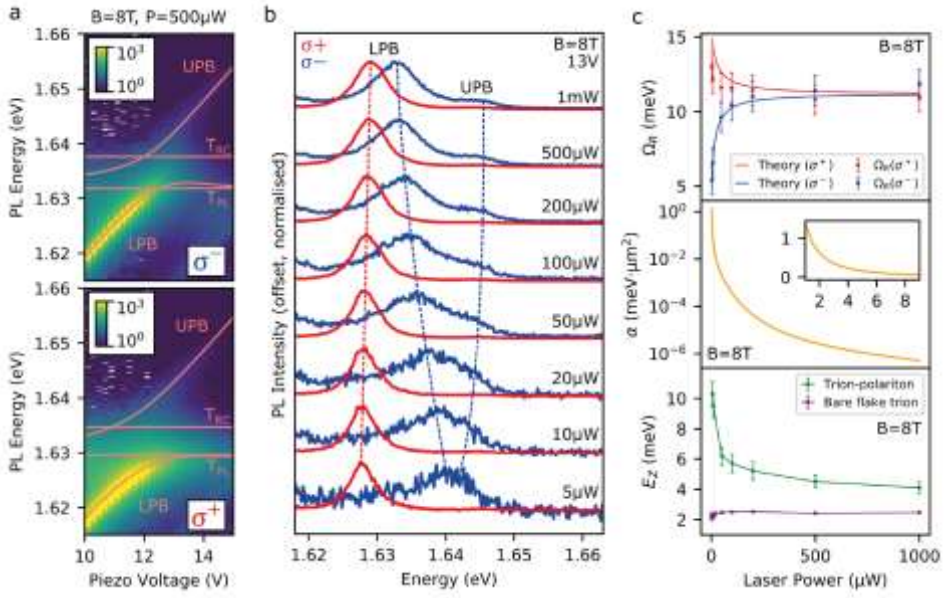


Figure 1: Trion-polariton effective nonliearity. (a) Cavity PL colourmaps in σ+ and σ- emission at a high laser power P = 500 μW. An anticrossing is seen in both polarisations despite the strong applied B-field. Polariton fitting curves incorporating the stokes shift effect are overlaid. (b) Cavity PL spectra at a fixed detuning close to trion-cavity resonance, taken at varying incident laser powers. As the power is decreased, the 2DEG spin polarisation increases and the anticrossing in σ- is suppressed, amplifying the effective Zeeman splitting between σ+ and σ- lower polariton branches (LPB). (c) (top panel) Rabi splittings in σ+ and σ- against laser power. Nonlinear breakdown of strong coupling in σ- is observed as the power is decreased. Solid curves are simulated results. (middle panel) The calculated effective trion-polariton interaction strength, α, as a function of pump power. Inset shows α at very low power. (bottom panel) The maximum LPB Zeeman splitting, E_Z, against laser power. The splitting increases dramatically at the lowest powers when the 2DEG spin polarisation is highest. For comparison the bare trion Zeeman splitting is shown, which is independent of laser power. All data shown is at B = +8 T.

Magnetization signature of topological surface states in a superconductor

Irina Grigorieva
W. Kuang, G. Lopez-Polin, H. Lee, F. Guinea, G. Whitehead, I. Timokhin, A. I. Berdyugin, R. K. Kumar, O. V. Yazyev, N. Walet, A. Principi, A. K. Geim
University of Manchester, Oxford Road, Manchester M13 9PL, UK
Irina.V.Grigorieva@manchester.ac.uk

Abstract

Superconductors with non-trivial band structure topology represent a class of materials with potentially useful properties for quantum technologies. Recent years have seen much success in creating artificial hybrid structures exhibiting main characteristics of two-dimensional (2D) topological superconductors. Yet, bulk materials known to combine inherent superconductivity with nontrivial topology remain scarce, largely because distinguishing their central characteristic – topological surface states – proved challenging due to a dominant contribution from the superconducting bulk. I will present our recent work [1] where we found a highly anomalous behaviour of surface superconductivity in a topologically nontrivial 3D superconductor In_2Bi. Topologically protected surface states in this material result from its nontrivial band structure, which itself is a consequence of the non-symmorphic crystal symmetry and strong spin-orbit coupling. In contrast to smoothly decreasing diamagnetic susceptibility above the bulk critical field H_{c2}, as seen for surface superconductivity in conventional superconductors, we observe near-perfect, Meissner-like screening of low-frequency magnetic fields nearly up to the critical field of surface superconductivity, H_{c3}. We show that the anomalous screening and finite bulk diamagnetism above H_{c2} result from the contribution of superconducting topological surface states. Our experiments demonstrate the possibility to detect such states using macroscopic magnetization measurements, providing a new tool for discovery and identification of topological superconductors.

References

[1] W. Kuang et al, *Adv. Mater.* **33** (2021) 2103257.

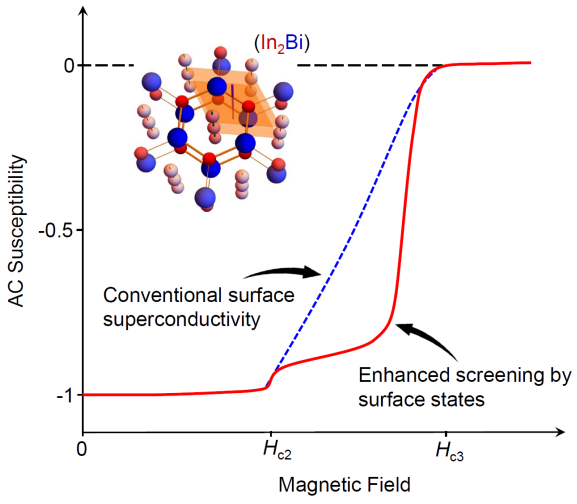


Figure 1: Crystal structure of In_2Bi and schematic magnetic susceptibility illustrating the contribution from topological surface states.

Controlling dark intervalley excitons for strain sensing in WS_2

Gabriele Grosso
Saroj B. Chand, John M. Woods, Enrique Mejia
Photonics Initiative, Advanced Science Research Center, City University of New York, New York, NY 10031, USA
Physics Program, Graduate Center, City University of New York, New York, NY 10016, USA
ggrosso@gc.cuny.edu

Dark excitonic states in transition metal dichalcogenides (TMDs) are attracting growing interest because they represent the lowest excitonic states of the system [1] and can deeply affect transport, dynamics and coherence of bright excitons, hampering optoelectronic properties and device performance [2]. Therefore, it is crucial to create conditions in which these excitonic states can be visualized and controlled. Here, we show that compressive strain in WS_2 change the band alignment and enables phonon scattering of photoexcited electrons between momentum valleys [3], enhancing the formation of dark intervalley ($K\Lambda$) excitons. This mechanism is illustrated in Fig.1a. Our photoluminescence (PL) and hyperspectral experiments indicate that dark excitons appear around compressive strain pockets that are created in the monolayer during the transfer process onto a hexagonal boron nitride (hBN) substrate (Fig.1c) [4]. Moreover, the emission and spectral properties of intervalley excitons are accessible and strongly depend on the local strain environment. Fig. 1b shows how the intensity and energy of $K\Lambda$ excitons change as a function of compressive strain that is characterized by a blueshift of the bright intravalley *KK* excitons. This mechanism is further exploited for strain sensing in two-dimensional semiconductors revealing an optical gauge factor exceeding 10^4, as shown in Fig. 1d.

References

[1] Malic, E. *et al. Phys. Rev. Mater.* **2**, 014002 (2018).
[2] Selig, M. *et al. Nat. Commun.* **7**, 13279 (2016).
[3] Feierabend, M. *et al. Phys. Rev. B* **99**, 195454 (2019).
[4] S. B. Chand, *et al.* arXiv:2201.03090 (2022) – To appear in *Nano Letters*

Figures

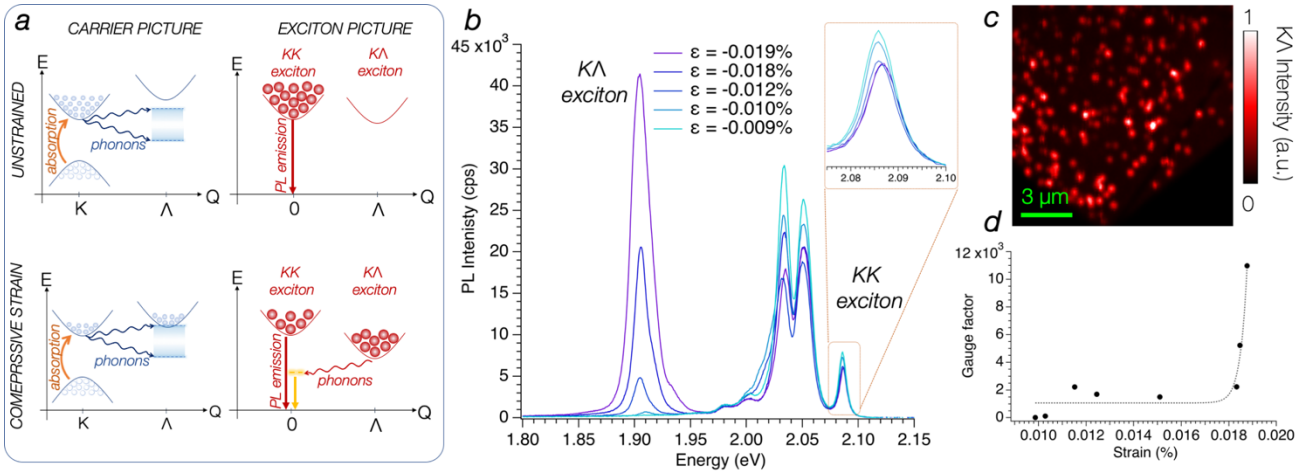


Figure 1: a - Top (bottom) panel shows a cartoon of the band diagram in the carrier and exciton picture for the unstrained (compressive strain) case. With compressive strain the band alignment allows intervalley phonon-assisted scattering and the formation of $K\Lambda$ excitons. b - Emission spectra at different compressive strain levels at T=60 K. The increase of compression in the WS_2 monolayer is characterized by a rise of the $K\Lambda$ exciton peak as well as a blueshift of the *KK* excitons. c - PL map of a WS_2 monolayer with the signal filtered to collect only photons with E<1.94 eV to include only $K\Lambda$ excitons. d - Optical gauge factor shows a nonlinear dependency on the strain with a maximum approaching 12000.

Atomic Layer Deposition of Layered BN

Jiyoung Kim
Su Min Hwang, Yong Chan Jung, Jaebeom Lee, Lanxia Cheng, Luigi Colombo
University of Texas at Dallas, 800 W. Campbell Rd., Richardson, TX 75080, USA
Jiyoung.kim@utdallas.edu

Abstract

Hexagonal boron nitride is a promising dielectric for two-dimensional (2D) material based electronics due to its atomically smooth and charge-free interface with an in-plane lattice constant similar to that of graphene.[1] In this work, we studied the deposition of boron nitride thin films using atomic layer deposition (ALD) with BCl_3/NH_3 precursors directly on various substrates including HOPG, SiO2 as well as 2D channel materials. X-ray photoelectron spectroscopy (XPS) shows that the ALD-BN thin films grow linearly with a growth rate of 0.042 nm/cycle at 600 °C. This growth temperature is significantly lower than chemical vapor deposition of *h*-BN. In Addition, our atomic force microscopy (AFM) results confirmed the formation of uniform and smooth ALD-BN thin films with a low roughness of 0.45 nm. Electrical characterization suggests that the ALD-BN film shows a high breakdown field of 8.5 MV/cm and a dielectric constant of 3.8 which is close to the theoretical value of *h*-BN.2 This ALD-BN thin film also shows reduced charge scattering for graphene devices as evidenced by a twice increase in carrier mobility of graphene field effect transistor (G-FETs) in comparison to that fabricated on thermal SiO_2. Therefore, this work indicates the feasibility of using low temperature ALD-BN as a substrate for futuristic 2D materials.

References

[1] Molaei, Younas, Rezakazemi, ACS Appl.Electron.Mater. 3 (2021) 5165
[2] J. Lee et al, ACS Appl. Mater. Interfaces, 12 (2020) 36688

Figures

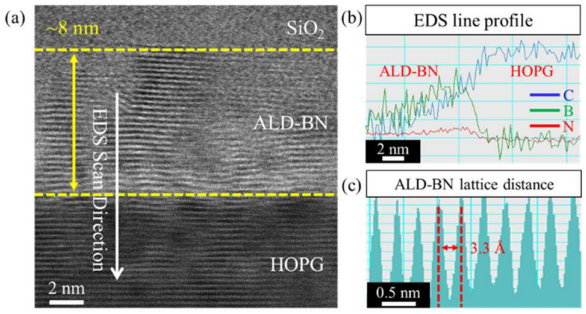


Figure 1: (a) HR-TEM image, (b) EDS line profile (along the solid white arrow in Fig. 2(a)), and (c) a lattice distance of the 200 cycles ALD-BN deposited on HOPG at 600 °C.

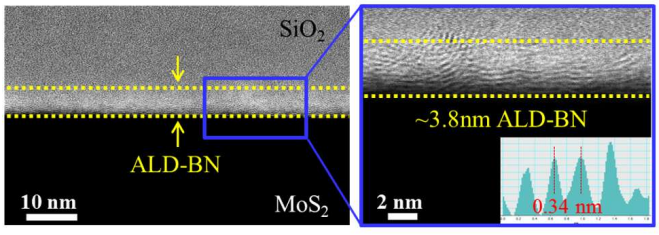


Figure 2: Cross sectional images of ALD -BN on top of MoS2

Electronic properties of sharp junctions in nitrogen doped graphene

Jérôme Lagoute[1,]
Mehdi Bouatou[1], Cyril Chacon[1], Aleksander Bach Lorentzen[2], Huu Thoai Ngo[1], Yann Girard[1], Vincent Repain[1], Amandine Bellec[1], Sylvie Rousset[1], Mads Brandbyge[2], Yannick J. Dappe[3]
[1] *Laboratoire Matériaux et Phénomènes Quantiques (MPQ), CNRS, Université de Paris, Paris, France*
[2] *Center for Nanostructured Graphene, Technical University of Denmark, Denmark*
[3] *SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, France*
jerome.lagoute@u-paris.fr

Tuning the physical properties of graphene is one of the current challenges in the field of 2D materials. Soon after the first isolation of graphene, its chemical doping has been investigated with particular attention in nitrogen doping which is an n-type dopant [1,2]. To bring graphene to a new level, one bottleneck is to control the spatial distribution of dopants in order to realize band engineering at the nanometer scale. Here, we show that a nanopatterning of nitrogen dopants in graphene can be achieved by using monolayer islands of adsorbed molecules as a resist during the doping procedure. The resulting formation of domains with different nitrogen concentrations allows obtaining nn' and pn junctions in graphene. This method leads to the formation of a large collection of domains on a sample, allowing to address the junctions at the atomic scale by scanning tunneling microscopy (STM). Using STM and scanning tunneling spectroscopy, the electronic properties of the junctions have been measured. In particular, the evolution of the Dirac point along the junction makes it possible to measure the width of the space charge zone (Figure 1) which appears to be smaller than the Fermi wavelength [4].

References

[1] F. Joucken, L. Henrard and J. Lagoute, Phys. Rev. Materials 3, (2019) 110301
[2] F. Joucken et al., Scientific Reports 5 (2015) 14564
[3] M. Bouatou et al., (submitted)

Figures

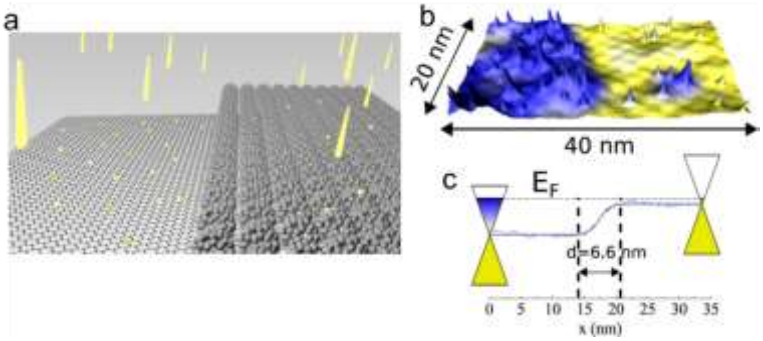


Figure 1: (a) 3D representation of a monolayer resist used to achieve nanodomains of different concentration of nitrogen dopants in graphene. (b) STM topography color code with a differential conductance map showing the variation of the Dirac point on a junction between two domains of different nitrogen concentration in graphene. (c) Linescan of the conductance map used in (b) showing the variation of the Dirac point across the junction.

Monitoring 2D Atomic Layers and Surface Chemistry of Graphene Dispersions Using NMR Proton Relaxation

Sofia Marchesini
Keith R Paton, Piers Turner, Benjamen P Reed, Barry Brennan, and Andrew J Pollard
National Physical Laboratory, Hampton Road, Teddington, TW11 0LW, UK
sofia.marchesini@npl.co.uk

Graphene related 2D products are now produced on an industrial scale in either powder form or as a dispersion. Properties such as the number of 2D atomic layers and surface chemistry are known to vary greatly depending on the production method and these can strongly affect the performance of graphene-containing products. Therefore, there is a growing need to develop fast methods for their quality control.

Microscopy and spectroscopy techniques, some of which have recently been standardised (ISO/TS 21356-1), can be combined to characterise thickness and surface chemistry of graphene samples. However, these are time-consuming, require expensive instruments, and can only characterise a small portion of the sample, making them unsuitable for quality control by graphene manufacturers.

We have recently showed that nuclear magnetic resonance (NMR) proton relaxation has the potential to be used for rapid characterisation of graphene samples [1,2]. In this talk we will demonstrate the use of NMR spin-spin relaxation to monitor changes in different structural properties of graphene particles such as particle size, specific surface area, and exfoliation yield. Moreover, we show that the relaxation time is sensitive to the surface chemistry of graphene as well as its solubility in a selected solvent, providing a route to characterise this important property quickly and at low cost. This is important for formulations of graphene flakes in liquids for inks and paints.

NMR proton relaxation exhibits advantages over conventional characterisation techniques including measurement speed, little to no sample preparation, and low costs using benchtop spectrometers. Moreover, this technique could be integrated into an industrial production line, making this a promising tool for graphene quality control. Improved quality control measurements can accelerate adoption of graphene in applications such as energy storage, coatings, and many more.

References

[1] S. Marchesini, K. R. Paton, B. Brennan, P. Turner, A. J. Pollard, Nanoscale,13 (2021), 6389-6393
[2] S. Marchesini, P. Turner, K. R. Paton, B. P. Reed, A. J. Pollard, Nanoscale 13 (2021), 14518-14524

Figures

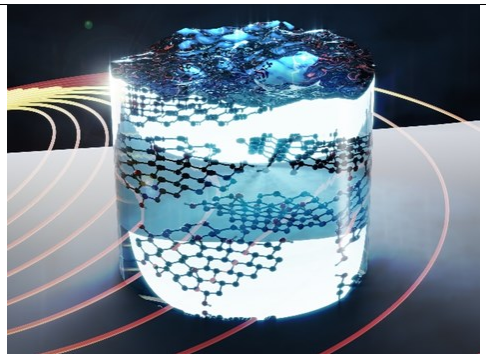


Figure 1: Nanoscale cover image representing graphene flakes in a liquid within the presence of a magnetic field for NMR relaxation measurements.

Mesoscopic Schwinger effect in ballistic graphene transistors

Bernard Plaçais[1]
Aurélien Schmitt[1], Pierre Vallet[2], Takashi Taniguchi[3], Kenji Watanabe[3], Jean-Marc Berroir[1], Erwann Bocquillon[1,4], Gwendal Fève[1], Christophe Voisin[1], Mark-Oliver Goerbig[5], Jérôme Cayssol[2,1], Jan Troost[1], Emmanuel Baudin[1]

1 *Laboratoire de Physique de l'Ecole normale supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université de Paris, 24 rue Lhomond, 75005 Paris, France.*
2 *Laboratoire Ondes et Matière d'aquitaine, 351 cours de la libération, 33405 Talence, France*
3 *Advanced Materials Laboratory, NIMS, Tsukuba, Ibaraki 305-0047, Japan*
4 *II. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln*
5 *Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, F-91405 Orsay, France*

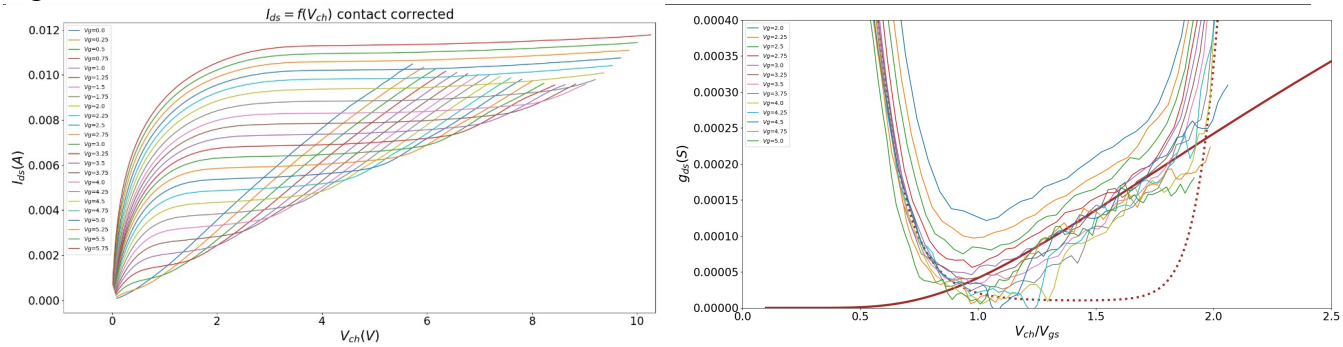
bernard.placais@phys.ens.fr

Vacuum breakdown by particle-antiparticle pair creation in a strong electric field, introduced by Sauter [1] and Schwinger [2], is a basic non-perturbative prediction of quantum electro-dynamics (QED). Its demonstration remains however elusive as Schwinger fields, $E_S = m^2c^3/e\hbar$, are beyond reach even for the light electron-positron pairs. Here we put a mesoscopic variant of Schwinger-effect to test in graphene, which hosts massless Dirac fermions with electron-hole symmetry. Using DC transport and RF noise, we report on universal 1d-Schwinger conductance at the pinch-off of long, hBN-encapsulated, graphene transistors [3]. In ballistic transistors the pinch-off electric fields are confined in a Klein junction of length $\lambda \sim 0.1\mu m$ at the transistor drain, inducing giant Klein-collimation at high bias and a transport gap set by the Fermi energy. They confer an apparent mass to Dirac fermions, leading to a Schwinger breakdown voltage, $V_S = E_S\lambda$, reaching pinch-off bias at large doping, while remaining smaller than the Pauli-blocked onset of Zener transport [4]. The ensuing Schwinger electron-hole conductance is measured in quantitative agreement with prediction (Figure). The mesoscopic Schwinger effect not only gives clues to current saturation limits in graphene electronics, but also opens new routes for QED experiments in the laboratory.

References

[1] F. Sauter, Z. Phys. 69 (1931) 742.
[2] J. S. Schwinger, Phys. Rev. 82 (1951) 664.
[3] A. Schmitt et al., (2022), in preparation
[4] W. Yang et al., Nature Nanotechnol. 13 (2018) 47.

Figure



Left: Current saturation by giant Klein collimation in a LxW=15x10μm, hBN-encapsulated, ballistic graphene transistor with a graphite gate. Gate voltages V_{gs} correspond to Fermi energies distributed in the range $0 \le \mu \le 0.2$eV. Ballistic pinch-off, at bias voltage $V_{ch}=V_{gs}$, is followed by a transition toward an ohmic Zener regime (conductivity $\sigma_Z \sim 1$mS), which onset is rejected, by efficient Pauli blocking in long transistors, at twice the pinch-off voltage. **Right:** differential conductance scaling $g_{ds}(V_{ch}/V_{gs})$. It highlights the Klein-collimation, with a giant conductance suppression $g(1.5) \le g(0)/5000 \sim 1\mu S$, leading to a broad conductance gap in the $V_{gs} \le V_{ch} \le 2V_{gs}$ range (dotted line) within which the Schwinger conductance, $g_S(x=V_{ch}/V_S) \approx 16e^2/\pi h \times (1.523x - 0.943)$, is observed (solid line). Schwinger formula is fitted here to the $V_{gs}=3.25$V data for an onset at $V_{ch} \equiv 0.619V_S \approx 0.87V_{gs}$. Universality lies in the observation of a doping- and sample-independent zero-bias extrapolate of the linear dependence at $g_0 \approx -0.18$ mS.

Thin films of transition Metal Dichalcogenides for optical applications: a GW+BSE approach

Alexandre Reily Rocha[1]
Enérsio Marinho Júnior,[1] Cesar Perez Villegas,[2] Pedro Venezuela[3]
1. Instituto de Física Teórica, São Paulo State University (UNESP), São Paulo, Brazil
2. Departamento de Ciencias, Universidad Privada del Norte, Lima 15434, Peru
3. Departamento de Física, Universidade Federal Fluminense, Niterói, Brazil
alexandre.reily@unesp.br

Transition metal dichalcogenides (TMDCs) are semiconductors with chemical configuration MX_2 [1], where M is a transition metal such as Mo, W, and X is a chalcogen atom such as S, Se, or Te. TMDCs constitute a class of layered materials of significant interest for optoelectronics due to their scalability and thickness-dependent electrical and optical properties. While significant attention has been given to single layer TMDCs, a limited number of works have addressed the few layer case.
Herein, we studied the electronic and optical properties of few layer TMDCs composed of Mo, W, S, and Se within the G_0W_0 and Bethe-Salpeter approach. First-principles calculations based on density functional theory were carried out using the Quantum ESPRESSO package [2]. The many-body perturbation theory and Bethe-Salpeter calculations were performed using YAMBO code [3,4]. We address the photovoltaic performance of these TMDCs estimating the spectroscopic limited practical efficiency (SLME) as a function of the thickness of the semiconductor. We compared the different TMDCs to known materials used in photovoltaics paving the way for efficient nanoscopically thin solar cells.

References

1. S. Shree, I. Paradisanos, X. Marie, C. Robert, and B. Urbaszek, Nat. Rev. Phys., 3 (2021) 39.
2. P. Giannozzi and et. al., J. Phys. Condens. Matter, 21 (2009) 395502.
3. D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite,I. Marri, E. Cannuccia, P. Melo, M. Marsili, F. Paleari, A. Marrazzo, G. Prandini, P. Bonfa, M. O. Atambo, F. Affinito, M. Palummo, A. Molina-Sánchez, C. Hogan, M. Grüning, D. Varsano, and A. Marini, J. Phys.: Condens. Matter, 31 (2019).
4. A. Marini, C. Hogan, M. Grüning, and D. Varsano, Computer Physics Communications, 180 (2009), 1392

Comparing Cr-Doped $(Bi_xSb_{1-x})_2Te_3$ to Graphene as a Future Platform for Quantum Hall Resistance Standards

Albert F. Rigosi
Linsey K. Rodenbach, Alireza R. Panna, Shamith U. Payagala, Ilan T. Rosen, Joseph A. Hagmann, Peng Zhang, Lixuan Tai, Kang L. Wang, Dean G. Jarrett, Randolph E. Elmquist, Jason M. Underwood, David B. Newell, and David Goldhaber-Gordon
National Institute of Standards and Technology (NIST), Gaithersburg, MD 20899, United States
afr@nist.gov

Since 2017, epitaxial graphene has been the base material for the US national standard for resistance. A future avenue of research within electrical metrology is to remove the need for strong magnetic fields, as is currently the case for devices exhibiting the quantum Hall effect. New materials, like magnetically doped topological insulators (MTIs), offer access to the quantum anomalous Hall effect, which in its ideal form, could become a future resistance standard needing only a small permanent magnet to activate a quantized resistance value [1-3]. Furthermore, these devices could operate at zero-field for measurements, making the dissemination of the ohm more economical and portable. Here we present results on precision measurements of the h/e^2 quantized plateau of Cr-Doped $(Bi_xSb_{1-x})_2Te_3$ and give them context by comparing them to modern graphene-based resistance standards. Ultimately, MTI-based devices could be combined in a single system with magnetic-field-averse Josephson voltage standards to obtain an alternative quantum current standard.

This material is based upon work supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

References

[1] E. J. Fox, I. T. Rosen, Y. Yang, G. R. Jones, R. E. Elmquist, X. Kou, L. Pan, K. L. Wang, D. Goldhaber-Gordon. *Phys. Rev. B,* 98, 075145, 2018.
[2] M. Götz, K. M. Fijalkowski, E. Pesel, M. Hartl, S. Schreyeck, M. Winnerlein, S. Grauer, H. Scherer, K. Brunner, C. Gould, F. J. Ahlers. *Appl. Phys. Lett*. 112, 072102, 2018.
[3] Y. Okazaki, T. Oe, M. Kawamura, R. Yoshimi, S. Nakamura, S. Takada, M. Mogi, K. S. Takahashi, A. Tsukazaki, M. Kawasaki, Y. Tokura. *Nat. Phys*. 13, 1-5, 2021

Figures

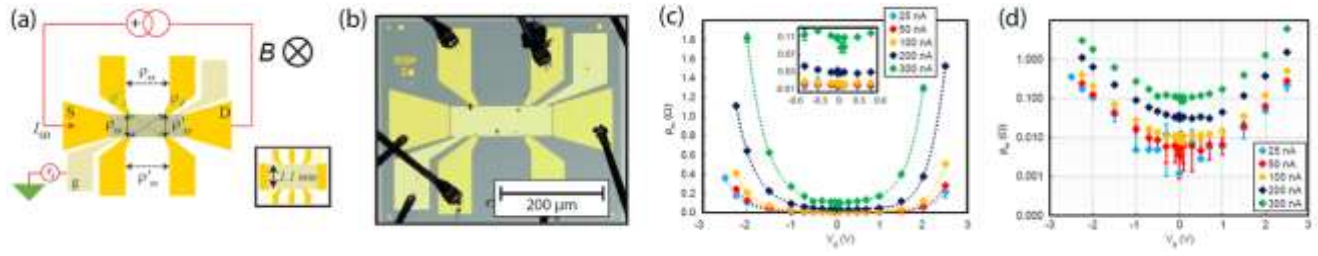


Figure 1: Fabrication of a MTI-based device and a basic top gate characterization of the longitudinal resistance.

Aharonov-Bohm oscillations on a network of trajectories joined by magnetic breakdown as a precursor of Brown-Zak fermions in twistronic graphenes

Sergey Slizovskiy,
Folkert K. de Vries, Petar Tomić, Aitor Garcia-Ruiz, Giulia Zheng, Peter Rickhaus, Thomas Ihn, Klaus Ensslin, Vladimir Fal'ko
National Graphene Institute,University of Manchester, UK and ETH, Zurich, Switzerland.
Sergey.Slizovskiy@manchester.ac.uk

Brown-Zak magnetic minibands for electrons are common for metals with a rational value of magnetic field flux, $\phi = \phi_0 p/q$, piercing the unit cell of a crystal [1]. Here, we study how this ultra-quantum phenomenon, usually, attributed to strong magnetic fields emerges at low magnetic fields and moderate temperatures from the interplay between peculiar dynamics and interference of electrons at the fundamental Lifshitz transition (LT), realised using moire superlattice miniband in twistronic graphene. We show that precursors of Brown-Zak minibands appear in the form of Aharonov-Bohm oscillations of conductivity produced by electrons propagating along entwining paths with a kagom\'e network topology, Fig.1(left). We report the observation of coinciding features in the vicinity of LT of both in twisted tetralayer graphene and in highly aligned graphene - hexagonal boron nitride heterostructures. In particular, the maximal amplitude of conductance oscillations is located in the vicinity of LT, displacing from the LT by the amount growing linearly in the magnetic field Fig.1 (right). These findings are naturally explained by the topology of interfering paths.

References

[1] R. K. Kumar, X. Chen, G. Auton, A. Mishchenko, D. A. Bandurin, S. V. Morozov, Y. Cao, E. Khestanova, M. B. Shalom, A. Kretinin, et al., Science 357, 181 (2017).

Figures

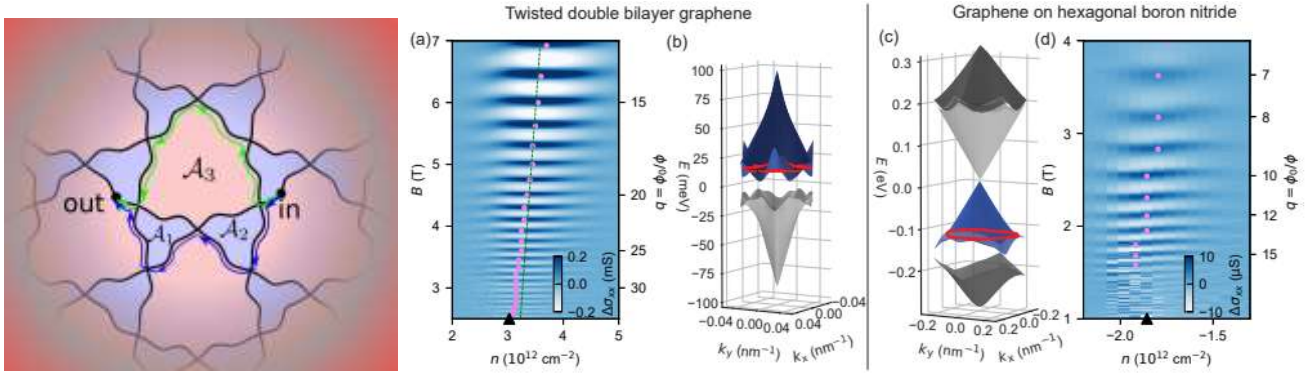


Figure 1: Left: At the LT, ballistic trajectories of electrons in a magnetic field form a kagome network. Green and blue lines in (b) exemplify the shortest paths responsible for quantum magneto-oscillations at the LT. Due to magnetic breakdown, electrons scatter at the intersections of chiral paths (linked to the saddle points in the band dispersion.
Right: The shift of the oscillations maxima in twisted double bilayer graphene (a,b) and graphene aligned to boron nitride (c,d). Pink dots are the maxima of the oscillations, bending away from LT. The green dashed line is a theoretical fit to this data. The LT density is indicated with the solid triangle.

Germanene derivatives synthesis and application

Zdenek Sofer
Tomas Hartman, Marco Serra, Ksenia Mosina, Jiri Sturala
Dept. of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic)
Zdenek.sofer@vscht.cz

The 14th group of elements consisting from carbon, silicon, germanium, tin and lead. In this group only carbon form thermodynamically stable layered allotrope, which is broadly studied in last two decades. On the other Silicon and germanium doesn't form layered compounds in bulk and chemical exfoliation of suitable precursors is necessary. Zintl phases of general formula AB2, where A is alkaline earth (e.g. Ca) and B is silicon/germanium exhibit layered structure containing honeycomb hexagonal motive of covalently bonded silicon / germanium atoms. By chemical etching can be calcium removed and germanene or its derivatives depending on method is formed. [1] In this work are introduced various methods for layered Zintl phase exfoliation and synthesis of germanen derivatives are discussed. The main explored methods are based on direct exfoliation of Zintl phases with alkyl halides. This method was performed under solvothermal condition as well as at room temperature with phase transfer agent. The second method is based on activation of germanane (hydrogenated form of germanene) with alkali metal using NaK liquid alloy as well as by sodium naphthalenide and subsequent reaction with alkyl halides. Scheme of reactions used for germanene functionalization are shown on Figure 1.
The properties of these materials were explored for possible application in photodetectors. The low temperature synthesis provide large area sheet of few layered germanene derivatives suitable for device fabrication. These materials shows fast response time in milsecond time scale and high sensitivity in UV-VIS-NIR region. The possible applications were explored also for use of germanene derivatives for photo-electrochemical water splitting showing excellent performance in alkaline environment and broad spectral range responsivity as well as good sensitivity for application as photo-electrochemical photodetector.

References

[1] Tomáš Hartman, Zdeněk Sofer, ACS Nano, 13 (2019) 8566.

Figures

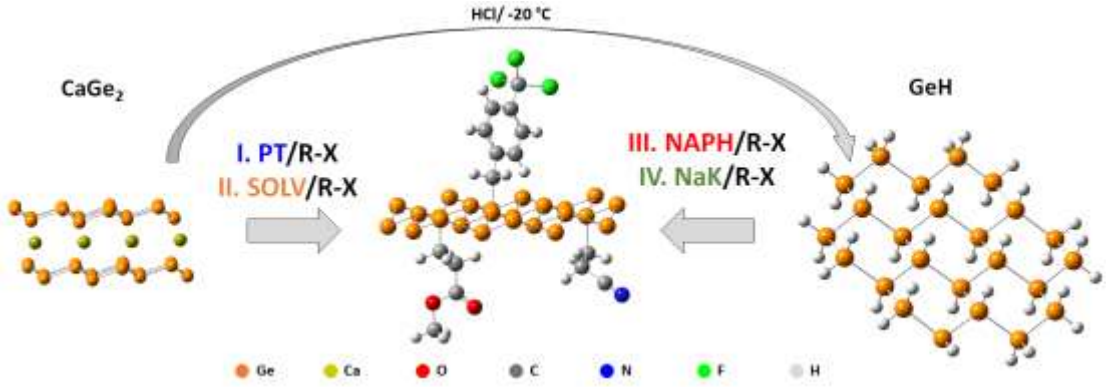


Figure 1: Schematic drawing of germanene functionalization using direct reaction of Zintl phase with alkyl halide and activation of hydrogenated germanene with alkali metal and subsequent reaction with alkyl halide.

Can TMDs compete with silicon in terms of thermal properties?

Klaas-Jan Tielrooij
Catalan Institute of Nanoscience and Nanotechnology (ICN2), BIST & CSIC, Campus UAB, 08193 Bellaterra (Barcelona), Spain
Klaas.tielrooij@icn2.cat

Proper thermal management of electronic and optoelectronic devices is extremely important for correct device functioning and preventing damage. The first line of defense in thermal management is formed by the active semiconductor material – usually silicon, which has a relatively high thermal conductivity of ~150 W/m/K. When considering technological applications based on semiconducting layered crystals, such as transition metal dichalcogenides (TMDs), it is crucial to take their thermal properties into account.

Together with co-workers at ICN2 (Spain), ICFO (Spain), Université de Liège (Belgium) and Utrecht University (the Netherlands), we have studied the thermal conductivity of the TMD $MoSe_2$ as a function of crystal thickness, down to the monolayer [1]. This joint experimental-theoretical work shows that bulk $MoSe_2$ has a somewhat lower thermal conductivity than bulk silicon: ~40 W/m/K. However, $MoSe_2$ starts outcompeting silicon for thin films below ~100 nm. And even monolayer $MoSe_2$ has almost the same thermal conductivity as bulk crystals: ~20 W/m/K. Furthermore, highly efficient out-of-plane dissipation to air molecules occurs for the thinnest crystals. This shows that TMDs are an excellent choice of material system for applications that require ultrathin semiconducting films with uncompromised thermal management properties, such as flexible devices.

References

[1] D. Saleta Reig, et. al. *Advanced Materials*. 2108352, (2022)

Figures

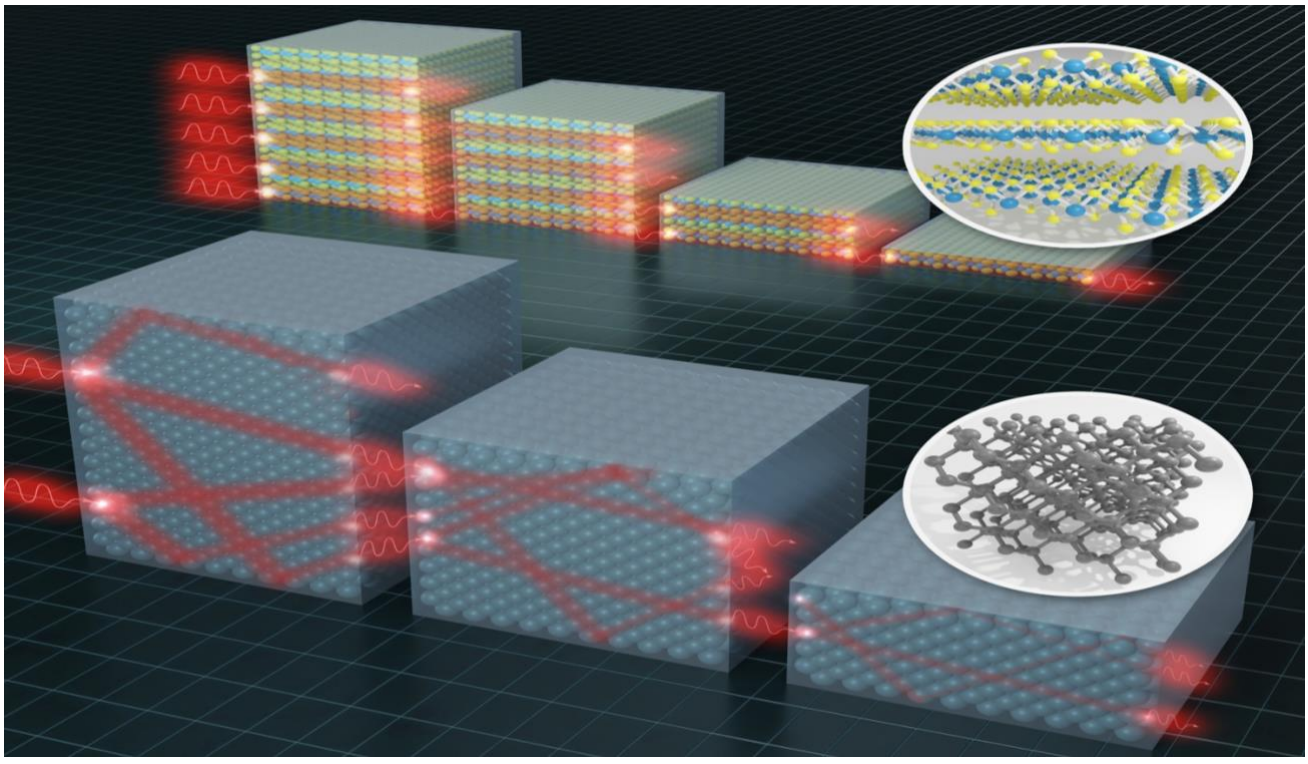


Figure 1: Comparison between in-plane thermal transport in increasingly thin films of layered TMDs and 3D-bonded silicon, where the latter suffers more strongly from increasing surface scattering.

Observation of competing, correlated ground states in the flat surface band of rhombohedral graphite

Péter Vancsó[1]
I. Hagymási[2,3,4], M. Syahid Mohd Isa[1], Z. Tajkov[1,5], K. Márity[1], L. Oroszlány[6], J. Koltai[5], A. Alassaf[6], P. Kun[1], K. Kandrai[1], A. Pálinkás[1], L. Tapasztó[1], P. Nemes-Incze[1]
[1]*Centre for Energy Research, Institute of Technical Physics and Materials Science, Budapest, Hungary*
[2]*Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany*
[3]*Wigner Research Centre for Physics, Budapest, Hungary*
[4]*Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, Freie Universität Berlin, Berlin, Germany*
[5]*Department of Biological Physics, ELTE Eötvös Loránd University, Budapest, Hungary*
[6]*Department of Physics of Complex Systems, ELTE Eötvös Loránd University, Budapest, Hungary*
vancso.peter@ek-cer.hu

In crystalline solids the interactions of charge and spin can result in a rich variety of emergent quantum ground states. A prime example is twisted bilayer graphene, where measurements have demonstrated the presence of superconductivity, ferromagnetism, and Mott insulator quantum states due to the enhanced correlation effects of the partially filled flat bands. Rhombohedral graphite (RG) is perhaps the simplest and structurally most perfect condensed matter system to host a flat band, which is also protected by the symmetry [1]. In this talk we provide detailed investigation of the flat band in RG by using low temperature (9 K) Scanning Tunneling Microscopy (STM) measurements combined with electronic structure calculations [2]. By STM we map the flat band charge density of 8, 10 and 17 layers and identify a domain structure emerging from a competition between a sublattice antiferromagnetic insulator and a gapless correlated paramagnet state up to a temperature of 20 K. Our density-matrix renormalization group (DMRG) calculations explained this observation by revealing a degenerate ground state of the system and demonstrate the important role of the correlation effects. Our work establishes RG as a new platform to study many-body interactions beyond the mean-field approach, in a topological 2D electron system.

References

[1] S. Slizovskiy et al., Communications Physics **2**, 164 (2019)
[2] I. Hagymási et al., arXiv:2201.10844 (2022)

Figures

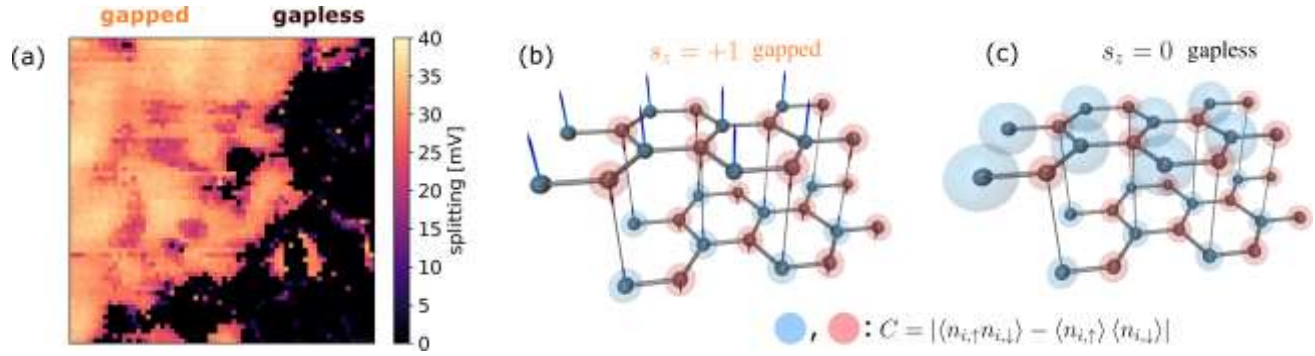


Figure 1: (a) Gapped and gapless domains measured over an 80×80 nm area of the sample. (b-c) DMRG calculations of the sublattice antiferromagnetic and correlated paramagnetic states. Colored arrows show the distribution of magnetic moments, while the radius of the opaque spheres is proportional to the local electronic correlation C values, as defined by the relation shown.

Spin and Valley Relaxation in Single-Electron Graphene Quantum Dots

Christian Volk[1,2]
L. Banszerus[1,2], K. Hecker[1,2], S. Möller[1,2], E. Icking[1,2], K. Watanabe[3], T. Taniguchi[4], and C. Stampfer[1,2]
[1]*JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany*
[2]*Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany*
[3]*Research Center for Functional Materials, NIMS, 1-1 Namiki, Tsukuba 305-0044, Japan*
[4]*International Center for Materials Nanoarchitectonics, NIMS, 1-1 Namiki, Tsukuba305-0044, Japan*
volk@physik.rwth-aachen.de

The relaxation time of single-electron states in a quantum dot (QD) is an important parameter for solid-state spin and valley qubits, as it directly limits the lifetime of the encoded information. Thanks to the low spin-orbit interaction and low hyperfine coupling, graphene and bilayer graphene (BLG) have long been considered promising platforms for spin qubits. Only recently, it has become possible to control single-electrons in BLG QDs and to understand their spin-valley texture [1], while the relaxation dynamics have remained mostly unexplored [2]. Here, we present spin and valley relaxation times (T_1) of single-electron states in BLG QDs. Using pulsed-gate spectroscopy, we extract spin relaxation times T_{1s} exceeding 200 µs at a magnetic field of B = 1.9 T [3] and valley relaxation times T_{1v} of around 6 µs at B = 0.1 T. The strong dependence of T_{1s} on the spin splitting, promises even longer T_{1s} at smaller B, where our measurements are limited by the signal-to-noise ratio. The spin relaxation times are more than two orders of magnitude larger than those previously reported for carbon-based QDs, further suggesting that graphene is a promising host material for scalable spin qubits.

References

[1] L. Banszerus, S. Möller, C. Steiner, E. Icking, S. Trellenkamp, F. Lentz, K. Watanabe, T. Taniguchi, C. Volk, and C. Stampfer, Nat. Commun.12, 5250 (2021).
[2] L. Banszerus, K. Hecker, E. Icking, S. Trellenkamp, F. Lentz, D. Neumaier, K. Watanabe, T. Taniguchi, C. Volk, and C. Stampfer, Phys. Rev. B 103, L081404 (2021).
[3] L. Banszerus, K. Hecker, S. Möller, E. Icking, K. Watanabe, T. Taniguchi, C. Volk, and C. Stampfer, arXiv:2110.13051 (2021).

Figures

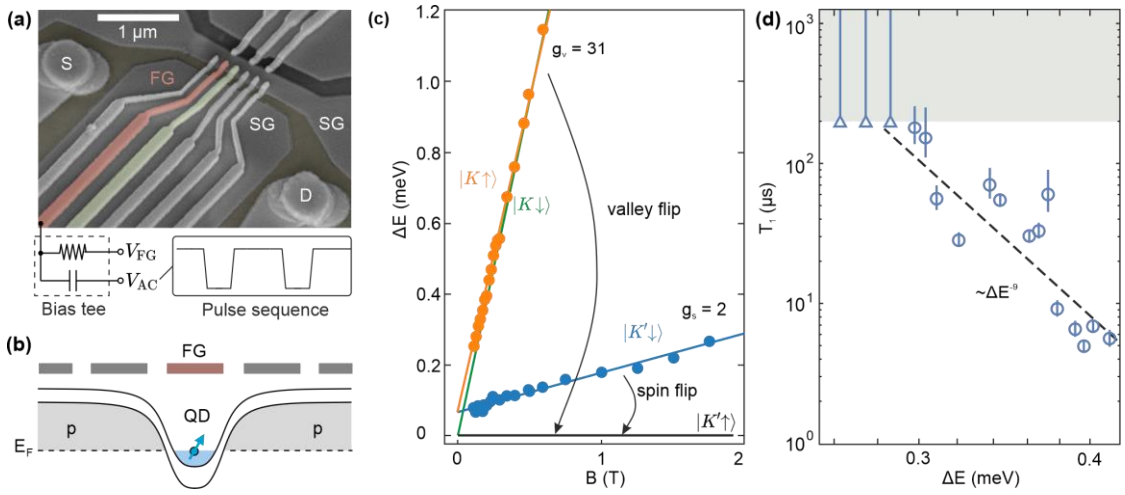


Figure 1: (a) Scanning electron micrograph of the device. AC and DC voltages are applied to the finger gate (FG). (b) Band edge diagram along the p-type channel, illustrating the formation of a QD. (c) Measured energy splitting of the states. (d) Spin relaxation time T_1 as a function of the energy splitting.

Chiral nonlocal currents in single layer graphene from orbital valley Hall effects

Mario Amado
Juan Salvador-Sánchez, Ana Pérez Rodríguez, Vito Clericò, Daniel Vaquero, José M. Caridad and Enrique Diez
Nanotechnology Group, USAL-NanoLab, University of Salamanca, E-37008, Salamanca, Spain
mario.amado@usal.es

Takashi Taniguchi and Kenji Watanabe
National Institute for Materials Science. J-305-0044, Tsukuba, Japan.

Yuriko Baba, and Francisco Domínguez-Adame
GISC, Departamento de Física de Materiales, Universidad Complutense, E- 28040, Madrid, Spain

Tatiana G. Rappoport
Instituto de Telecomunicações, Instituto Superior Técnico, University of Lisbon, P-104900, Lisbon Portugal
Instituto de Física, Universidade Federal do Rio de Janeiro, B-21941-972, Rio de Janeiro RJ, Brazil

Luis Canónico Armas and Stephan Roche
Catalan Institute of Nanoscience and Nanotechnology ICN2. 08193 Cerdanyola del Vallès, Spain

In this work we report on electrical measurements on single layer graphene Hall-bars encapsulated within hexagonal boron nitride thin films with controlled twisting angle between the layers. The samples have been fabricated by means of a cryo-etching method [1], permitting an unprecedented control of the roughness of the edges. The whole structure was placed onto a thin graphite back gate, preventing dopants or trapped charges arising from the standard semiconductor substrates [2].

We have carried out an exhaustive study of the electrical response at different temperatures when an in-to-out-of-plane external magnetic field has been exerted with special attention to the possible effects arising due to the Moiré pattern. Local and non-local signals are presented and a striking chiral behaviour at low magnetic fields of the nonlocal currents resulting from a charge carrier-valley coupling is found, in stark contrast with previous results of similar structures at different twisting angles [3]. Orbital valley Hall effect [4,5] has been found responsible for the presented chiral response with thorough theoretical calculations supporting the experimental results [6].

References

[1] V. Clericò, J. A. Delgado-Notario, M. Saiz-Bretín, A. V. Malyshev, Y. M. Meziani, P. Hidalgo, B. Méndez, M. Amado, F. Domínguez-Adame, and E. Diez, Scientific Reports, 9 (2019) 13572
[2] A.A. Zibrov, C. Kometter, H. Zhou, E. M. Spanton, T. Taniguchi, K. Watanabe, M. P. Zaletel and A. F. Young, Nature. 549 (2017) 360
[3] A. Aharon-Steinberg, A. Marguerite, D. J. Perello, K. Bagani, T. Holder, Y. Myasoedov, L. S. Levitov. A. K. Geim, and E. Zeldoz, Nature 593 (2021) 528
[4] S. Bhowal and G. Vignale, Physical Review B. 103 (2021) 195309
[5] S. Roche, S. R. Power, B. K. Nikolić, J. H. García, and A.-P. Jauho, Journal of Physics: Materials 5 (2022) 021001
[6] J. Salvador-Sánchez *et al.* Submitted.

Local nanomechanical properties in twisted double bilayer graphene

Alessandra Canetta
Jean Spiece (1), Sergio Gonzalez-Munoz (2), Viet-Hung Nguyen (3), Pauline de Crombrugghe (1), Khushboo Agarwal (2), Yuanzhuo Hong (4), Sambit Mohapatra (4), Kenji Watanabe (5), Takashi Taniguchi (5), Rebeca Ribeiro-Palau (4), Jean-Christophe Charlier (3), Oleg Kolosov (2), Pascal Gehring (1)
(1) IMCN/NAPS, Université Catholique de Louvain (UCLouvain), 1348 Louvain-la-Neuve, Belgium
(2) Physics Department, Lancaster University, Lancaster, UK
(3) IMCN/MODL, Université Catholique de Louvain (UCLouvain), 1348 Louvain-la-Neuve, Belgium
(4) Centre de Nanosciences et de Nanotechnologies (C2N), CNRS, Université Paris Sud, Université Paris-Saclay, Palaiseau, France
(5) National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
alessandra.canetta@uclouvain.be

Van der Waals heterostructures are tremendously versatile designer materials whose functionality can be engineered to an extend that goes far beyond the properties of the individual materials the heterostructure consists of [1]. In particular, by twisting two graphene layers, it is possible to induce an atomic reconstruction in the two-dimensional stack, which leads to a dramatic modification of the lattice symmetry [2]. This has important repercussions on its mechanical and electro-mechanical properties [3,4]. Here we investigate the local mechanical properties of double bi-layer graphene twisted by an angle ~1.1°. To this end, we employ three force microscope techniques, Piezoresponse Force Microscopy, Ultrasonic Force Microscopy and Electric Heterodyne Force Microscopy, respectively. We demonstrate that these methods are reliable and effective to visualize the Moiré pattern, to evidence the presence of strain solitons [5], and – for the first time – to extract the local Young's modulus in such systems. Our results bring on a comprehensive study of such complex structures and unlock critical understanding of these materials.

References

[1] Geim, A., Grigorieva, I., Nature, 499 (2013) 419–425.
[2] Dai, S., Xiang, Y., Srolovitz, D. J., Nano Lett., 16, 9 (2016) 5923–5927.
[3] De Sanctis, A., Mehew, J. D., et al., Nano Lett., 18, 12 (2018) 7919–7926.
[4] Li, Y., Wang, Xet al., Adv. Mater., 33 (2021) 2105879.
[5] Alden, J. S., Tsen, A. W., et al., PNAS, 110 (2013) 11256–11260.

Figures

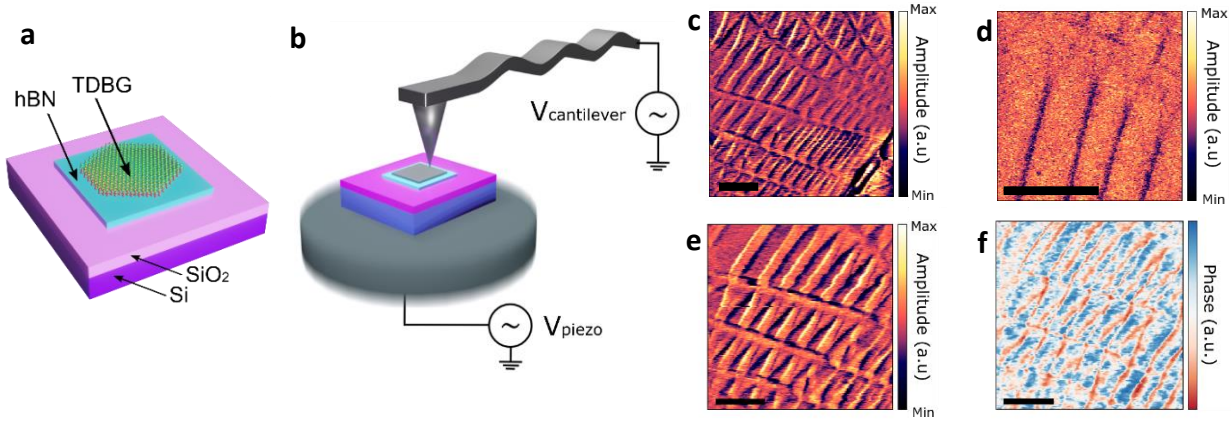


Figure 1: (a) Structure of the measured sample. (b) Schematic of the measurement system to image Moiré pattern in Twisted Double-Bilayer Graphene. (c) Piezoelectric Force Microscopy, (d) Ultrasound Force Microscopy and (e,f) Electric-Heterodyne Force Microscopy amplitude and phase, respectively. Scalebars: 200 nm.

Tuning van der Waals heterostructures by pressure

Szabolcs Csonka[1]
Bálint Szentpéteri[1], Bálint Fülöp[1], Albin Márffy[1], S. Zihlmann[3], Peter Rickhaus[2], Folkert K. de Vries[2], Endre Tóvári[1], C. Schönenberger[3], Andor Kormányos[4], Péter Makk[1]
[1]*Department of Physics, Budapest University of Technology and Economics and Correlated van der Waals phases Momentum Research Group of the Hungarian Academy of Sciences, 8 Budafoki street, 1111 Budapest, Hungary*
[2]*Solid State Physics Laboratory, ETH Zürich, CH-8093 Züurich, Switzerland*
[3]*Department of Physics, University of Basel, 82 Klingenbergstrasse, Basel, Switzerland*
[4]*Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary*
szabolcs.csonka@ttk.bme.hu

In van der Waals heterostructures the layer distance strongly affects the interaction between the layers. Therefore, pressure is an ideal tool to engineer the band structure of van der Waal materials [1].
In this talk I will show two examples for the versatility of this method. First, I will show, that in WSe_2/Gr structures spin-orbit coupling can be induced in graphene using proximity effects, which can be boosted using hydrostatic pressure [2]. The enhancement is confirmed using weak anti- localization measurements. Moreover, I will also demonstrate the band structure tuning of magic-angle twisted double bilayer graphene [3]. We have performed thermal activation and magneto-transport measurements to reveal changes in the bandgaps of the system. We have observed a strong tuneability with pressure, which is confirmed by our theoretical calculations. Finally, we have also observed changes in the strength of electron-electron interactions and in the topological phases at the charge neutrality point in magnetic fields.

References

[1] B. Fülöp et al., Journal of Appl. Phys., 130 (2021), 064303
[2] B. Fülöp, A. Márffy, S. Zihlmann, M. Gmitra, E. Tóvári, B. Szentpéteri, M. Kedves, K. Watanabe, T. Taniguchi, J. Fabian, C. Schönenberger, P. Makk, Sz. Csonka, npj 2D Materials and Applications 5 (2021), 82
[3] B. Szentpéteri, P. Rickhaus, F. K. de Vries, A. Márffy, B. Fülöp, E. Tóvári, K. Watanabe, T. Taniguchi, A. Kormányos, Sz. Csonka, and P. Makk, Nano Letters, 21 (2021), 8777

Figures

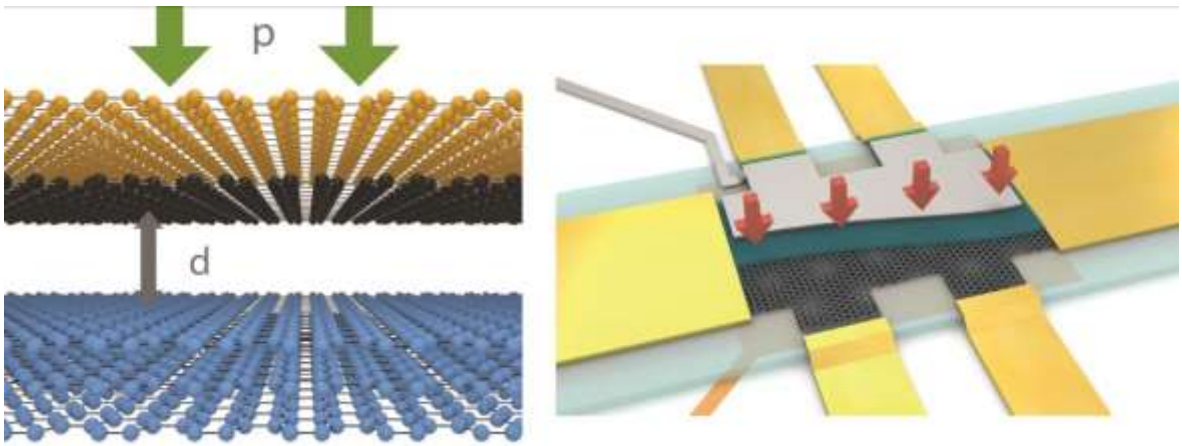


Figure 1: Illustration of the working principle of our pressure cell and an artistic view of the device architecture at study.

Indications of spatially correlated electrons near the band insulators in twisted bilayer graphene

Robin J. Dolleman[1]
A. Rothstein[1], L. Klebl[2], A. Fischer[2], T. Fabian[3], C. Schattauer[3], B. Beschoten[1], F. Libisch[3], D. M. Kennes[2], C. Stampfer[1]
[1] *JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Aachen, Germany*
[2] *JARA-FIT and Institut für Theorie der Statistischen Physik, RWTH Aachen University, Aachen, Germany*
[3] *Institute for Theoretical Physics, Vienna University of Technology, Vienna, Austria*
dolleman@physik.rwth-aachen.de

Twisted bilayer graphene at small angles has band insulators at full filling of the moiré superlattice, which are absent the Bernal stacked material [1]. Furthermore, multiple experiments have shown correlated electronic phases near fractional filling of the moiré lattice [2]. In our experiments, we observe periodic conductance oscillations near the band insulators of twisted bilayer graphene, with a remarkably high frequency that depends on the gate voltage [Figure 1(a—c)]. These oscillations are interpreted as the Coulomb blockade effect in localized regions on the sample, which are periodic because the charging energy is large compare to the quantum level spacing [3]. Remarkably, the frequency of these oscillations increases as we tune the Fermi level into the band gap. This implies that the capacitance of the localized region increases near this point. However, we expect the geometric and chemical quantum contributions to result in a minimum total capacitance near this bandgap. We therefore consider a negative quantum capacitance contribution, and find that a simple model for spatially correlated electrons in a 2D electron gas [4] can describe the observed increase in capacitance remarkably well [Figure 1(d)], which strongly indicates the relevance of correlated electrons near the band insulators of twisted bilayer graphene.

References

[1] Cao, Y., et al. Phys. Rev. Lett. 117.11 (2016): 116804
[2] Balents, L., et al. Nat. Phys. 16 (2020): 725—733
[3] Staring, A.A.M. et al. Phys. Rev. B. 45 (1992): 9222
[4] M. S. Bello, et al. Zh. Eksp. Theor. Fiz. 83 (1981): 1596

Figures

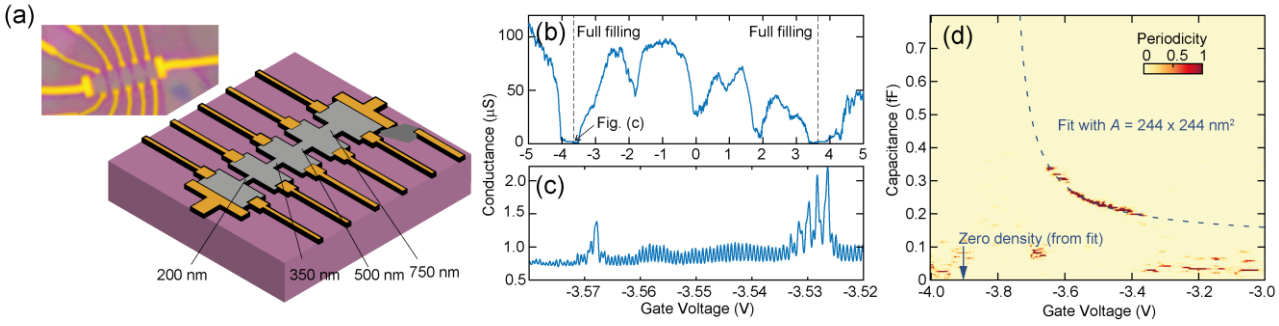


Figure 1: (a) Optical image and drawing of the sample, which consists of twisted bilayer graphene in a constricted Hall-bar geometry and a global graphite gate. (b) Conductance as a function of gate voltage for the 750 nm constriction (twist angle 1.02°), showing the band insulators (labelled "full filling") and further insulating states near -1/2, +1/4, +1/2 and +3/4 filling of the superlattice. (c) Zoom-in of the conductance, showing the periodic high-frequency conductance oscillations. (d) Frequency component converted to capacitance at full filling on the hole-side and a fit to the data considering spatial electron correlations.

Valley-polarized Hyperbolic-Exciton–Polaritons in Multilayer 2D Semiconductors at Visible Frequencies

Itai Epstein[1,2,3],
Tomer Eini[1], Tal Asherov[1], Yarden Mazor[1]
[1] School of Electrical Engineering, Faculty of Engineering, Tel Aviv University, Tel Aviv 6997801, Israel.
[2] Center for Light-Matter Interaction, Tel Aviv University, Tel Aviv 6997801, Israel.
[3] QuanTAU, Quantum Science and Technology center, Tel Aviv University, Tel Aviv 6997801, Israel
itaieps@tauex.tau.ac.il

Abstract
We show that resonant exitonic-based hyperbolicity can be induced in transition-metal-dichalcogenides (TMDs), leading to the existence of hyperbolic-exciton-polaritons (HEPs). Furthermore, we show that owing to the valley properties of TMDs, the HEPs are coupled to the valley degree-of-freedom, leading to a hyperbolic spin-valley hall effect. We analyze the HEPs' confinement and loss properties, finding large momentum modes with losses that increase slower than the confinement. Such highly confined and valley-polarized HEPs provide new opportunities and means of controlling strong light-matter interaction at the atomic scale.

Hyperbolic materials exhibit opposite signs of the real part of the in-plane ($\varepsilon_\perp$) and out-of-plane ($\varepsilon_\parallel$) components of the permittivity tensor: $Re\{\varepsilon_\perp\} \cdot Re\{\varepsilon_\parallel\} < 0$. Such materials support hyperbolic modes of arbitrarily large wavevectors, making them highly important for photonics and optoelectronics. Recently, transient HEPs in thick (~450nm) layers of TMDs that stem from the Rydberg series transitions of TMD excitons in the MIR spectrum, have been observed via ultrafast photoexcitation of electron-hole pairs[1]. Here, we show for the first time that TMDs can obtain a hyperbolic material response at VIS-NIR frequencies, at the frequency of the main exciton resonance, and at steady-state conditions (fig1(a)). This hyperbolicity stems from the combination of an in-plane negative permittivity, induced via the use high-quality van der Waals heterostructures at cryogenic temperatures[2], and an out-of-plane positive permittivity. The dispersion relation of the resulting visible frequency HEPs supported by multilayer TMDs is presented in fig1(b), showing very large momenta. Furthermore, the inherent spin-valley selection rules for excitons in TMDs lead to HEPs that are coupled to the TMD's valley degree-of-freedom. This can be seen via the directional coupling of HEPs in response to left/right circular polarization (CP), introducing a spin-valley Hall effect for HEPs (fig1(c)).

References

[1] Sternbach, A. J. et al. Science 371, 617–620 (2021).
[2] Epstein, I. et al. 2D Materials 7, 035031 (2020).

Figures

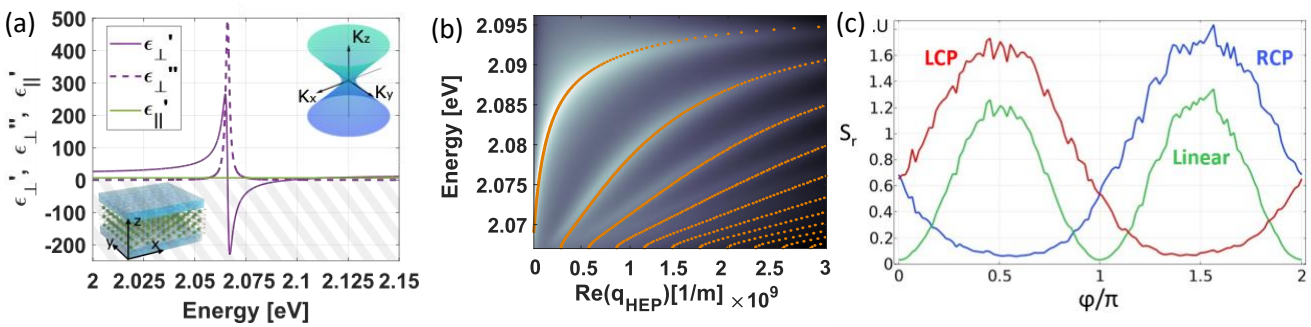


Figure 1: (a) Resonant exciton-induced hyperbolicity in multilayer TMDs. (b) Resulting HEPs dispersion relation in multilayer TMDs, carrying large momenta. (c) Radial component of the Poynting vector, S_r for the case of right/left CP and linear dipole, showing a symmetrical excitation for linear polarization, and an asymmetric one for CPs, demonstrating a spin-valley Hall effect for HEPs.

Ferroelectricity in twisted double bilayer graphene

Aitor Garcia-Ruiz
V. Enaldiev and V. I. Fal'ko
National graphene institute, University of Manchester, Booth St, M13 9PL, , Manchester, UK.
altor.garcia-ruiz@manchester.ac.uk

Abstract
Ferroelectric van der Waals heterostructures have attracted a lot of research attention, as they could be used on a wide range of device applications, such as non-volatile memory devices or pyroelectric sensors [1]. Experimentalists have constructed such structures using hexagonal boron nitride [2] or transition-metal dichalcogenides [3]. However, there has not been theoretical or experimental reports on single-element ferroelectric materials yet.
In this presentation, I will discuss the possibility of constructing a purely carbon-based ferroelectric structure. In particular, I present marginally twisted double bilayer graphene as a candidate material to observe ferroelectricity. Following previous works [4], we develop a method to compute the ferroelectric polarisation map across the moiré unit cell, as shown in Fig. 1. We find that the ferroelectric dipole moment has a definite orientation in each domain of the unit cell and propose experimental setups that enable us to observe this phenomenon.

References

[1] K. Uchino, Ferroelectric Devices (CRC Press, 2009).
[2] K. Yashuda et al., Science **372**, 1458 (2021).
[3] A. Weston et al., arXiv:2108.06489 (2021)
[4] A. Garcia-Ruiz et al., Phys. Rev. B, **104**, 085402 (2021).

Figures

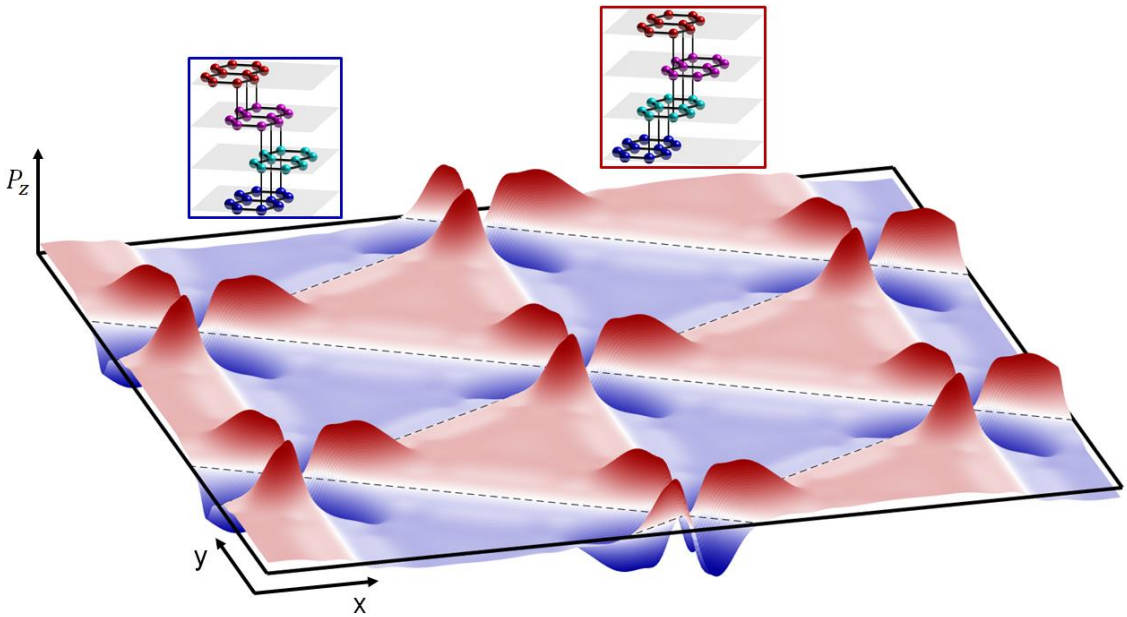


Figure 1: Ferroelectric polarisation across several moiré unit cells of AB/BA-twisted double bilayer graphene, with a twist angle of 0.5°. Inside the red (blue) coloured domains, where the system has a stacking configuration ABCB (ABAC), we observe a definite positive (negative) value for the ferroelectric polarisation.

Observation of flat bands in 57° twisted bilayer WSe_2

Gianmarco Gatti
J. Issing, F. Margot, L. Rademaker, A. Tamai, F. Baumberger

Department of Quantum Matter Physics, Quai Ernest-Ansermet 24, Geneva, Switzerland (CH)
gianmarco.gatti@unige.ch

Recent transport experiments revealed a correlated insulating phase and quantum criticality points in twisted transition metal dichalcogenides (TMDs)[1,2] that were predicted to host flat Moiré mini-bands [3,4]. Despite these exciting experimental observations and theoretical predictions, no direct measurements of the band structure of twisted TMD are available to date. We report here for the first time on the direct observation of flat band in twisted TMDs investigating 57° twisted bilayer WSe_2 by micro-focused angle-resolved photoemission spectroscopy. We resolve multiple Moiré mini-bands with strongly reduced dispersion and significant mini-gaps. By comparison with effective continuum band structure models, we attribute the origin of the flat states to a moderate Moiré potential of ≈50 meV emerging from the stacking of the two semiconducting layers. Our results establish a reference for future theoretical and experimental studies of the Moiré physics in twisted TMDs.

References

[1] A. Ghiotto *et al.* Nature **597** (2021), 345-349
[2] L. Wang *et al. Nat. Mater.* **19** (2020), 861–866
[3] Naik M. H. *et al.* Phys. Rev. Lett. **121** (2018) 266401
[4] M. Angeli and A. H. MacDonald, Proc. Natl. Acad. Sci. USA **118** (2021) 1–5

Figures

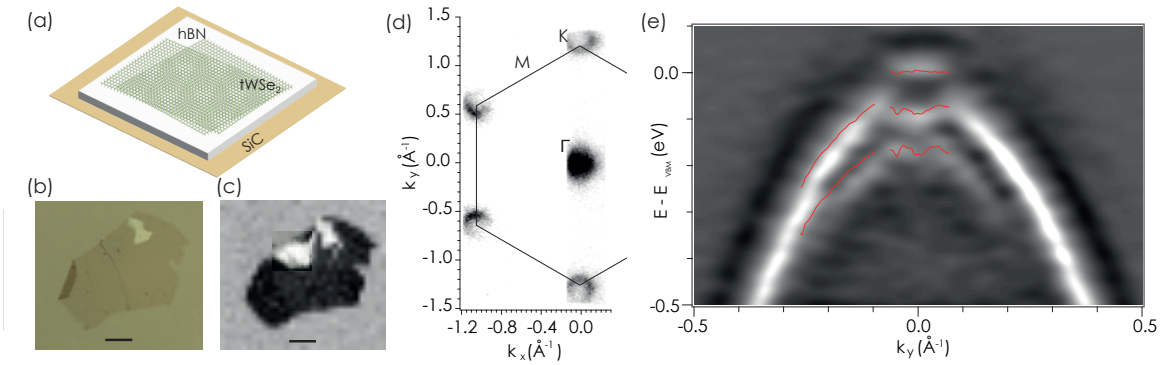


Figure 1: (a) Sketch of the 2D heterostructure. (b) Optical microscopy image of the heterostructure. (c) Real space mapping of the heterostructure by photoemission. The scale bar is 10 µm. (d) Momentum space mapping of the electronic structure 200 meV below the valence band maximum. (e) Close-up of the band dispersion along the K-Γ-K direction near the valence band maximum. Red curves indicate the fitted positions of the dispersing states.

Gate-defined electron interferometer in bilayer graphene

Shuichi Iwakiri
Folkert K. de Vries, Elias Portoles, Giulia Zheng, Takashi Taniguchi[1],Kenji Watanabe[2], Thomas Ihn, and Klaus Ensslin

Solid State Physics Laboratory, ETH Zurich, CH-8093 Zurich, Switzerland
1. *International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
2. *Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
Solid State Physics Laboratory, ETH Zurich, CH-8093 Zurich, Switzerland

siwakiri@phys.ethz.ch

Abstract

We present the fabrication of an electron interferometer in encapsulated bilayer graphene defined purely by electrostatic gating, minimizing the sample degradation which is introduced by conventional etching methods [1,2]. The device quality is demonstrated by observing Aharonov-Bohm (AB) oscillations with a period of h/e, $h/2e$, $h/3e$, and $h/4e$. The AB oscillations are tunable with gating; one can seamlessly tune the device geometry from the bulk transport to ring transport. The carrier type can also be changed from electron to hole, allowing us to perform an ambipolar operation of the ring. The temperature and magnetic field dependence of the oscillations indicate that ballistic electron transport is realized in the ring. Our gate-defined ring geometry is a first step to exploring novel quantum states in ring geometries for example superconductivity in twisted bilayer graphene [3].

References

[1] S. Russo, J. B. Oostinga, D. Wehenkel, H. B. Heersche, S. S. Sobhani, L. M. K. Vandersypen, and A. F. Morpurgo, Phys. Rev. B, **77**, 085413 (2008).
[2] J. Dauber, M. Oellers, F. Venn, A. Epping, K. Watanabe, T. Taniguchi, F. Hassler, and C. Stamper, Phys. Rev. B, **96**, 205407 (2017).
[3] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herello, Nature, **556**, 43-50 (2018).

Figures

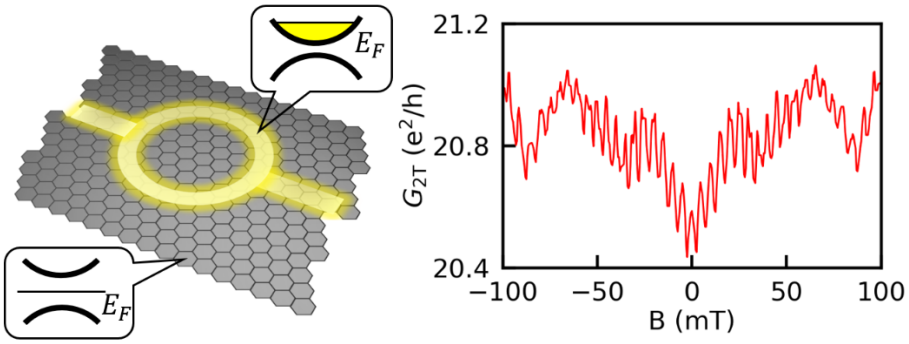


Figure 1: Left: Schematic image of the gate-defined ring in bilayer graphene. The ring-shaped area is conductive while the rest of the sample is tuned into the insulating state. Right: Magneto-conductance trace through the ring showing Aharonov-Bohm oscillations.

Spin-Charge Conversion in Twisted van der Waals Heterostructures

David T. S. Perkins[1]
Alessandro Veneri[1], Csaba G. Péterfalvi[2], Aires Ferreira[1]

[1]*Department of Physics and York Centre for Quantum Technologies, University of York, Heslington, YO10 5DD, York, United Kingdom*

[2]*Department of Physics, University of Konstanz, D-78464 Konstanz, Germany*

David.t.s.perkins@york.ac.uk(Century Gothic 10)

Spin-charge conversion processes in graphene-based van der Waals (vdW) heterostrucutres have been the subject of many theoretical and experimental studies over the past decade [1,2]. The field of spintronics prides itself on uncovering the novelty of these processes, with the perspectives of technology and fundamental physics in mind [3]. In recent years, research has turned towards studying the role played by misalignment between the layers of vdW heterostructures [4], i.e. twisting, leading to the birth of a new field known as twistronics.

In this talk, we look at the unification of spintronics with twistronics: we study the rich transport effects generated by proximity-induced spin-orbit coupling (SOC) in graphene on transition metal dichalcogenide (TMD) bilayers. Previous works [5-7] have found that the introduction of a twist between the graphene and TMD layers allows for the tuning of the SOC strength. Introducing a twist liberates the spin-texture of the Rashba-split graphene bands, such that it is no longer confined to be perpendicular to the momentum. Specifically, we study the generation of spin accumulation upon the application of an electrical current. We further demonstrate the robustness of our observations against twist-angle disorder.

References

[1] M. Offidani, M. Milletarì, R. Raimondi, and A. Ferreira, Phys. Rev. Lett., **119** (2017) 196801
[2] A. Avsar, H. Ochoa, F. Guinea, B. Özyilmaz, B.J. van Wees, and I.J. Vera-Marun, Rev. Mod. Phys., **92** (2020) 021003
[3] W. Han, R.K. Kawakami, M. Gmitra, and J. Fabian, Nat. Nanotechnol., **9** (2014) 794
[4] R. Ribeiro-Palau, C. Zhang, K. Watanabe, T. Taniguchi, J. Hone, and C.R. Dean, Science, **361** (2018) 690
[5] Y. Li, and M. Koshino, Phys. Rev. B, **99** (2019) 075438
[6] A. David, P. Rakyta, A. Kormányos, and G. Burkard, Phys. Rev. B, **100** (2019) 085412
[7] C.G. Péterfalvi, P. Rakyta, G. Burkard, and A. Kormányos, arXiv:2111.02781v2 [cond-mat.mes-hall]

Steering the Current Flow in Twisted Bilayer Graphene

Thomas Stegmann[1]
Jesús Arturo Sánchez-Sánchez[1], Montserrat Navarro-Espino[2], Yonatan Betancur-Ocampo[1], José Eduardo Barrios-Vargas[2]
1: Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, Cuernavaca, México
2: Departamento de Física y Química Teórica, Facultad de Química, Universidad Nacional Autónoma de México, Ciudad de México, México
stegmann@icf.unam.mx, jebarrios@quimica.unam.mx

A nanoelectronic device made of twisted bilayer graphene (TBLG) is proposed to steer the direction of the current flow. The ballistic electron current, injected at one edge of the bottom layer, can be guided predominantly to one of the lateral edges of the top layer. The current is steered to the opposite lateral edge, if either the twist angle is reversed or the electrons are injected in the valence band instead of the conduction band, making it possible to control the current flow by electric gates. When both graphene layers are aligned, the current passes straight through the system without changing its initial direction. The observed steering angle exceeds well the twist angle and emerges for a broad range of experimentally accessible parameters. It is explained by the twist angle and the trigonal shape of the energy bands beyond the van Hove singularity due to the Moiré interference pattern. As the shape of the energy bands depends on the valley degree of freedom, the steered current is partially valley polarized. Our findings show how to control and manipulate the current flow in TBLG. Technologically, they are of relevance for applications in twistronics and valleytronics.

Figures

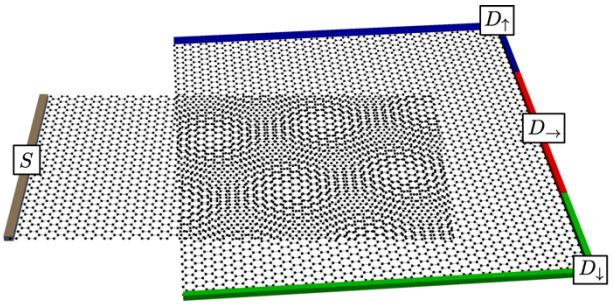


Figure 1: Schematic representation of the studied TBLG device. It consists of two stacked graphene nanoribbons, where the upper layer is twisted by the angle θ with respect to the lower one that remains fixed. Electrons are injected through the source contact at the left edge of the bottom layer. They pass through the twisted bilayer region and are detected by three drain contacts at the edges of the top layer (blue, red, and green bars).

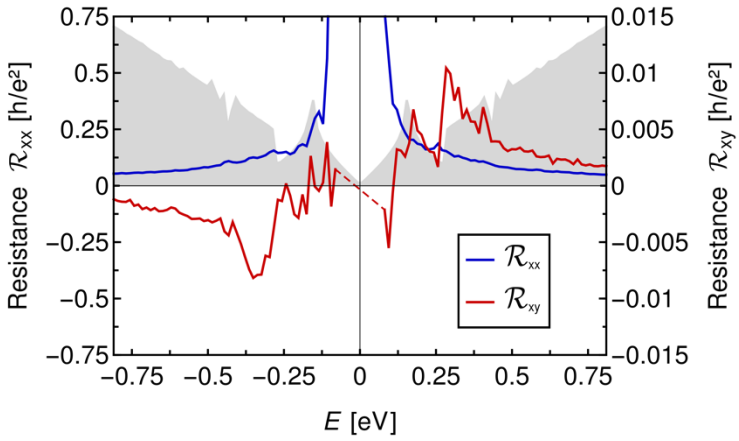


Figure 2: Longitudinal resistance R_{xx} (blue curve) and Hall resistance R_{xy} (red curve) as a function of energy for the TBLG device at a twist angle of θ=2.9 degree. The steering of the current flow to one of the lateral edges generates a non-local Hall resistance. The DOS (in arbitrary units) is indicated by the gray color shading.

References

[1] J. A. Sánchez-Sánchez, M. Navarro-Espino, Y. Betancur-Ocampo, J. E. Barrios-Vargas, T. Stegmann, J. Phys. Mater. 5: 024003 (2022).

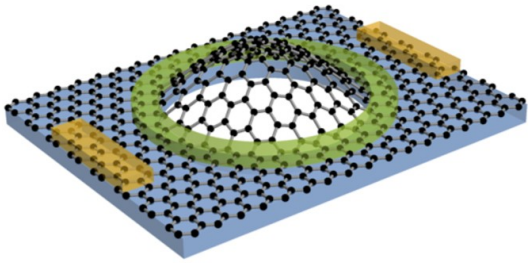
Graphene nanodrums as valleytronic devices

Nikodem Szpak[1]
Walter Ortiz[2], Thomas Stegmann[2]
1: Fakultät für Physik, Universität Duisburg-Essen, Germany
2: Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México, México
nikodem.szpak@uni-due.de, stegmann@icf.unam.mx

We investigate the electronic transport in graphene nanoelectromechanical resonators (GrNEMS), known also as graphene nanodrums or nanomembranes. We demonstrate that these devices, despite small values of out-of-plane strain, between 0.1 and 1%, can be used as efficient and robust valley polarizers and filters. Their working principle is based on the pseudomagnetic field generated by the strain of the graphene membrane. They work for ballistic electron beams as well as for strongly dispersed ones and can be also used as electron beam collimators due to the focusing effect of the pseudomagnetic field. We show additionally that the current flow can be estimated by semiclassical trajectories which represent a computationally efficient tool for predicting the functionality of the devices.

Figures

Figure 1: A graphene membrane deposited on an insulating substrate with a circular cavity forming a nanodrum. Current is injected and detected at the edges of the system.



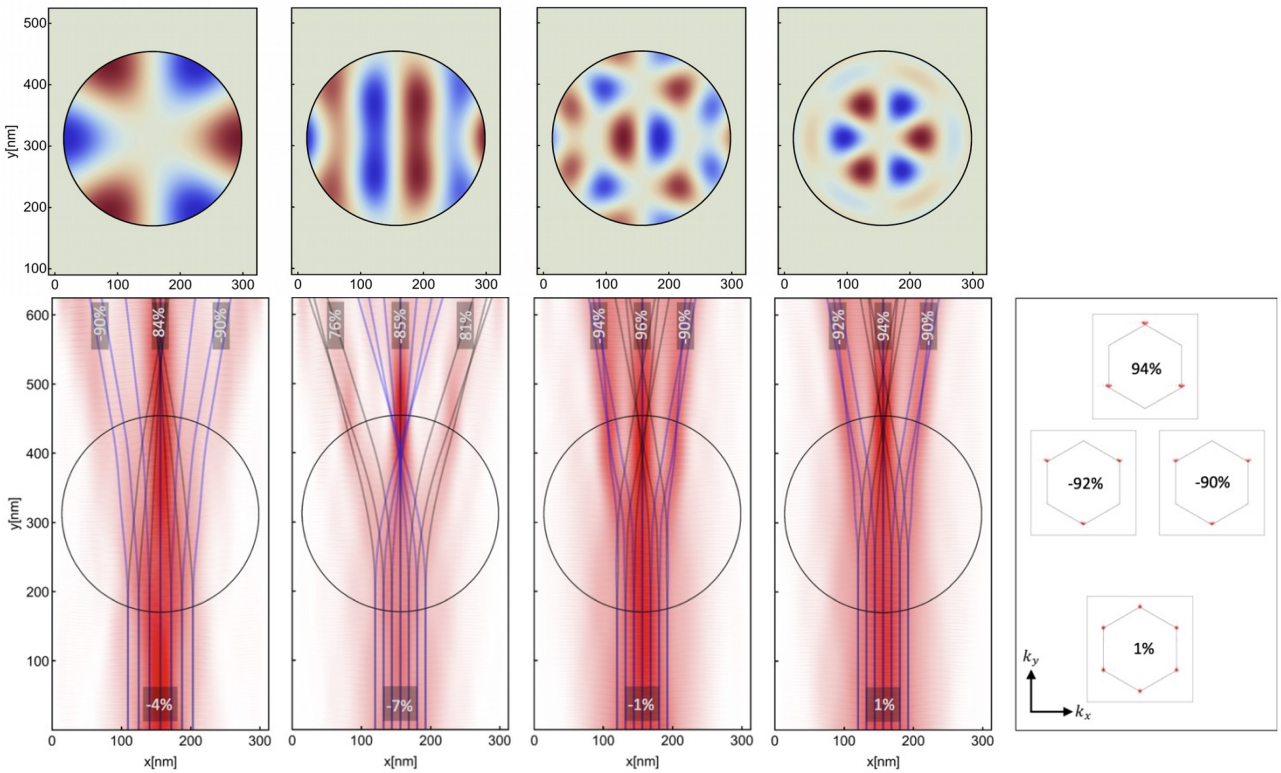


Figure 2: Nanodrum modes with pseudomagnetic field generated by the strain (top). Current flow split into three beams due to the pseudomagnetic field (bottom). Black and blue solid lines are semi-classical trajectories. The valley polarisations are measured in the Fourier space (right).

References

[1] W. Ortiz, N. Szpak, T. Stegmann: Graphene nanodrums as valleytronic devices, arXiv:2202:01739

Revealing the topological phase diagram of $ZrTe_5$ using the complex strain fields of microbubbles

Zoltán Tajkov[1]
Dániel Nagy[2], Konrád Kandrai[1], Oroszlány László[2,3], János Koltai[4], Péter Süle[1], Zsolt E. Horváth[1], Péter Vancsó[1], Levente Tapasztó[1], and Péter Nemes-Incze[1]
[1]Centre for Energy Research, Institute of Technical Physics and Materials Science, 1121 Budapest, Hungary
[2]Department of Physics of Complex Systems, ELTE Eötvös Loránd University, 1117 Budapest, Hungary
[3]Budapest University of Technology and Economics, 1111 Budapest, Hungary
[4]ELTE Eötvös Loránd University, Department of Biological Physics, 1117 Budapest, Hungary
tajkov.zoltan@ek-cer.hu

Abstract
Topological materials host robust properties, unaffected by microscopic perturbations, owing to the global geometric properties of the bulk electron system. Materials in which the topological invariant can be changed by easily tuning external parameters are especially sought after. Zirconium pentatelluride ($ZrTe_5$) is one of a few experimentally available materials that reside close to the boundary of a topological phase transition, allowing the switching of its invariant by mechanical strain. We unambiguously identified a topological insulator - metal transition as a function of strain, by a combination of *ab initio* calculations and direct measurements of the local charge density. Our model quantitatively describes the response to complex strain patterns found in bubbles of few layer $ZrTe_5$ without fitting parameters, reproducing the direction dependent closing of the band gap observed using scanning tunnelling microscopy. We calculated the topological phase diagram of $ZrTe_5$ and identify the phase at equilibrium, enabling the design of device architectures which exploit the unique topological switching behaviour.

Figures

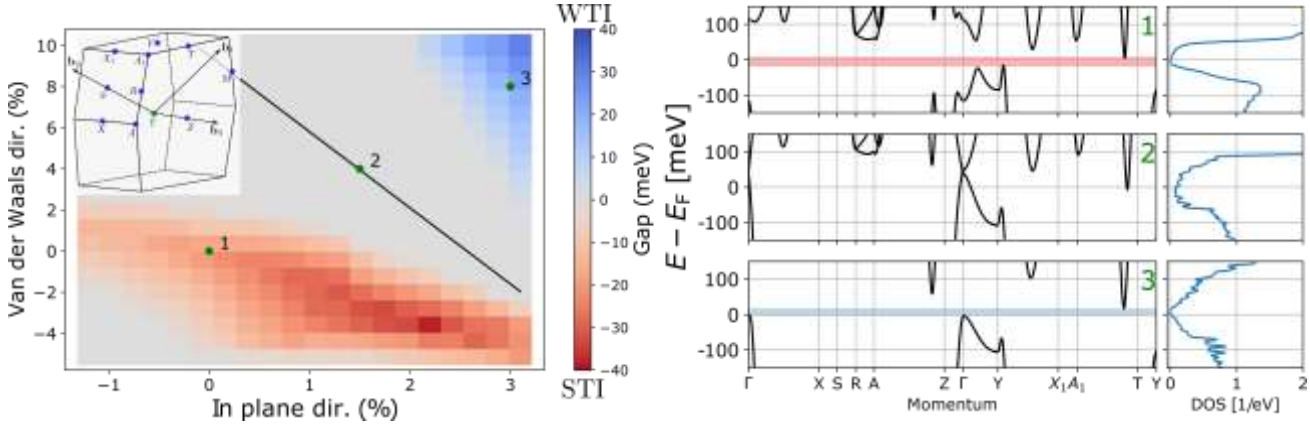


Figure 1: Left: The phase diagram of the electronic structure of the crystal under mechanical strain. At every point the size of the gap was calculated (SIESTA) and a sign has been assigned to it according to the topological flavour of the gap. The negative gap corresponds to the strong topological insulating phase, while the positive gap to the weak topological phase. The green dots assigned with a number denote the corresponding band structure on the right panel. The inset shows the corresponding Brillouin zone indicating the high symmetry points. Right: The calculated band structure along the path of the high symmetry points. The opaque band shows the size of the gap and colour indicates the topological favour.

Tuning the Topological Band Gap of Bismuthene with Silicon-based Substrates

Nils Wittemeier[1]
Pablo Ordejón[1] and Zeila Zanolli[2]
[1]*Catalan Institute of Nanoscience and Nanotechnology - ICN2 (CSIC-BIST), 08193 Barcelona, Spain*
[2]*Chemistry Department and, Debye Institute for Nanomaterials Science, Utrecht University, 3508 TA Utrecht, The Netherlands*
nils.wittemeier@icn2.cat

Bismuth plays a crucial role in many compounds with Topological Insulator [1] properties due to its strong intrinsic spin-orbit interaction. Some meta-stable polymorphs of bismuth monolayer (bismuthene) can host topologically nontrivial phases. [2, 3] However, it remains unclear if these polymorphs can become stable through interaction with a substrate, and, in that case, whether their topological properties are preserved, and how to design an optimal substrate to make the topological phase more robust.

To answer these questions, we performed a comprehensive DFT study of the interactions between bismuthene and silicon-based substrates. [4] We demonstrate that bismuthene polymorphs can become stable over silicon carbide (SiC), silicon (Si), silicon dioxide (SiO2) and that the proximity interaction in the heterostructures has a significant effect on the electronic structure of the monolayer, even when bonding is weak. We further show that the van der Waals interactions and the breaking of the sublattice symmetry are the main factors driving changes in the electronic structure. Our work demonstrates that substrate interaction can strengthen the topological properties of bismuthene polymorphs and make them accessible for experimental investigation and technological applications.

References

[1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 4 (2010), 3045
[2] S. Singh *et al.*, J. Phys. Chem. Lett., 23 (2019), 7324-7332
[3] F. Reis *et al.*, Science, 6348 (2017), 287-290
[4] N. Wittemeier, P Ordejón, and Zeila Zanolli, arXiv.org (2022), arXiv:2203.00114

Figures

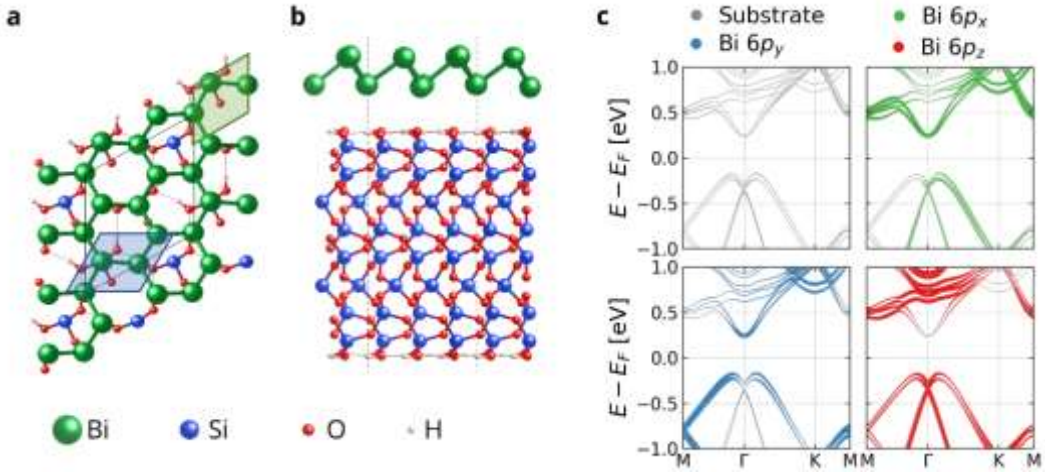


Figure 1: Crystal structure of buckled hexagonal bismuthene on hydroxylated SiO_2 ((a) top and (b) side views) and orbital projected band structure (c). Signature of band inversion is visible in the projection of Bi $6p_y$ orbitals.

Acoustically-induced pseudo-gauge fields and anomalous transport phenomena in graphene

P. Zhao[1]
C. H. Sharma[1], R. Liang[2], L. Mourokh[3], V. M. Kovalev[4, 5], L. Tiemann[1], R. H. Blick[1]
[1]*Center for Hybrid Nanostructures, University of Hamburg, Luruper Chaussee 149, Hamburg 22761, Germany*
[2]*School of Integrated Circuits, Tsinghua University, Beijing 100084, China*
[3]*Department of Physics, Queens College of the City University of New York, Flushing, NY 11367, USA*
[4]*A.V. Rzhanov Institute of Semiconductor Physics, Siberian Branch of Russian Academic of Science, Novosibirsk 630090, Russia*
[5]*Novosibirsk State Technical University, Novosibirsk 630073, Russia*
pzhao@chyn.uni-hamburg.de

Abstract

We will demonstrate that acoustically stimulated carrier transport in graphene at 4 Kelvin signals the presence of artificial gauge fields through the build-up of a transversal voltage at zero magnetic field. We fabricated a gate-tunable graphene Hall bar on a hybrid piezoelectric $LiNbO_3$ on insulator substrate. A nearby interdigitated transducer (IDT) can launch a surface acoustic wave (SAW) that acoustically accelerates the carriers in the graphene layer. The propagating SAW induces an acoustic current whose sign and magnitude reflect the carrier concentration and type reversal at the charge neutrality point. (Fig. 1a). At zero magnetic field, we observe large anomalous acoustically-induced synthetic Hall voltages up to ~200 µV, depending on the carrier type, concentration and the SAW power (Fig. 1b). The synthetic Hall voltage can modulate a conventional Hall voltage arising in a large external magnetic field (Fig. 1c). Our observation is consistent with studies of strain-induced pseudo-gauge fields [1-4]. We developed a model that successfully maps the mechanical deformation within the graphene, precipitated by the SAW in the substrate, to the presence of a gauge field and the observed synthetic Hall voltage [5].

References

[1] N. Levy, et al, Science 329 (2010) 544.
[2] F. Guinea, M. I. Katsnelson and A. K. Geim, *Nat. Phys.* 6 (2010) 30.
[3] S. Z. Zhu, J. A. Stroscio and T. Li, Phys. Rev. Lett. 115 (2015) 245501.
[4] M. Oliva-Leyva and G. G. Naumis, J. Phys.: Condens. Matter 28 (2016) 025301.
[5] P. Zhao *et al.*, https://arxiv.org/abs/2112.11888 [*under consideration*].

Figures

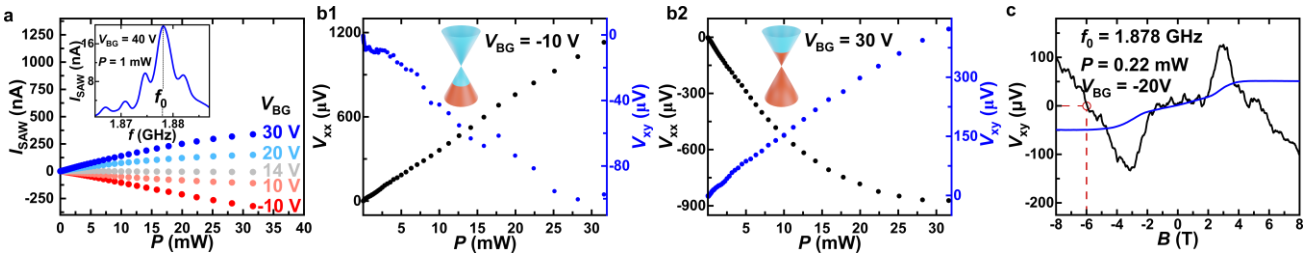


Figure 1: (a) Acoustic current measured at the resonance frequency f_0 of the IDT (inset) for different gate voltages and SAW powers. (b) Exemplary acoustically induced longitudinal and artificial Hall voltages in the hole (b1) and electron (b2) regime. (c) Transversal voltage component under an external magnetic field measured with a regular current superimposed on an acoustic current (black) shows the complete compensation of V_{xy} at finite B. The conventional Hall voltage (blue) [that measured separately] is shown for comparison.

Particle-hole symmetry protects spin-valley blockade in graphene quantum dots

Luca Banszerus[1,2] ,Samuel Möller[1,2], Eike Icking[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Fabian Hassler[5], Christian Volk[1,2], Christoph Stampfer[1,2]

1JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany, EU
2Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich,~Germany,EU
3Research Center for Functional Materials,
National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
4International Center for Materials Nanoarchitectonics,
National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
5JARA-Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany, EU
Luca.banszerus@rwth-aachen.de

Particle-hole symmetry plays an important role for the characterization of topological phases in solid-state systems. Graphene is a textbook example of a gapless particle-hole symmetric system, where topological phases can be understood by studying ways to open a gap by breaking symmetries [1]. An important example is the intrinsic Kane-Mele spin-orbit gap of graphene, which renders graphene a topological insulator in a quantum-spin Hall phase [2]. Here, we show that the Kane-Mele spin-orbit gap leads to a lifting of the spin-valley degeneracy in bilayer graphene quantum dots [3], resulting in Kramer's doublets with different ordering for electron and hole states preserving particle-hole symmetry. We observe the creation of single electron-hole pairs with opposite quantum numbers and use the electron-hole symmetry to achieve a protected spin-valley blockade in electron-hole double quantum dots. The latter will allow spin-to-charge conversion and valley-to-charge conversion, which is essential for the operation of spin and valley qubits

References

[1] F. Haldane, Phys. Rev. Lett. **61**, 2015 (1988)

[2] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95,** 226801 (2005)

[3] L. Banszerus et al., Nat. Commun **12**, 5250 (2021)

Figures

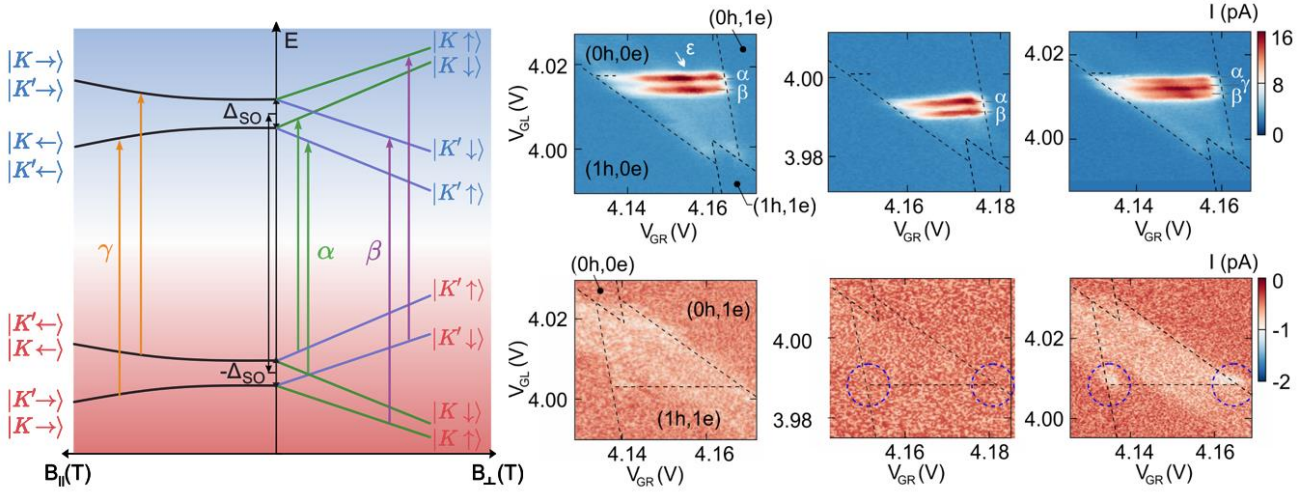


Figure 1: Single particle Pauli-Blockade in an ambipolar electron-hole DQD in bilayer graphene

Coupled Bilayer Graphene Quantum Dots

Angelika Knothe[1]
Vladimir Fal'ko[1,2,3]

1) National Graphene Institute, University of Manchester, Booth Street East, Manchester M13 9PL, United Kingdom
2) *Department of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom*
3) *Henry Royce Institute for Advanced Materials, University of Manchester, Booth Street East, Manchester, M13 9PL, United Kingdom*

Angelika.Knothe@gmail.com

Bilayer graphene quantum dots are promising for spin and valley qubits [1,2,3]. A functional quantum information architecture requires scalable multi-qubit systems. We theoretically study electrostatically confined double-dots and few-dot arrays in bilayer graphene. We quantify the inter-dot couplings for different dot parameters such as the field-induced gap, the confinement shape, and the inter-dot distance. This dependence on external parameters allows tuning the dot arrays into different regimes for which we study the extended Hubbard Hamiltonians and identify the spin and valley level structure. Our results will help to advance the use of bilayer graphene quantum dots for quantum technologies.

References

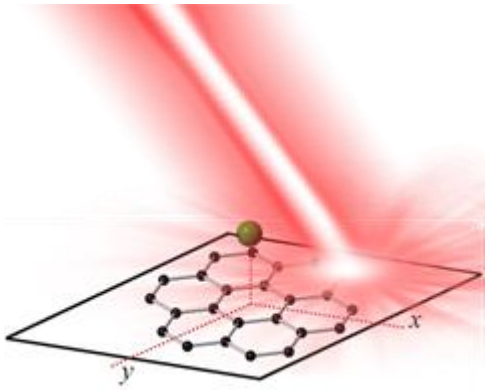
1. A. Knothe, L. I. Glazman, V. Fal'ko, arXiv:2104.03399
2. S. Möller, L. Banszerus, A. Knothe, C. Steiner, E. Icking, S. Trellenkamp, F. Lentz, K. Watanabe, T. Taniguchi, L. Glazman, V. Fal'ko, C. Volk, C. Stampfer, Phys. Rev. Lett. 127, 256802 (2021)
3. A. Knothe, V. Fal'ko, Phys. Rev. B 101, 235423 (2020)

Interaction of a graphene nanoflake with an adatom under optical illumination

Marta Pelc[1]
M. Kosik[1], M. Müller[2], G. Bryant[3], A. Ayuela[4], C. Rockstuhl[2,5], K. Słowik[1]
[1] *Institute of Physics, Faculty of Physics Astronomy and Informatics, Nicolaus Copernicus University, Torun, Poland*
2 Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
3 Joint Quantum Institute, University of Maryland and National Institute of Standards and Technology, College Park and Nanoscale Device Characterization Division, National Institute of Standards and Technology, Gaithersburg, Maryland, USA
4 Donostia International Physics Center (DIPC) and Centro de Física de Materiales, CFM-MPC CSIC-UPV/EHU, San Sebastián / Donostia, Spain
5 Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
mpelc@umk.pl

Graphene nanoantennas sustain strong electro-magnetic field localization upon resonant illumination. To exploit the local field enhancement, quantum emitters such as atoms or molecules should be positioned close to the flake, where electron tunneling may influence the optical response of the system. In our work, we develop an analytical framework and numerical tools to account for dynamics and optical properties of hybrid systems made of graphene nanoflakes coupled to adatoms in the presence of an external electromagnetic field.
We use this framework to investigate the optical phenomena, including plasmons and spontaneous emission of an atom in proximity to graphene antennas. We focus the analysis on the interplay of two distinct physical mechanisms that may influence the optical response, namely the optical coupling between the atom and the antenna and electron tunneling between them. We distinguish different regimes in adatom – flake distances where these effects determine optical properties. While optical coupling dominates at larger distances, the tunneling may be significant at distances of the order of a nanometer leading to hybridization of the antenna and adatom orbitals. In consequence, transition energies and transition dipole moment elements of the coupled system are modified. These quantities determine the spontaneous emission rate. As a result, we find that the spontaneous emission, optically enhanced at moderate atom-antenna distances, can be modified and quenched at short distances.

Figures



Coherent Oscillations in a Bilayer Graphene Charge Qubit

Aaron Johannes Schäpers[1]
Katrin Hecker[1,2], Luca Banszerus[1,2], Anton Peters[1], Samuel Möller[1,2], Eike Icking[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Christian Volk[1,2] and Christoph Stampfer[1,2]

[1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany, EU
[2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany, EU
[3]Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
[4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

aaron.schaepers@rwth-aachen.de

Semiconductor quantum dots (QDs) serve as hosts for charge and spin qubits. Charge qubits are a straight-forward realization of qubits in double quantum dots (DQDs), where quantum information is encoded in the position of an excess electron within the DQD [1]. Bilayer graphene (BLG) has proven particularly suitable for realizing highly tunable QDs [2], and its potential to host qubits is currently explored. However, no coherent manipulation of charge or spin states in BLG has been reported so far. We demonstrate coherent oscillations of a charge qubit in a BLG DQD. We operate the device in the few-electron regime and tune the interdot tunnel coupling to the low GHz regime, which we verify by photon-assisted tunnelling spectroscopy. The charge qubit is controlled by square voltage pulses that allow to non-adiabatically transfer the system from the initialization regime of high detuning to the vicinity of zero detuning, where we observe free charge oscillations. The oscillation frequency shows a strong dependency on the detuning. From the damping of the charge oscillations, we determine the decoherence time T^*_2 which exceeds 200 ps.

References

[1] K. D. Petersson, J. R. Petta, H. Lu, and A. C. Gossard, Phys. Rev. Lett. 105, 246804 (2010)
[2] L. Banszerus, B. Frohn, A. Epping, D. Neumaier, K. Watanabe, T. Taniguchi, and C. Stampfer, Nano Lett. 18, 4785 (2018)

Figures

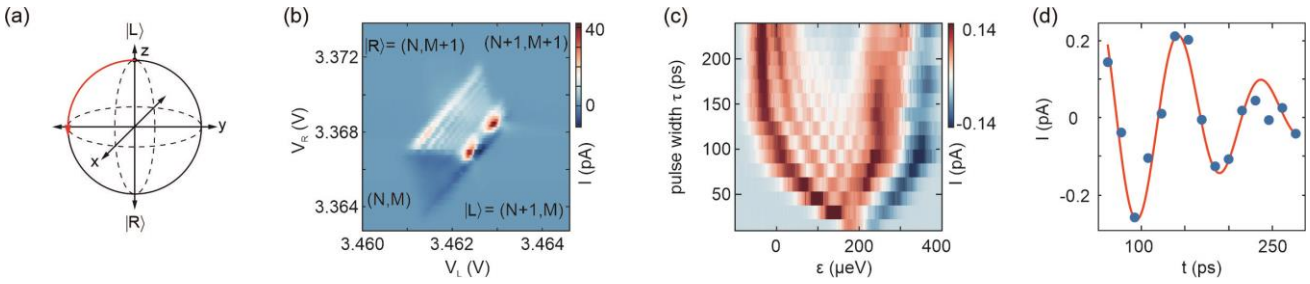


Figure 1: (a) Bloch sphere representation of charge oscillations. (b) Charge stability diagram in the presence of a square voltage pulse, showing multiple features of charge oscillations. (c) Charge oscillations in the time domain as function of detuning. (d) Line cut along the time axis in (c). The red line is a fit to the data.

Entanglement-based order parameter for Kondo phase transitions in graphene quantum dots

Lidia Stocker[1]
Oded Zilberberg[2]
[1]*Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland*
[2]*Department of Physics, University of Konstanz, D-78457 Konstanz, Germany*
stockerl@ethz.ch

Quantum dots in bilayer graphene (see Fig.1) have showcased experimental signatures of a SU(4) Kondo breaking and spin-1 underscreened Kondo singlet formation [1]. To characterise strongly-correlated many-body effects in graphene quantum dots, we apply a recently proposed entanglement witness for quantum impurity systems: the purity of the impurity [2]. With our novel method, we identify phase transitions where Kondo effects compete with dot valley-valley and spin-spin singlets (see Fig.2). Our results demonstrate how entanglement-based order parameters capture short- and long-ranged correlations. Thus, we advance a promising experimental prospect; the measurement of these entanglement-based observables in graphene quantum dots and other mesoscopic systems.

References

[1] A. Kurzmann et al., Nat. Commun. 12, 6004 (2021).
[2] L. Stocker et al., arXiv:2201.07461 (2022).

Figures

Figure 1: Left: Scanning electron micrograph of the experimental device from [1]. Right: The effective Hamiltonian of the graphene dot system [1] couples the closed quantum dot (QD) Hamiltonian (yellow) to two infinite leads (grey).

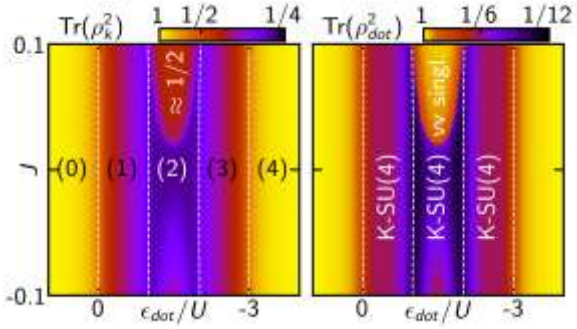


Figure 2: Characterisation of the strongly-correlated effects establishing in a graphene dot system. We show the purity of a single dot valley (left) and the whole quantum dot (right) as a function of the dot on-site energy ϵ_{dot} and the valley-valley magnetic interaction J, where U is the intra-dot Coulomb repulsion energy. Dashed lines separate the different Fock blocks of the closed system. The indicated value is the dot occupation (n_{dot}). The purity of a system with density matrix ρ is given by $\mathrm{Tr}(\rho^2)$. For an isolated system, the purity is 1, for a subsystem-environment singlet is 1/2, and for an impurity-environment Kondo SU(4) it is 1/6 for n_{dot}=2 and ¼ for n_{dot} =1,3.

Van-der-Waals nano-photonics

Panaiot G. Zotev[a*], Yue Wang[b], Luca Sortino[c], Toby Severs Millard[a], Nic Mullin[a], Donato Conteduca[b], Mostafa Shagar[a], Armando Genco[a], Jamie Hobbs[a], Thomas F. Krauss[b], A.I. Tartakovskii[a**]

[a]*Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK*
[b]*Department of Physics, University of York, York, YO10 5DD, UK*
[c]*Nanoinstitute Munich, Faculty of Physics, Ludwig-Maximilians-Universität, München, 80539, Munich, Germany*
[*]p.zotev@sheffield.ac.uk [**]a.tartakovskii@sheffield.ac.uk

Van-der-Waals materials have been the focus of many research efforts since the discovery of graphene [1]. Works based on the metallic properties of single layers of graphite, and further discoveries of the semiconducting properties of monolayer transition metal dichalcogenides (TMDs) [2] have bolstered the importance of materials which consist of covalently bonded layers stacked into bulk crystals due to van-der-Waals interactions. In the past, the use of these layered materials in nano-photonics has only proceeded as far as integration of few-layers with nano-photonic structures fabricated from other more traditional materials such as silicon [3] or gallium phosphide [4]. More recent works have involved the etching of nano-photonic architectures directly into layered materials such as hBN [5] and TMDs [6]. These are promising for the fabrication of such structures due to large refractive indices [6], low absorption within a large portion of the visible spectrum and the advantages which result from their van-der-Waals attractive nature to a wide variety of substrates. In our work, we utilize well established techniques to fabricate nano-photonic resonators with a range of geometries (see Fig. 1(a)) from a diverse set of van-der-Waals materials which exhibit Mie resonances as shown in Figs. 1(b)-(e). Signatures of strong coupling between excitonic features of TMDs and anapole modes were also observed as most clearly seen in Figs. 1(c)-(e). We demonstrate Purcell enhancement of emission from a TMD monolayer due to a nano-resonator mode induced in another material of the same family. Our subsequent observation of the formation of bright single photon emitters in a WSe_2 monolayer transferred onto WS_2 nano-antennas may lead to Purcell enhancement of quantum emission in a structure fabricated entirely of layered materials. Due to the weak van-der-Waals interaction with the SiO_2 substrate, we were able to employ an atomic force microscopy (AFM) cantilever in the repositioning of double-pillar (dimer) nano-antennas to achieve ultra-small gaps ($\approx$ 10 nm, shown in the left inset of Fig. 1(f)). This may enable applications such as stable, low-power optical trapping of quantum emitters with Purcell enhancement factors above 150 as shown by the simulations in Fig. 1(f).

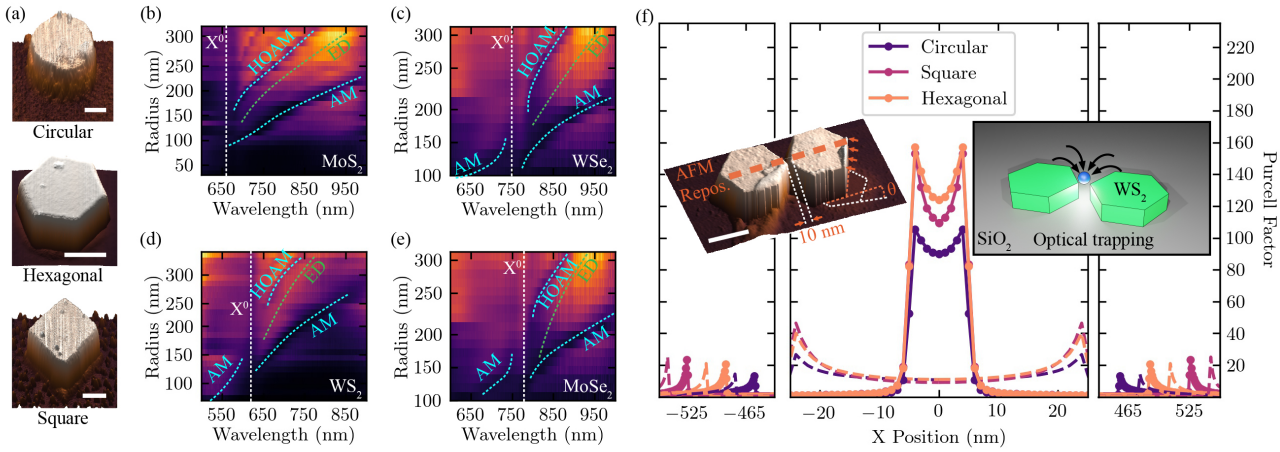


Figure 1: **Van-der-Waals nano-antenna experiments and simulations.** **(a)** AFM of fabricated geometries of layered material nano-antennas. **(b)-(e)** Dark field spectra of fabricated nano-antennas in different TMD materials exhibiting an electric dipole (ED) resonance, anapole (AM) and higher order anapole (HOAM) modes which anti-cross with the neutral exciton resonance (X^0). **(f)** Purcell enhancement of emission for an AFM repositioned 10 nm dimer gap (solid lines) and an as fabricated 50 nm dimer gap (dashed lines) at positions shown by the thick dashed line in the left inset. Left inset: AFM repositioning method to achieve a 10 nm dimer gap. Right inset: Schematic of optical trapping simulation of single photon emitters. Scale bars = 200 nm.

References

[1] Novoselov, K. et al. *Science*, 306(2004), 666-669.

[2] Mak, K. et al. *Physical Review Letters*, 105(2010), 136805.

[3] Li, Y. et al. *Nature Nanotechnology*, 12(2017), 987-992.

[4] Sortino, L. et al. *Nature Communications*, 10(2019), 5119.

[5] Fröch, J. et al. *Advanced Optical Materials*, 7(2019), 1801344.

[6] Verre, R. et al. *Nature Nanotechnology*, 14(2019), 679-683.

High-grip and hard-wearing graphene-polyurethane coatings

Monica Alberto
Maria Iliut, Mohan Pitchan, Aravind Vijayaraghavan
University of Manchester, Oxford Road, Manchester, UK
monica.alberto@postgrad.manchester.ac.uk

Liquid polyurethane (PU) resins are used to form anti-slip surface coatings. In this work, we reinforce PU resin films with few-layer graphene (FLG) nanoparticles incorporated by high-shear mixing. This process gives excellent dispersion as evidenced by optical tomography. The FLG does not appreciably change the tensile strength or Shore hardness of the PU, but we report modest increase of 10% in tear strength and Young's modulus, accompanied by a similar decrease in elongation to failure. However, significant improvement of over 100% is observed in the abrasion resistance. At the same time, we report a 25% increase in the coefficient of static friction and 200% increase in the coefficient of dynamic friction. These results, taken together, suggests that graphene can significantly improve the grip and durability of PU anti-slip coatings, without significantly affecting the other mechanical properties of the coating.

References

[1] Alberto, M.; et al. High-grip and hard-wearing graphene reinforced polyurethane coatings. Composites Part B: Engineering, 2021, 213, 108727

Figures

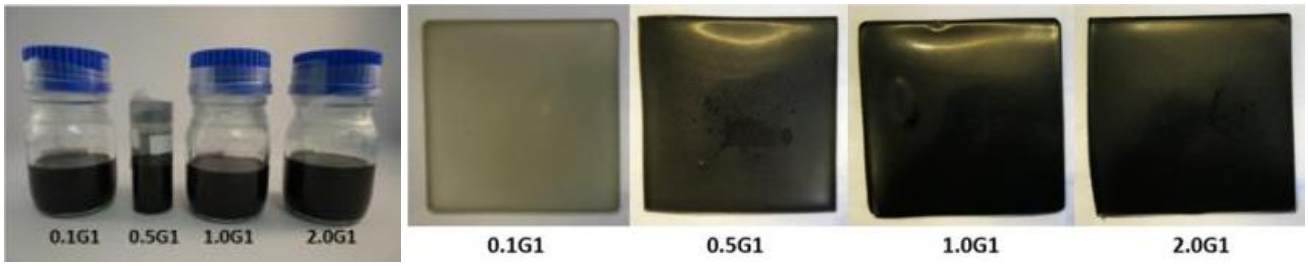


Figure 1: Optical images of graphene-PU composite resins and casted films with different loadings.

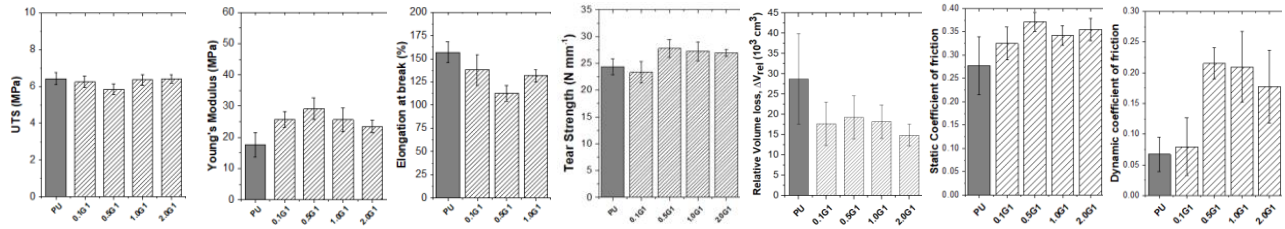


Figure 2: Mechanical property changes in PU resin films upon graphene addition – Ultimate tensile strength, Young's modulus, Ultimate elongation, Tear strength, Abrasion resistance, Coefficient of static friction and Coefficient of dynamic friction.

Conformation Effects and Charge Transfer Excitons in Organic-TMD Heterostructures

Cian Bartlam[1]
Nihit Saigal[2], Stefan Heiserer[1], Hendrik Lambers[2], Ursula Wurstbauer[2], Georg Düsberg[1]
[1]*Institut für Physik, Universität der Bundeswehr München, Germany.*
[2]*Physikalisches Institut, WWU Münster, Germany.*
cian.bartlam@unibw.de

Band alignment in transition metal dichalcogenide (TMD) heterostructures can give rise to a range of newly accessible excitonic states with large binding energies and lifetimes.[1] An alternative route to crystallographic stacking of individual TMD layers is the self-assembly of semiconductor molecules onto a TMD surface. Here the alignment between the band structure of the TMD and organic molecular orbitals can enable spatial separation of charge carriers between the two systems, leading to either free carrier generation or bound excitonic states. We describe the presence of interlayer charge transfer excitons between perylene derivatives (PBI) and bilayer MoS_2, constructed through liquid deposition of the organic molecule.[2] We observe and characterise variations in self-assembly on the MoS_2 surface that give rise to changes in the interfacial charge transfer and the density of interlayer excitons within different regions of the heterostructure. By further investigating the excitation intensity dependence of the intra and interlayer excitons, we find limits to charge transfer rates under poor molecular alignment, which has implications for the application of these materials in optoelectronic devices and sensors.

References

[1] Jiang *et al.*, Light: Science & Applications, 10 (2021) 72.
[2] Bartlam *et al.*, in preparation.

Figures

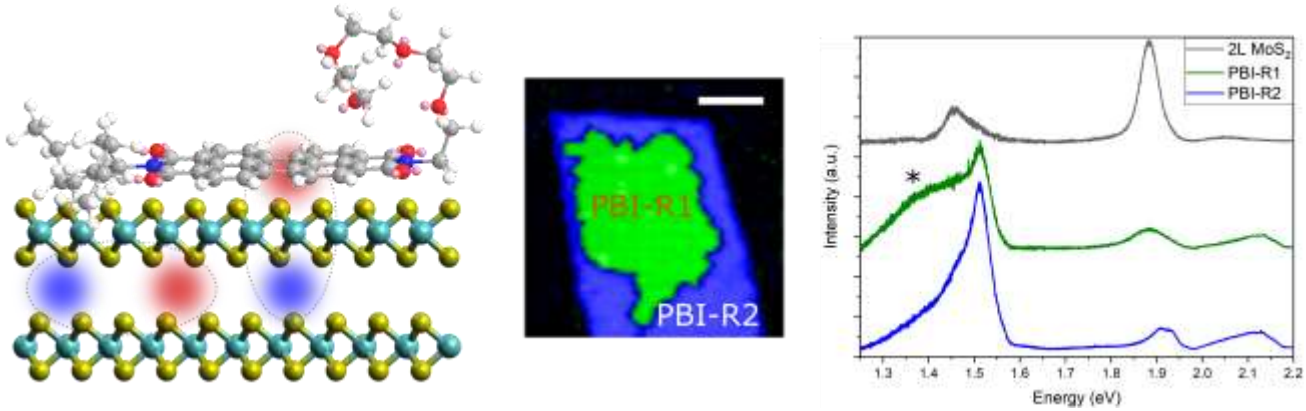


Figure 1: Left – schematic illustrating the presence of both interlayer and intralayer excitons in organic-TMD heterostructures. Centre – Raman map highlighting variations in the crystallographic alignment of the organic PBI molecule on a MoS_2 surface (5 µm scale). Right – Low temperature photoluminescence spectra highlighting the spectral variations between the two regions and an unfunctionalised bilayer (* denotes the energy of the interlayer exciton).

Patterned growth of transition metal dichalcogenides monolayers for electronic and optoelectronic device applications

Antony George[1], Ziyang Gan[1], Emad Najafidehaghani[1], Seung Heon Han[1], Sai Shradha[2], Fatemeh Abtahi[2], Christof Neumann[1], Julian Picker[1], Tobias Vogl[2], Uwe Hübner[3], Falk Eilenberger[2] and Andrey Turchanin[1] [1]*Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany,* [2]*Institute of Applied Physics, Friedrich Schiller University Jena, Albert-Einstein-Str 15, 07745 Jena, Germany,* [3] *Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745 Jena, Germany*
antony.george@uni-jena.de

Abstract

We present a simple, large area and cost effective soft lithographic method for the patterned growth of high-quality two-dimensional transition metal dichalcogenides (TMDs). Initially, a liquid precursor (Na_2MoO_4 in aqueous solution) is patterned on the growth substrate using micro-molding in capillaries (MIMIC) technique. Subsequently, a chemical vapor deposition (CVD) step is employed to convert the precursor patterns to monolayer, few layers, or bulk TMDs, depending on the precursor concentration. The grown patterns were characterized using optical microscopy, atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, scanning electron microscopy, and photoluminescence spectroscopy to reveal their morphological, chemical, and optical characteristics. Additionally, we have realized electronic and optoelectronic devices using the patterned TMDs and tested their applicability in field effect transistors (FETs) and photodetectors. The photodetectors made of MoS_2 line patterns shows a very high responsivity of 7674 A/W and external quantum efficiency of 1.49×10^6%. Furthermore, the multiple grain boundaries present in patterned TMDs enabled the fabrication of memtransistor devices. The patterning technique presented here may be applied to many other TMDs and related heterostructures, potentially advancing the fabrication of TMDs based device arrays.

References

[1] Ziyang Gan, Emad Najafidehaghani, Seung Heon Han, Sai Shradha, Fatemeh Abtahi, Christof Neumann, Julian Picker, Tobias Vogl, Uwe Hübner, Falk Eilenberger, Antony George and Andrey Turchanin, Submitted (2022)

Figure

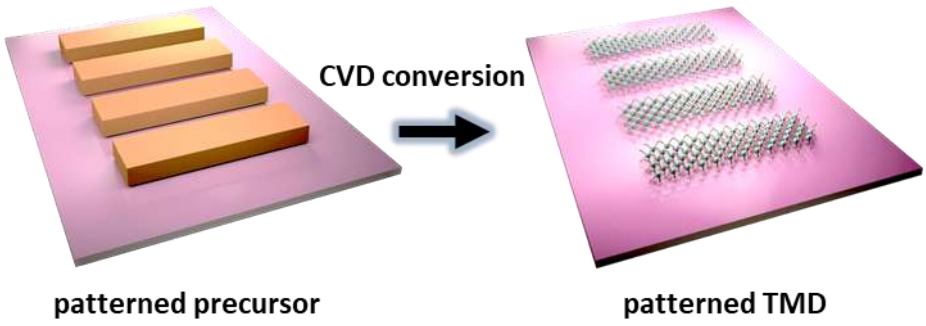


Figure 1: Schematic representation of the patterning process for transition metal dichalcogenides (TMDs)

Visible-Light Assisted Covalent Surface Functionalization of graphene based materials with Arylazo sulfones

Alessandro Kovtun
Lorenzo Lombardi, Sebastiano Mantovani, Giulio Bertuzzi, Laura Favaretto, Cristian Bettini, Vincenzo Palermo, Manuela Melucci, and Marco Bandini
*Istituto per la Sintesi Organica e la Fotoreattività ISOF CNR, Via Gobetti 101, Bologna, Italy*alessandro.kovtun@isof.cnr.it

We present an unprecedented environmentally benign methodology for the covalent functionalization [1] (arylation) of different sp^2 carbon-based materials with arylazo sulfones: from Graphene Oxide, to reduced Graphene Oxide (rGO), considering also the highly oriented pyrolytic graphite (HOPG) as ideal 100% sp^2 substrate. A variety of tagged aryl units were conveniently accommodated at the rGO surface via visible-light irradiation of suspensions of carbon nanostructured materials in aqueous media. Mild reaction conditions, absence of photosensitizers, functional group tolerance and high atomic fractions (XPS analysis) represent some of the salient features characterizing the present methodology. The late stage-functionalization of the modified rGO and a mechanistic proposal based on both experimental as well as spectroscopic analyses completed the study, control experiments for the mechanistic elucidation as Raman analysis on HOPG was successfully achieved [2]. The quantitative analytical determination of the tagged aryl units via XPS, represent a unique combination of factors electing the present methodology as a valuable synthetic alternative to the known protocols [3,4] for the covalent modification of reduced graphene oxide surface.

Graphene Flagship Core 3, grant N° 881603, PRIN-2017 project 2017W8KNZW.

References

[1] C. Sauer, Y. Liu, A. De Nisi, S. Protti, M. Fagnogni, M. Bandini, ChemCatChem 2017, 9, 4456-4459
[2] Lombardi L., Kovtun A., Mantovani S., Bertuzzi G., Favaretto L., Bettini C., Palermo V., Melucci M., Bandini M. *Chemistry—A European Journal*, accepted manuscript
[3] Sinitskii, A.; Dimiev, A.; Corley, D. A.; Fursina, A. A.; Kosynkin, D. V.; Tour, J. M. ACS Nano 2010, 4, 1949
[4] Greenwood, J.; Phan, T. H.; Fujita, Y.; Li, Z.; Ivasenko, O.; Vanderlinden, W.; Van Group, H.; Frederickx, W.; Lu, G.; Tahara, K.; Tobe, Y.; Uji-I, H.; Mertens, S. F. L.; De Feyter, S., ACS Nano 2015, 9, 5520

Figures

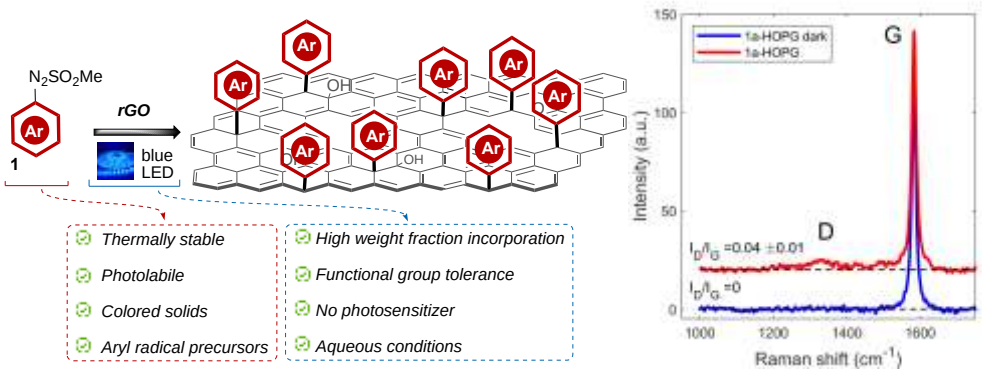


Figure 1: left: schematic representation of the present visible-light assisted covalent arylation of rGO with arylazo sulfones. Right: Raman spectrum of 1a-HOPG dark and 1a-HOPG. Linear background was subtracted, and spectra were shifted for clarity.

Optical and chemical study of two-dimensional lead iodide perovskite stability to ambient conditions

Marie Krecmarova[1],
Andrés F. Gualdrón-Reyes[2,3], Jesús Rodríguez-Romero[2,4], Iván Mora-Seró[2], Maria C. Asensio[5,6], Juan P. Martínez-Pastor[1,6], Juan F. Sánchez-Royo[1,6].
[1]*Instituto de Ciencia de Materiales, Universidad de Valencia (ICMUV), 46071 Valencia, Spain.*
[2]*Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castellón, Spain.*
[3]*Facultad de Ciencias, Instituto de Ciencias Químicas, Isla Teja, Universidad Austral de Chile, 5090000, Valdivia, Chile.*
[4]*Facultad de Química, Universidad Nacional Autónoma de México, Circuito Exterior s/n, C.U., Coyoacán, 04510 Mexico.*
[5]*Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC 28049 Madrid, Spain.*
[6]*MATIN ´ EE: CSIC Associated Unit (ICMM-ICMUV), Universidad de Valencia, Valencia, Spain.*
Marie2.Krecmarova@uv.es

Abstract

Two-dimensional (2D) halide perovskites hold a great promise for electronics and optoelectronics applications due to the structural diversity, high absorption and photoluminescence, and tunable bandgap. Especially, they are one of the most promising studied material for photovoltaics. However critical issue is their low stability to the ambient environment conditions. In this work, we have investigated their degradation processes upon external factors such as oxygen, humidity, light, heat and photo-induced degradation. We applied combination of optical (micro-photoluminescence, micro-Raman spectroscopy) and chemical (X-ray photoemission spectroscopy) characterization techniques. We demonstrate that 2D perovskites easy degrade upon heat and laser illumination in atmospheric conditions. Surprisingly, we have found a different aging chemical processes after the crystal exposition to long periods (up to 1 year) in atmospheric conditions with and without presence of external light (see Figure 1). Crystals exposed to light aged into morphology with penetrated micro-holes and their photoluminescence is degraded. On the other hand, crystals exposed to dark show wire-like morphology maintaining photoluminescence. The degradation processes finally results in removal of organic part from the crystal and formation of lead and iodine vacancies, which are probably related to side non-radiative recombination mechanisms responsible for the photoluminescence degradation. These vacancies are associated with the crystal decomposition into PbI_2, metallic Pb, and Pb oxides. Presented work is beneficial for development of long-term stable perovskite devices with an enhanced optical performance.

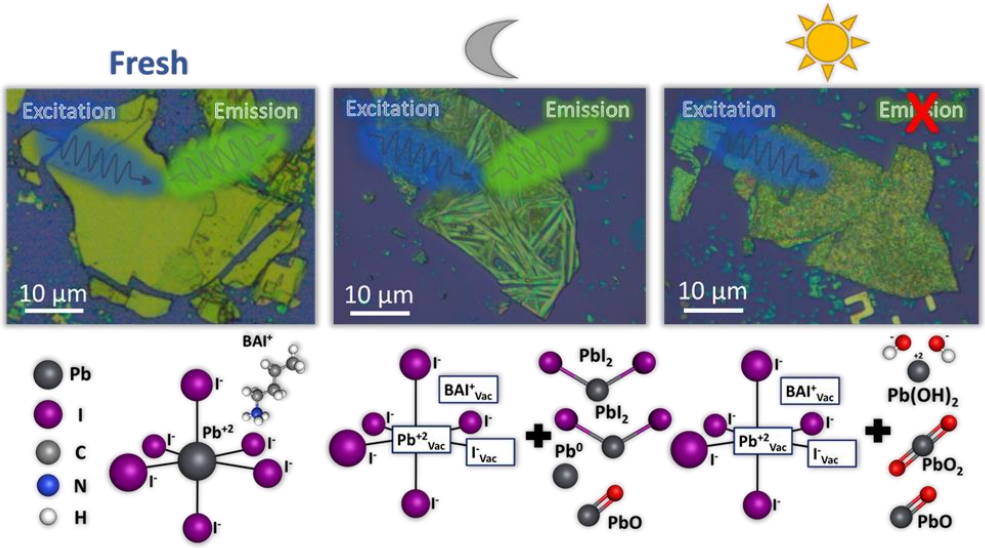


Figure 1: Degradation processes in 2D perovskites.

Electrical properties of large single-crystal tungsten disulfide grown by liquid precursor chemical vapor deposition

Leonardo Martini[1]
Niccolò Martinolli[3], Paolo Paletti[1,2], Domenica Convertino[1,2], Giorgio Orlandini[4], Hasret Agircam[1,5], Simona Pace[1,2], Stiven Forti[1], Vaidas Miseikis[1,2], Camilla Coletti[1,2]

1. *Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, 56127, Pisa, Italy*
2. *Graphene Labs, Istituto italiano di tecnologia, Via Morego 30, I-16163 Genova, Italy*
3. *Department of Civil and Industrial Engineering, University of Pisa, Largo Lazzarino 1, Pisa, 56122, Italy*
4. *Department of Condensed Matter Physics, University of Pisa, Largo Bruno Pontecorvo 3, 56127 Pisa, Italy*
5. *Department of Metallurgical & Materials Engineering Istanbul Technical University, 34469 Maslak, Istanbul, Turkey*

leonardo.martini@iit.it

The research in two-dimensional (2D) materials has attracted great interest in recent years, for electronic, spintronic and optoelectronics applications. One class of 2D materials of particular interest are transition metal dichalcogenides (TMDs), where one layer of transition metal atoms is packed between two layers of dichalcogenide atoms[1]. One of the most interesting properties of this class of material is the presence of a bandgap, which changes from indirect to direct when the thickness goes from bulk to monolayer[2].
One of the most promising TMDs is tungsten disulfide(WS_2)[3], due to the presence of a direct bandgap in the visible range (around 2 eV) that makes it suitable for electronics and optoelectronics applications. Hence, controlling the growth process in order to obtain highly crystalline WS_2 with appreciable electronic and optical properties is of primary importance.
Here we report on the growth, through liquid-phase chemical vapor deposition (LiP-CVD)[4], of monolayer single-crystal WS_2 on Silicon dioxide, with lateral size up to hundreds of micrometers.
The quality of the grown material is assessed through atomic force microscopy (AFM), Raman and photoluminescence spectroscopy, which confirm the single-crystal and monolayer nature of our samples. The electrical properties of LiP-CVD WS_2 are tested with transport measurements. To this end, Transfer Length Measurement (TLM) devices are defined via electron beam lithography (EBL), thermal metal evaporation and reactive ion etching (RIE). We demonstrate field-effect mobilities above 15 cm^2/Vs and an on/off ratio in the range of 10^6. Moreover, we also test the electrical photo-responsivity of the material, proving a wavelength-dependent photocurrent of hundreds of microampere and a photoresponsivity as high as 10 A/W.

Acknowledgment

This work has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement 881603.

References

[1] R. G. Dickinson and L. Pauling, "The crystal structure of molybdenite," *J. Am. Chem. Soc.*, vol. 45, no. 6, pp. 1466–1471, Jun. 1923.
[2] C. Cong, J. Shang, Y. Wang, and T. Yu, "Optical Properties of 2D Semiconductor WS 2," *Adv. Opt. Mater.*, vol. 6, no. 1, p. 1700767, Jan. 2018.
[3] S. Ulstrup *et al.*, "Spin and valley control of free carriers in single-layer WS 2," *RAPID Commun. Phys. Rev. B*, vol. 95, no. R, p. 41405, 2017.
[4] H. Y. Jeong *et al.*, "Heterogeneous Defect Domains in Single-Crystalline Hexagonal

WS2," *Adv. Mater.*, vol. 29, no. 15, Apr. 2017.

Figures

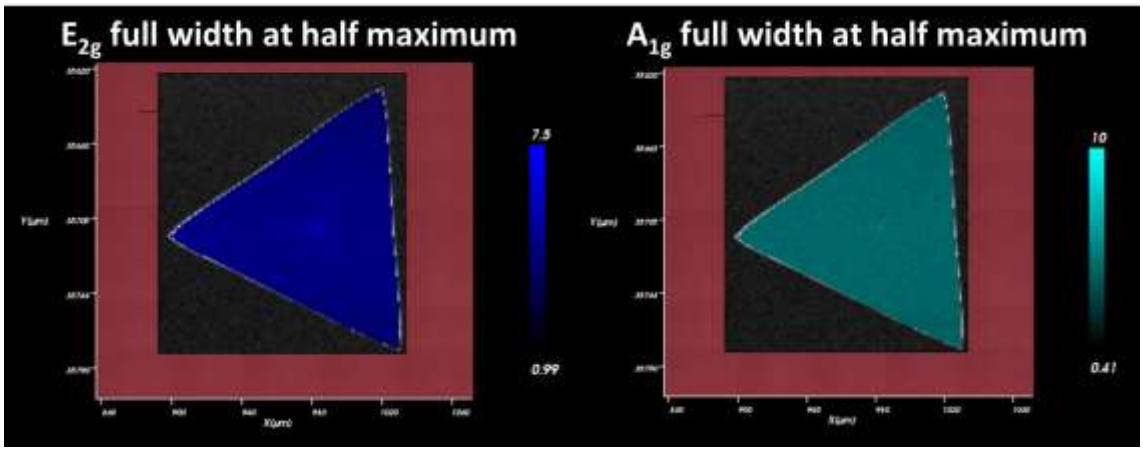


Figure 1: Raman characterization of a LiP-CVD grown WS_2 crystal: On the left, the map of the FWHM(E_{2g}) peak shows homogeneity of the strain on the sample and the high quality of the synthesized material. On the right, the map of the FWHM(A_{1g}) peak demonstrates high level of homogeneity of the sample. Raman characterization has been performed with laser excitation of 473 nm, 1.4 mW of power, the measurements were performed with a 100x (0.89 NA) magnification lens, that produces a spot size of 0,7 μm.

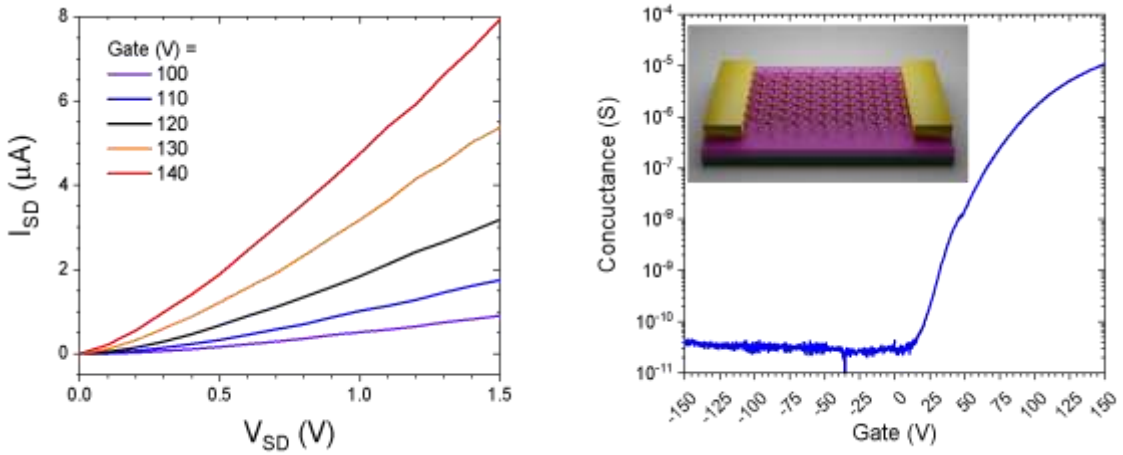


Figure 2: Electrical characterization of the WS_2-based FET device: On the left, the output characteristic of a device demonstrates current in the order of tens of μA; the super-linear onset for applied biases below 0.5 V suggests the presence of a contact-limited transport. On the right, a transfer curve in a semi-log scale, WS_2 FET device show a n-type behavior, with an on/off ratio above 10^5 and onset voltage around 20 V (over 285 nm of SiO_2); we obtained FET mobility of 15 cm^2/Vs.

Hexagonal boron nitride-reinforced polyisobutylene-based anticorrosive coatings

Miguel Angel Molina-Garcia[a]
Sebastiano Bellani[a], Antonio Esau del Rio Castillo[a], Irene Conticello[a], Luca Gabatel[a], Marilena Isabella Zappia[a], Matilde Eredia[a], Beatriz Martin-Garcia[b], Francesco Bonaccorso[a]
[a] BeDimensional S.p.A., Via Lungotorrente Secca 30R, Genova, 16163, Italy
[b] CIC nanoGUNE, Tolosa Hiribidea, 76, Donostia-San Sebastian, 20018, Spain
m.molina@bedimensional.it

The incorporation of inorganic nanofillers into polymeric matrices represents an effective strategy for developing smart coatings for corrosion protection [1,2]. In this work, we investigate the addition of hexagonal boron nitride (*h*-BN) flakes, produced through the wet jet milling method in BeDimensional SpA industrial plant [3,4], as functional anticorrosive filler into polymeric polyisobutylene (PIB) matrix to yield *h*-BN/PIB composites with different *h*-BN contents. Once casted onto structural steel substrates, the anticorrosion properties of the as-produced composites were evaluated in a 3.5 wt.% NaCl aqueous solution, following ASTM standards. The results demonstrate that the *h*-BN/PIB composite with an *h*-BN content of 5 wt.% is the most performant anticorrosive coating, exhibiting a corrosion rate that is two orders of magnitude lower compared to the one of the pristine PIB coating used as reference (7.42 x 10^{-6} mm $year^{-1}$ *versus* 4.47 x 10^{-4} mm $year^{-1}$), see Figure 1. Our composite coating maintained its corrosion protection efficiency over 1000 h of continuous immersion in saline water, resulting in an ideal long-term anticorrosion coating for steel operating in corrosive marine environments. The hydrophobic nature of the *h*-BN flakes, together with the capability of PIB to act as a moisture barrier, are the reasons behind the remarkable anticorrosion performance.

References

[1] G. Cui *et al*, Prog. Org. Coatings. 148 (2020) 105821.
[2] A. Kausar, J. Plast. Film Sheeting. 35 (2019) 181.
[3] A. E. del Rio Castillo *et al*, Mater. Horizons. 5 (2018) 890.
[4] A.E. Del Rio Castillo, A. Ansaldo, V. Pellegrini, F. Bonaccorso, WO 2017/089987 Al, 2019.

Figures

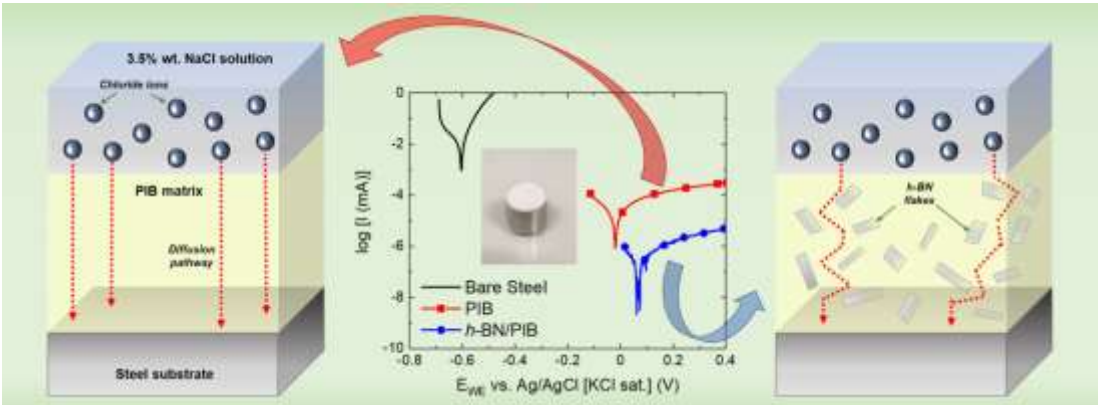


Figure 1: *Anodic polarisation curves (Tafel plots) of pristine PIB- and h-BN/PIB composite-coated structural steel. The Tafel plot measured for uncoated structural steel is also shown for comparison. The figure also shows schematic diagrams of diffusion pathways followed by chloride ions through pristine PIB and h-BN/PIB composite coatings from the NaCl aqueous solution to the surface of the steel substrate.*

"This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement GrapheneCore3 - 881603"

Environmentally friendly graphene-based membranes for water filtration

Siva Sankar Nemala
J. Fernandes[1], M. Barreiros dos Santos[1], B. Espiña[1], A. Tamburrano[2], P. Alpuim[1,3], A. Capasso[1]
[1]*International Iberian Nanotechnology Laboratory, 4715-330, Braga, Portugal*
[2]*Sapienza University of Rome, 00184 Rome, Italy*
[3]*University of Minho, 4710-057 Braga, Portugal*
siva.sankar@inl.int

Antibiotic contaminations present a serious threat to human and animal health security. Antibiotics removal from aqueous environments mostly relies on either adsorption or catalysis oxidation processes, which are rather inefficient[1]. Towards sustainable management of water and sanitation on a global scale, new classes of membrane materials and systems are required. Owing to atomic thickness, large surface area, and mechanical strength, graphene-based materials appear as a suitable choice. So far, graphene oxide membranes were proposed for water purification, efficiently blocking solutes with hydrated radii larger than 4.5 Å. These materials are however not ideal since they tend to swell and weaken when operating in water over a few days[2,3]. Liquid phase exfoliation (LPE) methods allow the large-scale production of atomic thick graphene flakes at low cost[4], but hazardous and toxic solvents (*i.e.*, NMP, DMF, and DMSO) are commonly used, hindering sustainable upscaling. Here we describe the preparation of LPE graphene by high-shear mixing in environmentally friendly, non-toxic solvent Cyrene[5,6]. The graphene dispersions have a 1 mg/mL concentration and high stability (over 9 months). Membranes were fabricated via vacuum-filtration on PVDF supports and tested in terms of mechanical strength, bacterial adhesion, and antibiotics (ampicillin and tetracycline) filtering. The membranes remain structurally stable over 90 days, without any noticeable swelling. When exposed to common bacterial pathogens (*Escherichia coli* and *Enterococcus)* in freshwater, they showed a very scarce level of bacterial adhesion, indicating a promising resistance to biofilm formation. Overall, the membranes showed more than 90% rejection of both antibiotics.

References

[1] X. Wang et.al., Environmental Pollution, 253 (2019) 100.
[2] J.N. Coleman et.al., Science, 331 (2011) 568.
[3] J. Fernandes et.al., Front. Chem., (2022) accepted.
[4] S. Tkachev et.al., Adv. Funct. Mater., 31(2021) 2103287.
[5] R.K. Joshi et.al., Science, 343 (2014) 752.
[6] W. Hirunpinyopas et.al., Carbon, 156 (2020) 119.

Figures

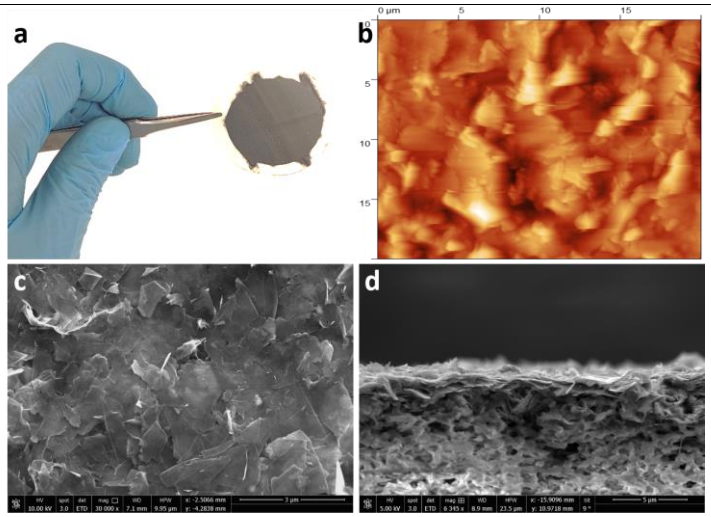


Figure 1: (a) Graphene-based membrane on PVDF. (b) AFM image of the top surface. SEM images of (c) top surface and (c) cross-section of the membrane.

Layer-by-Layer Films of Upconverting Perovskite Nanosheets

Özge Sağlam
Bensu Gunay
Department of Mechanical Engineering, Faculty of Engineering, Izmir University Economics, Sakarya Cad. 156, 35330, Balçova, İzmir, Turkey
ozge.saglam@ieu.edu.tr

Inorganic nanosheets are a class of two-dimensional materials obtained by chemical exfoliation of layered oxides, in which the A sites of the host structure can be modified via the doping of various combinations of the lanthanides [1]. These 2D materials have different optical, chemical, catalytic, and electronic properties according to the crystal structure and composition of the layered material [2]. The oxide nanosheets can also be self-assembled to fabricate multilayer films via bottom-up deposition techniques. Layer-by-layer assembly (LBL) method, which is a sequential adsorption driven technique by electrostatic interactions between oppositely charged oxide nanosheets and polycations, forms the nanofilms in a more cost-effective and easy-to-perform way [3]. In this study, upconverting LBL films were fabricated using Er^{+3}/Tm^{+3}, Yb^{+3}/Tm^{+3} and Er^{+3}/Yb^{+3} co-doped perovskite nanosheets. The single nanosheets in colloidal form with thickness in the range of 2-3 nm were obtained by the chemical exfoliation procedure. The UV-vis absorption spectra of LBL films of the exfoliated nanosheets confirmed that the deposition of upconverting nanosheets via the LBL procedure. The LBL films fabricated after 60 sequences of LBL tecnique using the nanosheets exfoliated from three different layered perovskites co-doped with various lanthanide pairs and concentrations have shown a white emission in the CIE diagram. On the other hand, the log-log dependence of the UC emission intensity of the LBL films fabricated after 30 sequences using the nanosheets derived from the 2.5% Er^{3+} + 5% Yb^{3+} co-doped layered perovskites, the two-photon processes were responsible for green and red UC emission due to the $_4F^{9/2} \rightarrow {}_4I^{15/2}$ and $_2H^{11/2}$, $_4S^{3/2} \rightarrow {}_4I^{15/2}$ transitions, respectively.

References

[1] Sağlam Ö., Optical Materials, 109 (2020) 110294.
[2] Gunay B, Sarıyar E, Unal U, Firtina Karagonlar Z, Sağlam Ö., Colloids and Surfaces A: Physicochemical and Engineering Aspects,612 (2021) 126003.
[3] Sasaki T, Ebina Y, Watanabe M, Decher G., Chemical Communications (2000); 2163–2164.

Figures

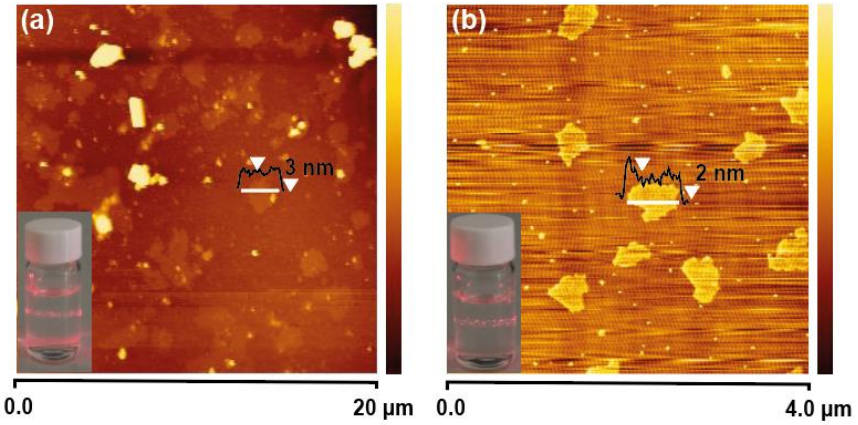


Figure 1 AFM images with height profile of nanosheets delaminated from layered perovskite co-doped with (a) 2.5% Er^{3+} + 5% Yb^{3+} (b) 2.5% Tm^{3+} + 20% Yb^{3+}

Semi-Layered Metal Diborides
Liquid Exfoliation and Processing of Metallic non-Van der Waals Crystals

Kevin Synnatschke
Alina Mueller, Adam Kelly, Claudia Backes, Jonathan Coleman
Trinity College Dublin, School of Physics, College Green, Dublin 2, Ireland
synnatsk@tcd.ie

Owning to their unique material properties, the field of two-dimensional materials is getting ever-growing attention. This can be attributed to their surface chemistry and high surface to volume ratio, as well as arising quantum effects, when going from bulk solid to the monolayer limit.[1,2] While more and more reports on the exfoliation of novel 2D materials with promising properties and interesting transport characteristics have been presented over the past decade, only few examples of metallic or semi-metallic 2D materials have successfully been exfoliated into nanosheets, especially in liquid processable media, offering scalable device fabrication.

In this contribution, a scalable exfoliation method for three different, commercially available, semi-layered metal diborides (CrB_2, MgB_2 and ZrB_2) is presented, using a novel approach of liquid phase exfoliation in inert atmosphere. This allows to fabricate nanosheet dispersions in versatile liquid environments, while established centrifugation-based protocols are used to remove initially oxidised starting material from the nanosheets and for size selection.[3,4]
After successful exfoliation, a modified Langmuir Schaefer deposition technique was used for processing the nanomaterial into tiled thin-film networks, revealing metallic conductivity of the nanosheet network. The deposited nanomaterial is characterised electrically and spectroscopically, and changes of the film characteristics are followed over time to provide insights in the sample degradation after exposure to ambient conditions. At last, oxidation preventive working procedures are presented.

References

[1] Fu, Q., *et al.*, Chem. Soc. Rev., 46 (2017), 1842-1874
[2] Backes, C., *et al.*, Nat Commun, 5 (2014), 4576-4586
[3] Synnatschke, K., *et al.*, Chem Mater, 31 (2019) 9127-9139
[4] Backes, C., *et al.*, ACS Nano, 10 (2016), 1589-1601

Figures

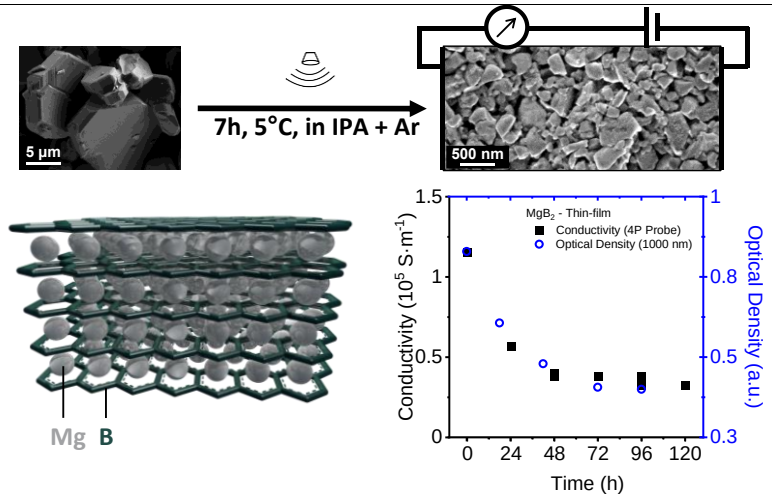


Figure 1: Schematic illustration of the processes addressed within the scope of this report. Liquid phase exfoliation and thin-film preparation from MgB_2 bulk crystallites. Thin films are contacted, and transport characteristics are studied over time.

Phthalocyanine-Based 2D Conjugated Polymers

Mingchao Wang
Renhao Dong, Xinliang Feng
Center for Advancing Electronics Dresden (cfaed) and Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Mommsenstasse 4, 01069 Dresden, Germany.
Mingchao.wang@tu-dresden.de

Two-dimensional conjugated polymers (2D CPs) are emerging as a unique class of 2D polymers with in-plane π-conjugation,[1] which have exhibited unique properties such as intrinsic crystallinity, porosity, conductivity/mobility, tailorable band gaps, etc. and displayed great potential in (opto)electronic and energy devices. However, understanding the intricate interplay between the chemical structure and charge transport remains a challenge.[2] In addition, the lack of rational design on the chemical structure—which effectively tailors the energy levels/gap and electronic structures of the frontier orbitals—hampers the development of highly conductive 2D CPs. Herein, we have rationally designed and synthesized a series of semiconducting phthalocyanine-based 2D CPs with low optical band gaps down to ~1 eV and charge carrier mobilities up to ~50 cm^2/Vs. The combination of Hall effect measurements, Terahertz spectroscopy and calculated electronic band structures provide a rational approach on how to assess structure-/doping-electronic property relationships.[2,3] These works highlight the great potential of high-mobility 2D CPs semiconductors for (opto)electronics.

References

[1] M. Wang, R. Dong, X. Feng, Chem. Soc. Rev., 50 (2021) 2764.
[2] M. Wang, M. Ballabio, M. Wang, H.-H. Lin, B. P. Biswal, X. Han, S. Paasch, E. Brunner, P. Liu, M. Chen, M. Bonn, T. Heine, S. Zhou, E. Canovas, R. Dong, X. Feng, J. Am. Chem. Soc., 141(2019) 16810–16816.
[3] M. Wang, M. Wang, H.-H. Lin, M. Ballabio, H. Zhong, M. Bonn, S. Zhou, T. Heine, E. Cánovas, R. Dong, X. Feng, J. Am. Chem. Soc., 142 (2020), 21622−21627.

Figures

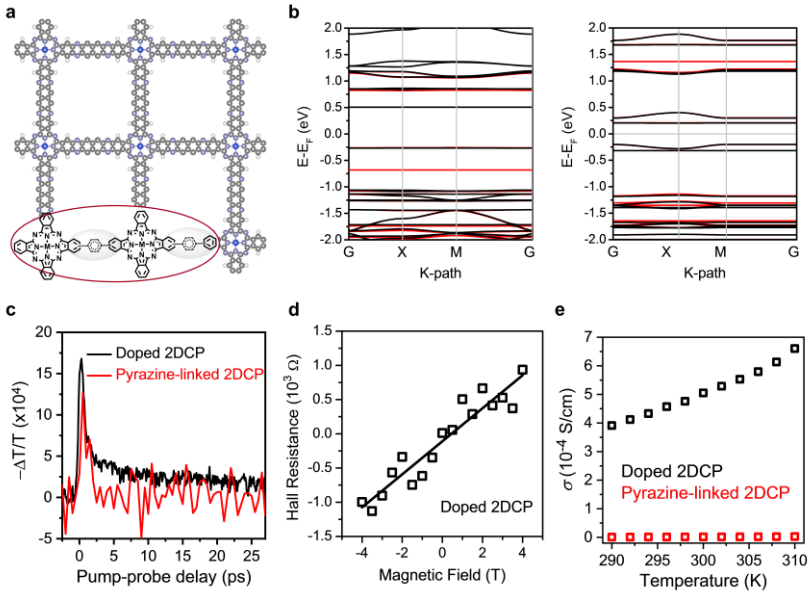


Figure 1: (a) Phthalocyanine-based 2D CPs. (b) Electronic band structures of different 2D CPs. (c–e) Terahertz spectroscopy, Hall effect and variable-temperature conductivity of pristine and doped pyrazine-linked 2D CPs.

2D Indium selenide (InSe)/indium tin oxide (ITO) hybrid films for photoelectrochemical (PEC)-type photodetectors

Marilena Isabella Zappia[1]
Gabriele Bianca,[2,4] Sebastiano Bellani,[1] Michele Ghini,[2,4] Nicola Curreli,[2] Joka Buha,[2] Valerio Galli,[1,4] Mirko Prato,[2] Aljoscha Soll,[86] Zdeněk Sofer,[86] Guglielmo Lanzani,[4,7] Ilka Kriegel[2] and Francesco Bonaccorso[1,2]
[1] 1BeDimensional S.p.A., via Lungotorrente Secca 30R, 16163 Genova, Italy
[2] Istituto Italiano di Tecnologia, via Morego 30, 16163, Genova, Italy
[3] Dipartimento di Chimica e Chimica Industriale, Università degli Studi di Genova, via Dodecaneso 31, 16146 Genoa, Italy.
[4] Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133, Milano, Italy
[6] Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic
[7] Center for Nano Science and Technology @PoliMi, Istituto Italiano di Tecnologia, via Pascoli 70/3, 20133, Milano, Italy
m.zappia@bedimensional.it

Two-dimensional (2D) metal monochalcogenides have recently attracted interest for their applications in photoelectrochemical (PEC) applications in aqueous electrolytes [1][2]. Their optical bandgaps in the visible and near-infrared spectral region are adequate for energy conversion and photodetection/sensing applications. Their large surface-to-volume ratio guarantees that the charge carriers are photogenerated at the material/electrolyte interface in which redox reactions take place, thus minimizing recombination processes. In particular, 2D indium selenide (InSe) has emerged as a promising candidate for these applications.[3] In this work, we report a PEC characterization of single-/few-layer flakes of InSe, produced in inks form through scalable liquid-phase exfoliation (LPE) [4,5,6], as photoactive material for PEC-type photodetectors. The PEC behaviour of 2D InSe-based photoelectrodes was evaluated in both acidic (0.5 M H_2SO_4) and alkaline (1 M KOH) media under different illumination wavelengths, *i.e.*, 455, 505, and 625 nm. The highest photoresponse of the InSe photoelectrodes was observed in acidic media, reaching promising responsivities up to 31.1 mA W^{-1} at 0.8 V vs. RHE under 0.5 mW cm^{-2} 455 nm illumination. In addition, to improve the performances of our devices by increasing the electrode thickness without lacking efficient charge carrier collection toward the current collectors, we also hybridized InSe flakes with conductive indium tin oxide (ITO) nanocrystals, achieving a responsivity up to 60.0 mA W^{-1} at +0.4 V vs. RHE in the 0.5 M H_2SO_4 under blue.

References

[1] M. I. Zappia, et al., The Journal of Physical Chemistry C, 125, 11857−11866 (2021).
[2] G. Bianca, M. I. Zappia, et al., ACS Appl. Mater. Interfaces, 12, 43, 48598-48613 (2020).
[3] E. Petroni, et al., Small 14, 1800749 (2018).
[4] F. Bonaccorso, et al., Materials today, 12, 564 (2012).
[5] A. E. Del Rio Castillo, et al., Materials Horizons 5, 890-904 (2018).
[6] S. Bellani et al., Chem Soc. Rev.11870-11965 (2021).

Figures

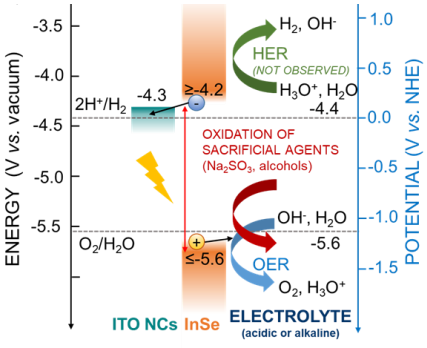


Figure 1: Energy level diagram of the PEC-type hybrid ITO/InSe

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement GrapheneCore3 - 881603

Modeling the influence of stuctural defects on the thermal transport properties of single layer MoS_2

Christophe Adessi
S. Pecorario S. Thebaud and G. Bouzerar
Institut Lumière Matière, UMR 5306 Université Claude Bernard Lyon 1 – CNRS, Université de Lyon, 69622 Villeurbanne cedex
christophe.adessi@univ-lyon1.fr

Transition metal dichalogenides like MoS_2 have received an increasing interest as a new family of two dmensional (2D) materials. Unlike graphene, MoS_2 exhibits a large band gap and seems promising for applications such as field effect transistors. Moreover, MoS_2 exhibits a rather low thermal conductivity of the order of 35 W/m/K for thin film[1] which is an important feature for thermoelectric applications.

One intriguing question is the role of structural defects on the thermal transport properties and the combine influence on the electronic transport properties in the framework of thermoelectricity[2]. In the present work, we have focussed on two kinds of defects: Sulfur vacancies, which are inherent within this material[3] and adsorbed alkali metal atoms (Li and K) which have been observed to be efficient n-type dopants[4].

We have used, for the present work, harmonic interatomic force constants derived from DFT calculations combined with non equilibrium Green's function technique to investigate the influence of these defects on the thermal transport properties (see Fig. 1). It has allowed us to study realistic disordered systems with various defects concentration. Moreover, this technique allows to disentangle the respective influence of phonon-defect and phonon-phonon (or Umklapp) scattering on the thermal conductivity.

References

[1] R. Yan, et al. ACS Nano, 8:986–993, 2014.
[2] Ch. Adessi, et al. Pysical Chemistry Chemical Physics, 22:15048–15057,2020.
[3] Wu Zhou et al. Nano Letters, 13(6):2615–2622, 2013.
[4] 4. Hui Fang et al. Nano Letters, 13(5):1991–1995, 2013.

Figures

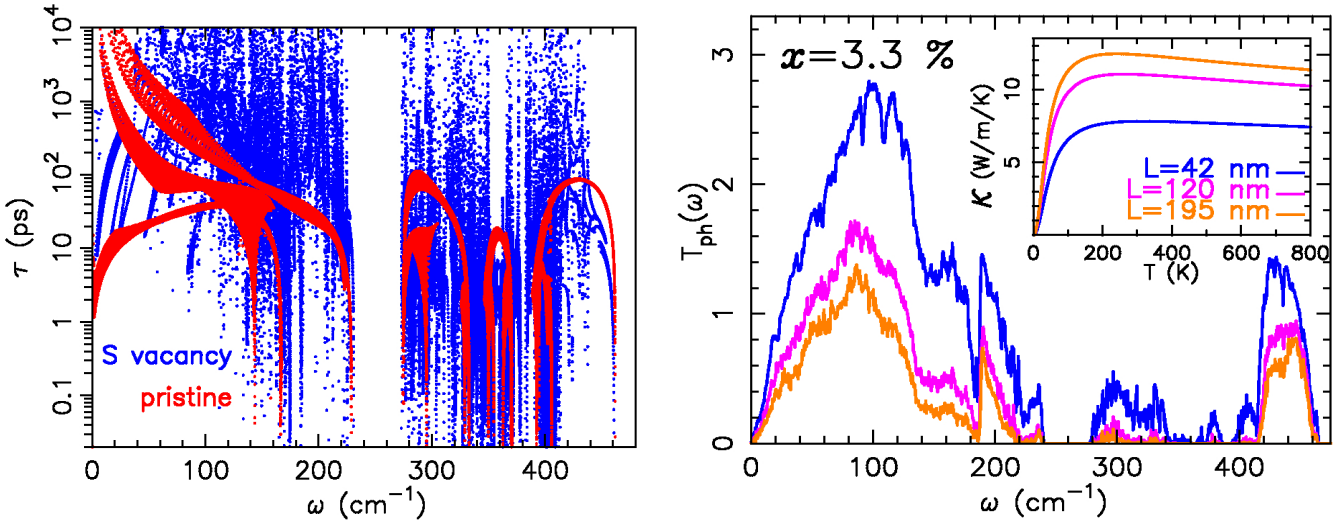


Figure 1: Phonon Lifetime (left) for pristine MoS_2 and MoS_2 with a sulfur vacancy. Phonon transmission (right) for MoS_{2-X} for increasing lengths of the material. In inset is given the thermal conductivity.

Asymmetric correlated states in twisted monolayer-bilayer graphene

Mohammed M. Al Ezzi
Alexandra Carvalho, Vladimir I. Fal'ko, Kostya S. Novoselov, Antonio Helio Castro Neto, Shaffique Adam
Centre for Advanced 2D Materials, National University of Singapore, Singapore
alezzi@u.nus.edu

In twisted monolayer-bilayer graphene massless and massive Dirac fermions mix together and lead to asymmetric correlated states and out-of-equilibrium criticalities characterized by superconductivity-like non-linear current-voltage characteristics. In this theoretical work, we first develop an analytical model to explain the observed asymmetry in formation of correlated states with respect to carrier density and displacement field [1]. Using the linearized gap equation method, we calculate the stability and critical temperature for different symmetry breaking phases, including spin density waves, charge density waves, and valley ordered phases. We compare our theoretical findings with available experimental data.
This work was supported by the Singapore National Research Foundation Investigator Award (Grant No. NRF-NRFI06-2020-0003).

[1] Shuigang Xu, et al. Nature Physics, 5 (2021)

Designing Metal and Semiconductor Contact Heterostructures to Two-Dimensional $MoSi_2N_4$ and WSi_2N_4

Yee Sin Ang
Qianqian Wang, Che Chen Tho and L. K. Ang
Singapore University of Technology and Design, 8 Somapah Road, Singapore 487372
yeesin_ang@sutd.edu.sg

The recent discovery of two-dimensional (2D) MA_2Z_4 monolayers unravels an exciting material platform for a plethora of device applications [1]. Here we study the heterostructures of MA_2Z_4 using density functional theory (DFT) simulations [2-5]. Focusing on $MoSi_2N_4$ and WSi_2N_4, we investigated three major classes of contacts: (i) 3D metals [2]; (ii) 2D metals [3]; and (3) 2D semiconductors [4,5]. For 3D metal contacts, we found that MoSi2N4 and WSi2N4 exhibit strongly suppressed Fermi level pinning effect [Figure 1(a)]. Intriguingly, the presence of an outer Si-N layer offers a *built-in* protective mechanism that preserves the transport states situating in the inner core layer, thus significantly suppressing interfacial tunnelling barrier and avoiding severe metallization of the VBM and CBM states. For 2D metal contacts, nearly Ohmic and electric-field tunable contacts can be obtained using graphene and NbS_2 [3]. We further perform a comprehensive cataloguing of 2D/2D van der Waals heterostructures (vdWHs) between MA_2Z_4 and other 2D semiconductors [4,5]. By simulating 52 different types of MA_2Z_4 vdWHs, several candidate structures with excellent solar cell conversion efficiency reaching well over 20% are identified. Furthermore, we found that $MoSi_2N_4$-and WSi_2N_4-based vdWHs typically exhibit strong optical absorption in the ultraviolet (UV) regime, suggesting their potential for UV photonics applications [Figure 1(b)]. Our findings uncover the contact properties of $MoSi_2N_4$ and WSi_2N_4 and reveal the opportunities of MA_2Z_4 as an emerging 2D material family towards the realization of novel solid-state technology beyond the silicon era.

References

[1] Y.-L. Hong et al, Science, **369** (2020) 670
[2] Q. Wang et al, NPJ 2D Mater. Appl., **5** (2021) 71
[3] L. Cao, G. Zhou, Q. Wang, L. K. Ang, Y. S. Ang, Appl. Phys. Lett., **118** (2021) 013106
[4] J. Q. Ng, Q. Wu, L. K. Ang and Y. S. Ang, Appl. Phys. Lett., **120** (2022) 103101
[5] C. C. Tho, Y. S. Ang, et al, manuscript in preparation (2022)

Figures

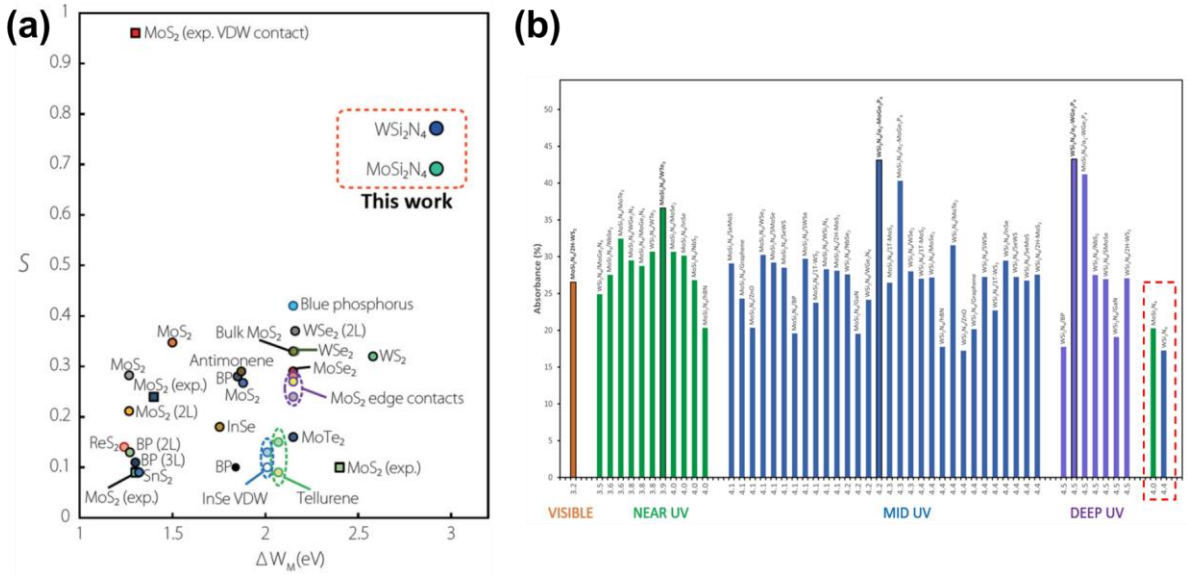


Figure 1: (a) Strongly suppressed FLP effect in $MoSi_2N_4$ and WSi_2N_4 metal contacts [2]. (b) 2D/2D VDWHs based on $MoSi_2N_4$ and WSi_2N_4 exhibit strong optical absorption in the UV regime [5].

Trilayer Rhombohedral Stacked Graphene being more Stable than its Bernal Counterpart

Raúl Guerrero-Avilés,† Marta Pelc,‡,† Fabian R. Geisenhof,¶ Thomas Weitz,§ and **Andrés Ayuela**∗ **,†**

†Material Physics Center CFM-MPC, Donostia International Physics Center (DIPC), Paseo Manuel Lardizabal 4-5, 20018 Donostia-San Sebastián, Spain
‡Institute of Physics, Nicolaus Copernicus University in Toruń, Grudziadzka 5, 87-100 Toruń, Poland
¶Physics of Nanosystems, Department of Physics, Ludwig- Maximilians- Universität München, Amalienstrasse 54, 80799 Munich, Germany
§I. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

*email: swxayfea@sw.ehu.es

Stackings in graphene have a pivotal role in properties to be discussed in the future, as seen in the recently found superconductivity of twisted bilayer graphene[1]. Beyond bilayer graphene, the stacking order of multilayer graphene can be rhombohedral, which shows flat bands near the Fermi level that are associated with interesting phenomena, such as tunable conducting surface states[2] expected to exhibit spontaneous quantum Hall effect[3], surface superconductivity[4], and even topological order[5]. However, the difficulty in exploring rhombohedral graphenes is that in experiments, the alternative, hexagonal stacking is the most commonly found geometry and has been considered the most stable configuration for many years. Here we reexamine this stability issue in line with current ongoing studies in various laboratories. We conducted a detailed investigation of the relative stability of trilayer graphene stackings and showed how delicate this subject is. These few-layer graphenes appear to have two basic stackings with similar energies. The rhombohedral and Bernal stackings are selected using not only compressions but anisotropic in-plane distortions. Furthermore, switching between stable stackings is more clearly induced by deformations such as shear and breaking of the symmetries between graphene sublattices, which can be accessed during selective synthesis approaches. We seek a guide on how to better control – by preserving and changing - the stackings in multilayer graphene samples [6].

References

[1] Cao, Y. et al. Nature 2018, 556, 43.
[2] Shi, Y. et al. Nature 2020, 584, 210–214.
[3] Zhang, F. et al. Phys. Rev. Lett. 2011, 106, 156801.
[4] Kopnin, N. et al. Phys. Rev. B 2013, 87, 140503.
[5] Slizovskiy, S. et al. Comm. Phys. 2019, 2, 1-10.
[6] Geisenhof, F. R. et al. ACS Appl. Nano. Mater. 2019, 2, 6067–6075.

Figures

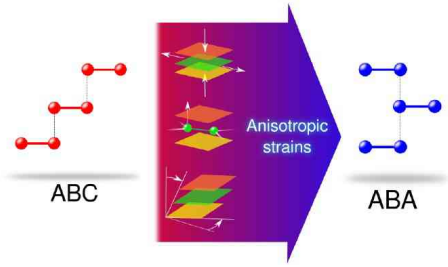


Figure 1: Graphene stacking changes from rhombohedral to Bernal due to small lattice deformations.

Ab Initio Simulations of Defective Metal Contacts in Beyond-CMOS Devices Based on Single-layer MoS_2: Impact of Small and Extended Defects

Gabriele Boschetto
Stefania Carapezzi, Aida Todri-Sanial
LIRMM, University of Montpellier, CNRS, 34095 Montpellier, France
gabriele.boschetto@lirmm.fr

Atomically thin single-layer molybdenum disulfide (MoS_2) is a two-dimensional material with highly desirable mechanical, electronic, and optical properties. These, combined with its reduced dimensionality and ultra-thin size, could enable the fabrication of a new generation of very compact and low-power devices which go beyond the conventional CMOS technology.
At present, wafer-scale production of MoS_2 is mainly achieved via CVD and PVD growth techniques, however, films have not yet reached the level of purity typical of the silicon technology. Small and extended defects are inevitably introduced in the material, and are expected to significantly affect not just the properties of MoS_2 itself but also the quality of the metal contact. For instance, poor electron injection and Fermi level pinning at the MoS_2-metal interface could lead to large Schottky barriers and contact resistances, which limit the device performance by introducing unwanted parasitic elements [1]. This is detrimental for devices like field-effect transistors (FETs). On the other hand, the functionality of some devices, such as memristors based on monolayer MoS_2, may even depend on the presence and nature of such defects [2].
Here, with the aim of bridging the gap between material's properties and device physics, we investigate defective single-layer MoS_2 in top contact with a metal electrode. To do so, we carry out ab initio computer simulations in the framework of Density Functional Theory (DFT) coupled with surface simulations based on the Green's function formalism [3]. Such a simulation scheme allows us to construct realistic MoS_2-metal interfaces and to carry out accurate interface simulations. To model the metal electrode, we choose the chemical inert Au as it is commonly employed at the lab scale to fabricate devices. We explore the impact of experimentally-observed vacancies and substitutions on the properties of MoS_2-Au contacts, and we predict relevant interface properties such as electron injection rates and tunnelling barriers.
Ultimately, our study constitutes the first step of a more comprehensive multi-scale modelling approach, in which the aim is to construct a full atomistic-to-device level model that can aid us in elucidating the physics of 2D devices based on single-layer MoS_2.

References

[1] A. Allain et al. "Electrical Contacts to Two-Dimensional Semiconductors," *Nat. Mater.*, 14, 1195–1205, **2015**.
[2] R. Ge et al., "Atomristor: Nonvolatile Resistance Switching in Atomic Sheets of Transition Metal Dichalcogenides," *Nano Lett.*, 18, 434-441, **2017**.
[3] S. Smidstrup et al. "First-Principles Green's Function Method for Surface Calculations: A Pseudopotential Localized Basis Set Approach," Phys. Rev. B, 96, 195309, **2017**.

Peierls phase formulas for periodic systems under magnetic field

Alessandro Cresti
Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, IMEP-LAHC, 38000 Grenoble, France
alessandro.cresti@grenoble-inp.fr

The Peierls phase describes the orbital effect of a relatively weak magnetic field $\boldsymbol{B}=\nabla\times\boldsymbol{A}$, where $\boldsymbol{A}$ is the vector potential, on atomistic systems within a tight-binding-like Hamiltonian representation [1]. It is proportional to the line integral of $\boldsymbol{A}$ along the straight path between couple of orbitals and it changes under gauge transformations $\boldsymbol{A}\rightarrow\boldsymbol{A}+\nabla\chi$, while its circulation and the physical observables are gauge independent. For periodic systems, under a generic gauge the Hamiltonian is not necessarily invariant under spatial translations, which could be inconvenient to allow the use of efficient techniques for electronic structure and transport simulations, as the so-called Sancho-Rubio algorithm [2] for determining the contact self-energies. In this contribution, I will provide a gauge choice and ready-to-use formulas to determine Peierls phase factors that preserve the translation symmetry of any periodic quasi-one-dimensional and two-dimensional systems under a homogeneous magnetic field [3]. I will show some interesting applications regarding a metallic carbon nanotube in high magnetic field and periodic 2D graphene with Gaussian bumps, where the induced strain makes Landau levels dispersive and lifts the valley degeneracy. The provided formulas represent a powerful tool for the simulation of electronic and transport properties of mesoscopic one- and two-dimensional systems in the presence of magnetic fields.

References

[1] R. Peierls, Zeitschrift für Physik, 80 (1933) 763
[2] M. P. Lopez Sancho et al., Journal of Physics F: Metal Physics, 15 (1985) 851
[3] A. Cresti, Physical Review B, 103 (2021) 045402

Figures

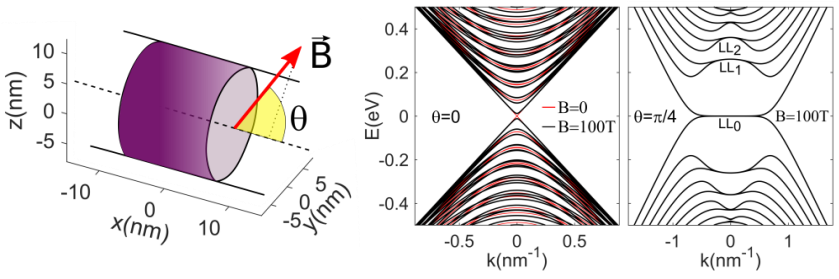


Figure 1: Sketch and band structure of a metallic carbon nanotube with 50 nm circumference in the presence of a magnetic field $\boldsymbol{B}$ at angle θ with the ribbon axis.

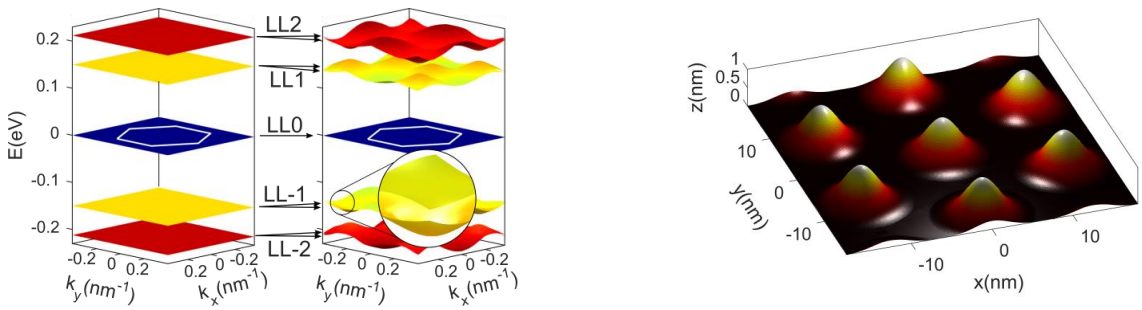


Figure 2: Low-energy bands in the absence (left) and in the presence (right) of the superlattice of a superlattice of bumps in two-dimensional graphene it (see sketch), under a 22.74 T orthogonal magnetic field. Strain makes Landau levels dispersive and removes the valley degeneracy, while the zero-energy Landau level does not change.

First-principles insights into the spin-valley physics of strained transition metal dichalcogenides monolayers

Paulo E. Faria Junior[1]
Klaus Zollner[1], Tomasz Woźniak[2], Marcin Kurpas[3], Martin Gmitra[4], Jaroslav Fabian[1]
1. Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany.
2. Wroclaw University of Science and Technology, 50-370 Wroclaw, Poland
3. Institute of Physics, University of Silesia, 75 Pulku Piechoty 1, 41-500 Chorzów, Poland
4. Institute of Physics, Pavol Jozef Šafárik University in Košice, Park Angelinum 9, 04001 Košice, Slovakia
fariajunior.pe@gmail.com / paulo.eduardo-faria-junior@ur.de

Transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of spin-valley physics under external stimuli. Here, we investigate the influence of strain on the spin and orbital angular momenta, effective g-factors, and Berry curvatures of several monolayer TMDCs (Mo and W based) using state-of-the-art first principles calculations of the spin and orbital angular momenta[1-4]. At the K-valleys, we find a surprising decrease of the conduction band spin expectation value for compressive strain, consequently increasing the dipole strength of the dark exciton by more than one order of magnitude. We also predict the behavior of direct excitons g-factors under strain: tensile (compressive) strain increases (decreases) the absolute value of g-factors. Strain variations of ~ 1% modify the bright (A and B) excitons g-factors by ~ 0.3 (0.2) for W (Mo) based compounds and the dark exciton g-factors by ~ 0.5 (0.3) for W (Mo) compounds. Our predictions could be directly visualized in magneto-optical experiments in strained samples at low temperature. Additionally, our calculations strongly suggest that strain effects are one of the possible causes of g-factor fluctuations observed experimentally. By comparing the different TMDC compounds, we reveal the role of spin-orbit coupling (SOC): the stronger the SOC, the more sensitive are the spin-valley features under applied strain. Consequently, monolayer WSe_2 is a formidable candidate to explore the role of strain on the spin-valley physics (summarized in Fig.1 for the K-valley). We complete our analysis by considering the side valleys, Γ and Q points, and by investigating the influence of strain in the Berry curvature. In the broader context of valley- and strain-tronics, our study provides fundamental microscopic insights into the role of strain in the spin-valley physics of TMDCs, which are relevant to interpret experimental data in monolayer TMDCs as well as to model TMDC-based van der Waals heterostructures.

References

[1] T. Woźniak, P. E. Faria Junior, G. Seifert, A. Chaves, J. Kunstmann, Phys. Rev. B, 101 (2020) 235408.
[2] T. Deilmann, P. Krüger, M. Rohlfing, Phys. Rev.Lett., 124 (2020), 226402.
[3] J. Förste, N. V. Tepliakov, S. Y. Kruchinin, J. Lindlau, V. Funk, M. Förg, K. Watanabe, T. Taniguchi, A. S. Baimuratov, A. Högele, Nature Communications 11 (2020) 4539.
[4] F. Xuan, S. Y. Quek, Phys. Rev. Research, 2 (2020), 033256.

Figures

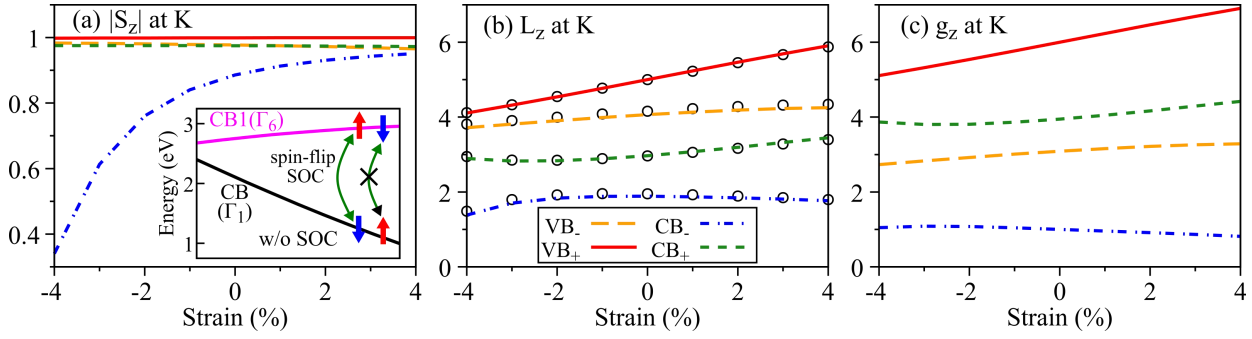


Figure 1: (a) Spin angular momenta, S_z, (b) orbital angular momenta, L_z, and (c) g-factors ($g_z = L_z + S_z$) for the low-energy bands at the K-valley for strained WSe_2 monolayer. The inset in Fig.(a) indicates the microscopic mechanism responsible for the drastic spin mixing in CB-.

Heat Transport in Transition Metal Dichalcogenides from first principles calculations

Roberta Farris[1]
D. Saleta Reig[1], S. Varghese[1], A. Block[1], O.Hellman[2], K. J. Tielrooij[1], P. Ordejón[1], Z. Zanolli[3], M. J. Verstraete[4]

[1]*Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193, Barcelona, Spain*
[2] Departament of Molecular Chemistry and Materials Science, *Weizmann Institute of Science, Rehovot 76100, Israel*
[3]*Chemistry Department & Debye Institute for Nanomaterials Science, Utrecht University, the Netherlands*
[4]*Université de Liège, Département de Physique, B-4000 Sart Tilman, Liège, Belgium*
roberta.farris@icn2.cat

Layered 2D Transition Metal Dichalcogenides (TMDs) have received significant attention because of their unique electrical, optical, and mechanical properties that may be in contrast with those of their bulk parent compounds. In contrast, thermal properties and how they change from a 3D crystal to a 2D layered structure have received less attention even though their understanding is crucial for several applications exploiting these materials, such as thermoelectricity and optoelectronics [1].
Here, we present a theoretical study of the intrinsic lattice thermal conductivity of bulk and monolayer WS_2, WSe_2, MoS_2 and $MoSe_2$ focusing on the dependence of heat transport on the atomic mass and atomic species present in the compounds.
This study allows us to understand the role of the different atomic species involved in the thermal transport when we pass from a 3D structure to a 2D structure and the implications at the microscopic level, including a complete inverstigation of the scattering rates and phonon frequencies.
The thermal conductivity κ of TMDs is calculated by solving the Boltzmann Transport Equation (BTE) including phonon-phonon scattering and phonon boundary scattering beyond the relaxation time approximation (RTA) [2].
First principles calculations are accurately performed by the SIESTA program [3] based on the Density Functional Theory (DFT) and the Temperature Dependent Effective Potential package (TDEP) [4] for finite temperature lattice dynamics calculations.
By employing this method we computed the thermal properties for the different TMDs at room temperature and we compare the results with recent and accurate experiments on a full range of thicknesses [5].

References

[1] Han, S.A., Bhatia, R. & Kim, SW. Nano Convergence 2, 17 (2015)
[2] Peierls, R. E. (1955). Quantum Theory of Solids. Clarendon Press.
[3] Garcia A. et al., J. Chem. Phys. 152, 204108 (2020)
[4] Hellmann, O. & Abrikosov, A. Phys. Rev. B 88, 144301 (2013)
[5] D. Saleta Reig, et. al. Advanced Materials. 2108352 (2022)

Proximity effects in graphene on alloyed transition metal dichalcogenides

Zahra Khatibi
Stephen Power
School of Physics, Trinity College Dublin, Dublin 2, Ireland
School of Physical Sciences, Dublin City University, Dublin 9, Ireland
khatibiz@tcd.ie

Stacked heterostructures of graphene and transition metal dichalcogenides (TMDs) are particularly interesting for spin- and valleytronics since spin-orbit coupling (SOC) can be induced in the graphene layer by proximity effects with a strong valley dependence [1]. The induced proximity SOC, and associated imprinted spin-valley locking, enable experimentally verified spin-charge conversion and anisotropic spin relaxation effects that are absent in pristine graphene [2-3]. The nature and strength of the induced SOC depends on the composition of the TMD layer and its interaction with the graphene. Recent experimental advances allow the synthesis of TMD layers with a mix of metal atoms, suggesting that metal-atom alloying of the TMD layer may be an effective route to tune proximity effects in graphene-based heterostructures [4]. In this study we investigate the proximity induced SOC in graphene/TMD heterostructures by deliberate defecting of the TMD layer. We analytically study simple alloyed G/$W_{1-\chi}Mo_\chi Se_2$ heterostructures with diverse concentrations (χ) and geometrical distribution of defects in the TMD layer. Utilizing density functional theory-computed electronic dispersions, spin textures, and an effective medium model, we evaluate the role of locally perturbed SOC on spin- and electronic signatures. We use the gained microscopic insight via tight-binding model to further examine the impact of defects in larger and more realistic heterostructures. We find that despite some dramatic perturbation of local SOC for individual defects, the low energy spin- and electronic behaviour yet follows the effective medium model. Since G/WSe_2 and G/$MoSe_2$ heterostructures individually maintain robust topological and trivial insulating phases, this finding yields that topological state of alloyed systems can be feasibly tuned via controlling the composition ratio of the metallic element.

References

[1] M. Gmitra, Phys. Rev. B 93 (2016) 155104
[2] A. W. Cummings, Phys. Rev. Lett. 119 (2017) 206601
[3] L. A. Benítez, Nat. Phys 14 (2018) 303
[4] F. A. Nugera, Small (2022), 2106600

Figures

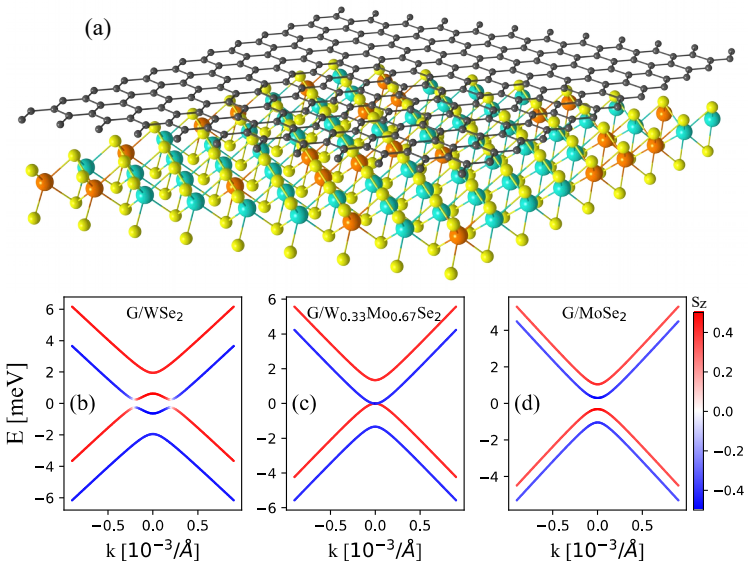


Figure 1: (a) Schematic representation of a composite G/$W_{1-\chi}Mo_\chi Se_2$ heterostructure. The electronic dispersion of G/$W_{1-\chi}Mo_\chi Se_2$ with (b) χ=0, (c) χ=0.67, and (d) χ=1.

Wannier Diagram and Brown-Zak Fermions of Graphene on Hexagonal Boron-Nitride

F. Libisch
T. Fabian, M. Kausel, L. Linhart, J. Burgdörfer
Institute for Theoretical Physics, TU Wien, Wiedner Haupstrasse 8-10/136, Vienna, Austria
Florian.libisch@tuwien.ac.at

The moiré potential of graphene on hexagonal boron nitride (hBN) generates a supercell sufficiently large as to thread a full magnetic flux quantum Φ_0 for experimentally accessible magnetic field strengths. Close to rational fractions of Φ_0, $p/q \cdot \Phi_0$, magnetotranslation invariance is restored giving rise to Brown-Zak fermions featuring the same dispersion relation as in the absence of the field. Employing a highly efficient numerical approach we have performed the first realistic simulation of the magnetoconductance for a 250 nm wide graphene ribbon on hexagonal boron nitride using a full ab-initio derived parametrization including strain [1]. The resulting Hofstadter butterfly is analysed in terms of a novel Wannier diagram for Landau spectra of Dirac particles that includes the lifting of the spin and valley degeneracy by the magnetic field and the moiré potential. This complex diagram (Fig. 1) can account for many experimentally observed features on a single-particle level [2,3,4], such as spin and valley degeneracy lifting and a non-periodicity in Φ_0.

References

[1] T. Fabian, M. Kausel, L. Linhart, J. Burgdorfer, and F. Libisch, arXiv:2111.01755 (2021).
[2] B. Hunt, J. D. Sanchez-Yamagishi, A. F. Young, M. Yankowitz, B. J. LeRoy, K. Watanabe, T. Taniguchi, P. Moon, M. Koshino, P. Jarillo-Herrero, and R. C. Ashoori, Science **340**, 1427 (2013)
[3] R. Krishna Kumar, X. Chen, G. H. Auton, A. Mishchenko, D. A. Bandurin, S. V. Morozov, Y. Cao, E. Khestanova, M. Ben Shalom, A. V. Kretinin, K. S. Novoselov, L. Eaves, I. V. Grigorieva, L. A. Ponomarenko, V. I. Fal'ko, and A. K. Geim, Science 357, 181 (2017)
[4] J. Barrier et al., Nature Comm **11**, 5756 (2020)

Figures

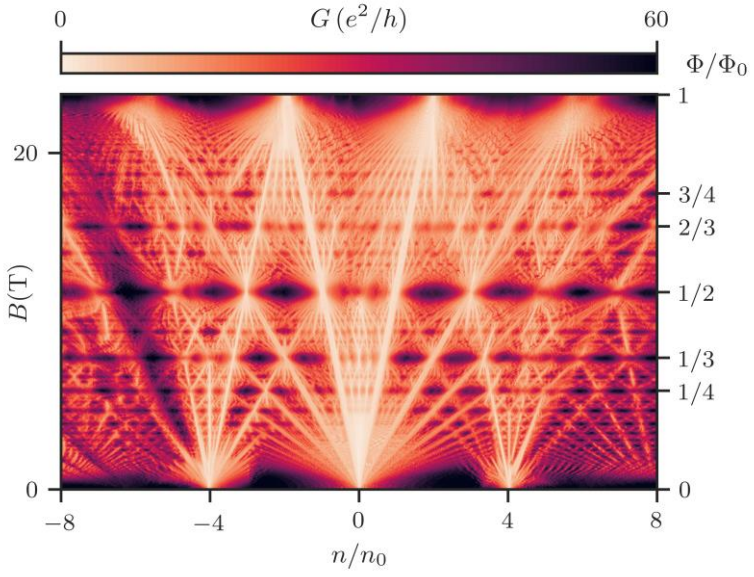


Figure 1: Conductance through graphene aligned on hBN as a function of charge carrier density and magnetic field.

Wave Packet Dynamical Simulation of Magnetic Effects in 2D Materials

Géza I. Márk[1]
Péter Vancsó[1], Alexandre Mayer[2]
[1]*Institute for Technical Physics and Materials Science, Centre for Energy Research, 1121 Budapest, Hungary*
[2]*Department of Physics, University of Namur, 5000, Namur, Belgium*
mark.geza@ek-cer.hu

Two dimensional (2D) materials and 2D heterostructures have extraordinary physical properties, determined both by the pristine crystal lattice and its defects. Understanding the effect of magnetic fields on the electronic structure and transport properties of these materials is important for several reasons: (1) magnetic fields arising near magnetic defects, (2) pseudo-magnetic fields [1] arising because of structural defects, and (3) one-dimensional (1D) defects (edges and 2D grain boundaries), where magnetic and topological phenomena may occur. We studied such effects utilizing two calculation methods based on wave packet (WP) dynamics. (1) We model the atomic- and electronic structure of the perfect 2D lattice by a local atomic pseudopotential [2] and calculate the time dependent scattering [3] of a Bloch WP on the defect represented by a scalar potential. (2) We describe the perfect crystal by a dispersion relation derived from band structure calculation [4] and study the scattering of a WP on a vector potential corresponding to the pseudo magnetic field of the defect. The model calculations were performed on a graphene sheet but the second method is applicable for any 2D material where electronic structure calculations are available.

References

[1] P. Kun et al, 2D Mat. Appl. 3 (2019) 11.
[2] A. Mayer, Carbon 42 (2004) 2057.
[3] G. I. Márk et al, Phys. Rev. B 85 (2012) 125443.
[4] P. Vancsó et al, Appl. Sci. 11 (2021) 4730.

Figures

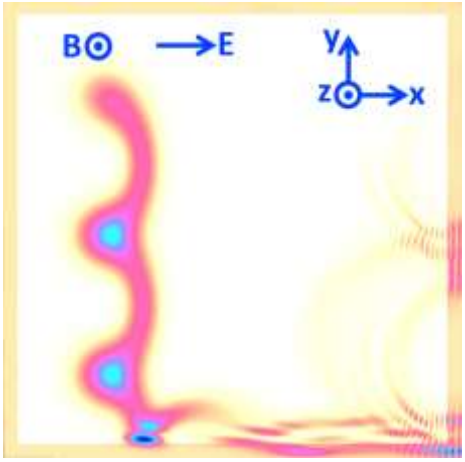


Figure 1: Wave packet scattering on a topological insulator model. The time integrated probability density of the wave packet propagating in perpendicular electric- and magnetic fields demonstrates that there is no conduction in the bulk but conduction occurs at the boundary.

Modelling of thermal properties of single-layer MoS_2-WS_2 alloys by using machine-learned interatomic potentials

Juan M. Marmolejo-Tejada
Martín A. Mosquera
Department of Chemistry and Biochemistry, Montana State University, Bozeman, MT 59717 USA
martinmosquera@montana.edu

Two-dimensional (2D) quantum materials are promising in the advancement of conventional electronic devices. For the study of thermal transport in single-layer (1L) or multi-layer transition metal dichalcogenides (TMDs), this work explores the combination of density functional theory (DFT) and artificial machine training for the generation of a moment-tensor potential (MTP) that models 1L-MoS_2, 1L-WS_2 and their alloys. This MTP model gives a convenient inter-atomic (or inter-molecular in other contexts) force field that can predict the response of quantum materials to thermal perturbations, or other driving forces. We show that our trained MTP successfully describes the vibrational properties of the systems, and their thermal conductivities. The trained potential displays consistent agreement with DFT calculations, as well as the Stillinger-Weber potential. We also find that the thermal conductivity of the 2D alloys is largely unaffected by sulfur vacancies. This is a behaviour that may aid the fine-tuning of material's thermal properties for heat management and energy storage and conversion applications.

References

[1] A. V. Shapeev, *Multiscale Modeling & Simulation*, 14.3 (2016) 1153-1173.
[2] B. Mortazavi *et al.*, *Applied Materials Today*, 20 (2020), 100685.
[3] B. Mortazavi *et al*, *Journal of Physics: Materials* 3.2 (2020), 02LT02.
[4] V. V. Ladygin *et al.*, *Computational Materials Science* 172 (2020), 109333.
[5] Y. Zuo *et al.*, *The Journal of Physical Chemistry A* 124.4 (2020), 731-745.
[6] P. K. Schelling *et al.*, *Physical Review B* 65 (2002), 144306.
[7] X. Zhang *et al.*, *Physical Review B* 89 (2014), 054310.
[8] Y. Cai *et al.*, *Physical Review B* 89 (2014), 035438.

Figures

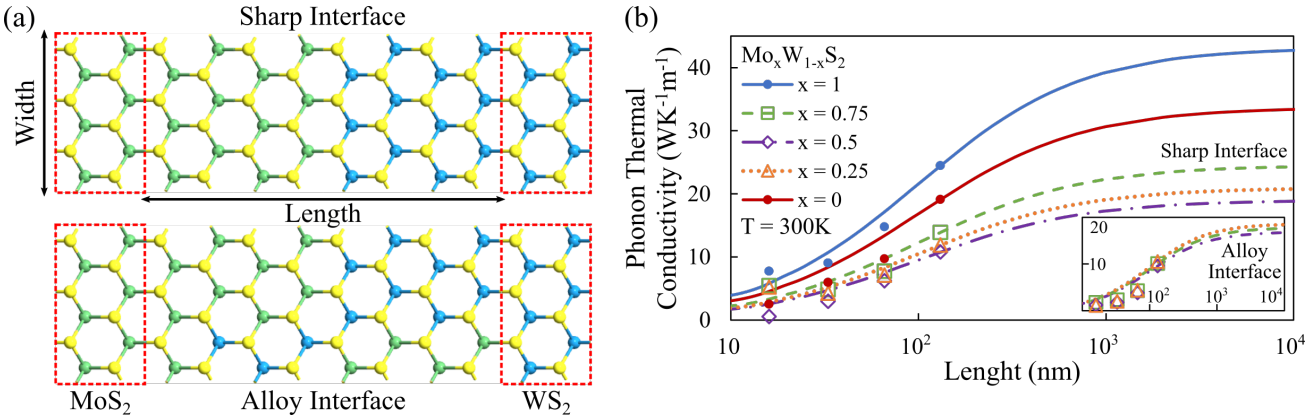


Figure 1: (a) Top view of a 1L-MoS_2/WS_2 heterostructure with sharp or alloy interface. Blue, green and yellow spheres correspond to W, Mo and S atoms, respectively. (b) Phonon thermal conductivity (κ) of 1L-$Mo_xW_{1-x}S_2$ systems at T=300K, obtained with our trained MTP. The symbols show the estimated conductivity at finite lengths, which are used to estimate the infinite length conductivity (κ_∞) by extrapolating the expression $1/\kappa = (1+\Lambda/l)/\kappa_\infty$., where l is the length of the sample and Λ is the effective phonon mean free path, assumed to be 100 nm for all cases. The lines show the estimation of κ with the previously calculated κ_∞ for each system.

Valley dependent optics in transition metal dichalcogenides

Pedro Miguel M. C. de Melo
Thibault Sohier, Matthieu J. Verstraete, Zeila Zanolli
Chemistry Department, Debye Institute for Nanomaterials Science, Condensed Matter and Interfaces, Utrecht University, PO Box 80.000, 3508 TA Utrecht, The Netherlands
p.m.monteirocamposdemelo@uu.nl

Transition metal dichalcogenides (TMDs) are strong contenders to optoelectronic applications. Thanks to spin-valley coupling, it is possible to use circularly polarized laser fields to create populations of excited electrons and holes with well-defined spin. These carrier densities can be tracked by optical measurements, such as time-dependent Kerr amplitude signal. However, such populations do not last long in pristine samples, due to scattering by phonons[1]. Here the energy splitting between the K and Q valleys plays a fundamental role in electron scattering mechanisms at higher temperatures[2,3]. This Q-K energy splitting is highly sensitive to thickness of the TMD sample, and can be changed even by encapsulation. Unfortunately, the changes in thickness of the TMD are hard to track once the device is built.
In this work we present a comprehensive study of the effects of Q-K valley energy splitting in the quenching of the Kerr signal. By setting up different valley alignments and excited configurations, we show how the different levels of density of excited carriers lead to a quenching of the Kerr signal amplitude. We relate these changes to the different levels of spin-orbit induced splitting in the band structure and show how the Kerr amplitude signal can be used to track the changes in layer thickness that are introduced in the TMD layer.

References

[1] A. Molina-Sánchez, D. Sangalli, L. Wirtz, A. Marini, Nano Letters 17 (8), (2017) 4549-4555
[2] M. Ersfeld, F. Volmer, P. Melo, R. de Winter, Ma. Heithoff, Z. Zanolli, C. Stampfer, M. J. Verstraete, B. Beschoten, Nano letters 19 (6), (2019) 4083-4090
[3] M. Ersfeld, F. Volmer, L. Rathmann, L. Kotewitz, M. Heithoff, M. Lohmann, B. Yang, K. Watanabe, T. Taniguchi, L. Bartels, J. Shi, C. Stampfer, B. Beschoten, Nano Letters 20 (5), (2020) 3147–3154

Figures

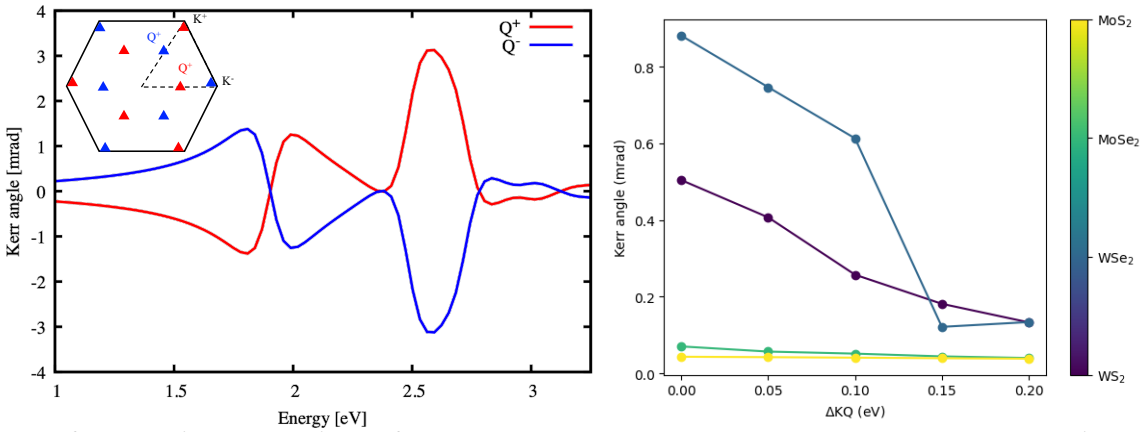


Figure 1: Left – Kerr signal amplitude for a WS_2 monolayer where the K and Q valleys are aligned. The inset marks the regions in the Brillouin zone where excited electrons are placed. Right – change in the Kerr amplitude for the A exciton of each TMD as a function of the energy splitting between the K and Q points.

Valley dependent optics in transition metal dichalcogenides

Pedro Miguel M. C. de Melo
Thibault Sohier, Matthieu J. Verstraete, Zeila Zanolli
Chemistry Department, Debye Institute for Nanomaterials Science, Condensed Matter and Interfaces, Utrecht University, PO Box 80.000, 3508 TA Utrecht, The Netherlands
p.m.monteirocamposdemelo@uu.nl

Transition metal dichalcogenides (TMDs) are strong contenders to optoelectronic applications. Thanks to spin-valley coupling, it is possible to use circularly polarized laser fields to create populations of excited electrons and holes with well-defined spin. These carrier densities can be tracked by optical measurements, such as time-dependent Kerr amplitude signal. However, such populations do not last long in pristine samples, due to scattering by phonons[1]. Here the energy splitting between the K and Q valleys plays a fundamental role in electron scattering mechanisms at higher temperatures[2,3]. This Q-K energy splitting is highly sensitive to thickness of the TMD sample, and can be changed even by encapsulation. Unfortunately, the changes in thickness of the TMD are hard to track once the device is built.
In this work we present a comprehensive study of the effects of Q-K valley energy splitting in the quenching of the Kerr signal. By setting up different valley alignments and excited configurations, we show how the different levels of density of excited carriers lead to a quenching of the Kerr signal amplitude. We relate these changes to the different levels of spin-orbit induced splitting in the band structure and show how the Kerr amplitude signal can be used to track the changes in layer thickness that are introduced in the TMD layer.

References

[1] A. Molina-Sánchez, D. Sangalli, L. Wirtz, A. Marini, Nano Letters 17 (8), (2017) 4549-4555
[2] M. Ersfeld, F. Volmer, P. Melo, R. de Winter, Ma. Heithoff, Z. Zanolli, C. Stampfer, M. J. Verstraete, B. Beschoten, Nano letters 19 (6), (2019) 4083-4090
[3] M. Ersfeld, F. Volmer, L. Rathmann, L. Kotewitz, M. Heithoff, M. Lohmann, B. Yang, K. Watanabe, T. Taniguchi, L. Bartels, J. Shi, C. Stampfer, B. Beschoten, Nano Letters 20 (5), (2020) 3147–3154

Figures

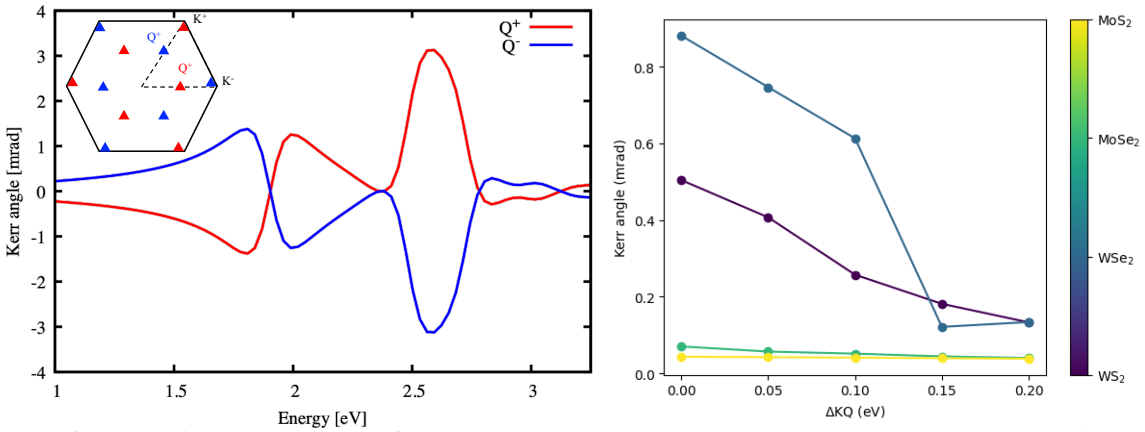


Figure 1: Left – Kerr signal amplitude for a WS_2 monolayer where the K and Q valleys are aligned. The inset marks the regions in the Brillouin zone where excited electrons are placed. Right – change in the Kerr amplitude for the A exciton of each TMD as a function of the energy splitting between the K and Q points.

First principle calculations of excitonic phases in van der Waal heterostructures

Fredrik Nilsson
Kristian Thygesen
CAMD, Technical University of Denmark (DTU), DK-2800 Kgs. Lyngby, Denmark
fanni@dtu.dk

Computational materials discovery has played a major role in the discovery of novel two dimensional materials, such as e.g. transition metal dichalcogenides. Different monolayers can be combined to form heterostructures with even richer phase diagrams. One interesting phenomenon in these heterostructures are long lived excitons formed by spatially separated electron-hole pairs. In double bilayer graphene experimental evidence of exciton condensation we found 2018 [1] while MoSe2/WSe2 bilayers have been shown to become excitonic insulators at certain electron and hole concentrations [2]. In both of these experimental setups the electron hole layers were separated by hBN barriers and the electron and hole concentrations were tuned using external gates. In this talk we will discuss how the newly developed excitonic density functional theory method [3] can be combined with the quantum electrostatic heterostructure model [4] to allow for realistic computations of the excitonic properties of stacked 2D materials. We will show how the relative band alignment as well as intrinsic dipole moments of some of these materials can be used to tailor their properties, without the need for hBN barriers or external fields, and propose new material combinations with interesting excitonic phases.

References

[1] W. Burg et. al Phys. Rev. Lett. 120 (2018)
[2] L. Ma et al, Nature 598 (2021)
[3] F. Nilsson et. al. Phys. Rev. Mat. 5 (2021)
[4] K. Andersen et al Nano Lett. 15 (2015)

Figures

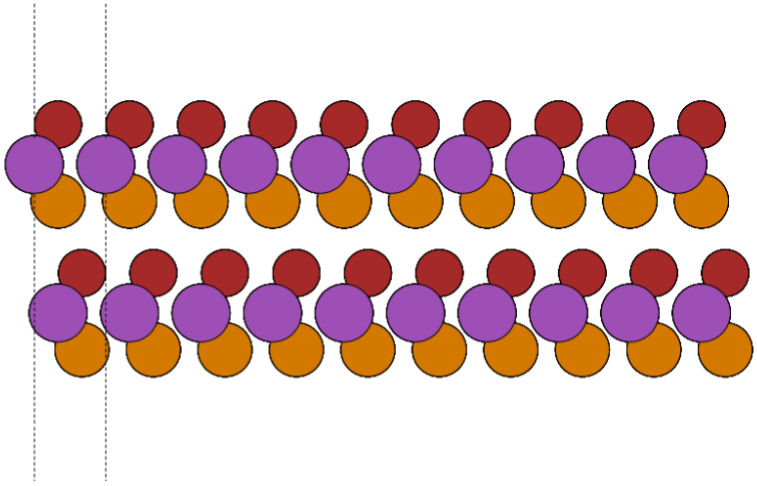


Figure 1: Schematic figure of a Janus bilayer

High-throughput stacking reveals emergent and switchable properties of 2D van der Waals bilayers

Sahar Pakdel
Asbjørn Rasmussen, Mads Kruse, Alireza Taghizadeh, Thomas Olsen, Kristian Sommer Thygesen
CAMD, Computational Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark
sahpa@dtu.dk

Abstract

Stacking atomically thin two-dimensional monolayers into van der Waals (vdW) heterostuctures [1] offer new opportunities to control physical properties of 2D materials. Here we provide a systematic ab initio-based study of homo-bilayers created by stacking several hundreds of stable monolayers containing up to 10 atoms per unit cell. We investigate all configurations commensurate with the primitive unit cell. We further verify the predictive power of our stacking approach by comparing our stacking orders when exfoliable bulk compounds of the same material exist. For the stable bilayers within a 3 meV/A^2 binding energy distance from our most stable configuration, we calculate a range of electronic and magnetic properties. We further explore switchable properties in bilayer pairs where two stable stacking configurations are related with a slide vector. Experimental evidence of switching such bilayers have been recently reported [2, 3]. Our work contributes to the systematisation of 2D materials and represents a step towards rational design of layered vdW materials. Our results will be available online and well-integrated with the Computational 2D Materials Database (C2DB) [4, 5] which allows for comparison between mono- and bilayer properties.

References

[1] Geim, A. K., & Grigorieva, I. V., Nature, 499(7459) (2013) 419-425.
[2] Yasuda, K., Wang, X., Watanabe, K., Taniguchi, T. and Jarillo-Herrero, P, Science, 372 (6549) (2021) 1458-1462.
[3] Wang, X., Yasuda, K., Zhang, Y., Liu, S., Watanabe, K., Taniguchi, T., Hone, J., Fu, L. and Jarillo-Herrero, P., Nature nanotechnology (2022) 1-5.
[4] Haastrup, S., Strange, M., Pandey, M., Deilmann, T., Schmidt, P. S., Hinsche, N. F., ... and Thygesen, K. S., 2D Materials, 5(4) (2018) 042002.
[5] Gjerding, M. N., Taghizadeh, A., Rasmussen, A., Ali, S., Bertoldo, F., Deilmann, T., ... and Thygesen, K. S., 2D Materials, 8(4) (2021) 044002.

DFTB study of the electronic and magnetic properties of titanium carbide Mxene

Taoufik Sakhraoui * and František Karlický **
Department of Physics, Faculty of Science, University of Ostrava, 30. dubna 22, 701 03 Ostrava, Czech Republic
https://nano.osu.cz/ *taoufik.sakhraoui@osu.cz **frantisek.karlicky.osu.cz

Two-dimensional (2D) materials metal carbide MXenes ($Ti_{n+1}C_n$; n=1, 2, 3, 4) has attracted a lot of attention recently [1, 2], due to its promising physical and chemical properties [3, 4]. It was shown that after the synthesis process, the MXenes are usually functionalized with O and F atoms, or -OH group [5, 6]. Moreover, the electronic, optical and magnetic properties of MXenes are affected by the surface termination [5-7].

Our computational study of the electronic and magnetic properties of MXenes have been performed using a calculation method that combines density functional theory (DFT) based ground state calculation with tight binding approach. The Self Consistent Charge Density Functional Tight Binding method (SCC-DFTB) which is an approximate, parametrised form of DFT [8] gives a response of the need for approximate methods. DFTB is is capable of targeting the studied MXene systems. This method allows us to optimize the "computational costs" with reasonable accuracy for large MXene systems. Here, we show good performance of DFTB approach to investigate the electronic and magnetic properties O-functionnalazed Titanium carbide MXene.

DFTB calculations provide a reasonable electronic structure and magnetic properties of the studies MXenes. We consider mainly Ti_2C which have magnetically ordered ground states. The magnetization is attributed, mainly, to the 3d electrons of surface Ti atoms. However, when two surfaces of Ti_2C monolayer are saturated by O atoms, the magnetism is spontaneously removed and Ti_2CO_2 shows a semiconducting behaviour.

References

[1] M. Nqguib, V. N. Mochalin, M. W. Barsoum and Y. Gogotsi, Adv, Mater., 26 (2014) 992.
[2] K. Hantanasirisakul and Y. Gogotsi, Adv. Mater., 30 (2018) 1804779.
[3] M. Naguib, O. Mashtalir, J. Carle, V. Presser, J. Lu, L. Hultman, Y. Gogotsi, and M. W. Barsoum, ACS Nano 6 (2012) 1322.
[4] A. Enyashin and A. Ivanovskii, Computational and Theoretical Chemistry 989 (2012) 27.
[5] M. Khazaei, M. Arai, T. Sasaki, C.-Y. Chung, N. S. Venkataramanan, M. Estili, Y. Sakka and Y. Kawazoe, Adv. Funct. Mater., 23 (2013) 2185.
[6] J. L. Hart, K. Hantanasirisakul, A. C. Lang, B. Anasori, D. Pinto, Y. Pivak, J. T. van Omme, S. J. May, Y. Gogotsi and M. L. Taheri, Nat. Commun., 10 (2019) 522.
[7] H. Zhang, G. Yang, X. Zuo, H. Tang, Q. Yang and G. Li, J. Mater. Chem. A, 4 (2016) 12913.
[8] M. Elstner, D. Porezag, G. Jungnickel, J. Elsner, M. Haugk, T. Frauenheim, S. Suhai, and G. Seifert, Phys. Rev. B 58 (1998) 7260.

Spin-textured ferroelectrics in InAs monolayer

Jiaqi Zhou[1], Marc Vila Tusell[2], and Jean-Christophe Charlier[1]
[1] *Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium*
[2] *Department of Physics, University of California, Berkeley, California 94720, USA*
jiaqi.zhou@uclouvain.be

Abstract

Two-dimensional materials have attracted the attention for next-generation electronic devices [1]. With practical band gaps and high carrier mobilities, group III–V compounds have become a mainstream part of semiconductor research [2]. In the present work, the electric properties of InAs monolayer are investigated by *ab initio* calculations. Rashba and out-of-plane spin textures are respectively discovered around conduction band minimum (CBM) and valence band maximum (VBM), as shown in Fig. 1. A third-order $k \cdot p$ model of C_{3v} symmetry is presented to explain the mechanism [3]. Moreover, with a buckling structure, the properties of InAs are tunable by external electric fields (EEFs), as shown in Fig. 2. With EEF increasing from -0.5 to 0.5 V/Å, InAs remains to be a semiconductor. Meanwhile, both the structural buckling heights and Rashba constants are increasing, while the energy gaps are decreasing. More intriguingly, the switchable ferroelectricity has been verified in InAs. This work reveals the potential of InAs to be applied in spintronic, piezoelectric, and ferroelectric devices.

References

[1] Wu *et al.*, *Nature* **603**, (2022) 259–264.
[2] Alamo *et al.*, *Nature* **479**, (2011) 317–323.
[3] Miyamoto *et al.*, *Phys. Rev. B* **97**, (2018) 085433.

Figures

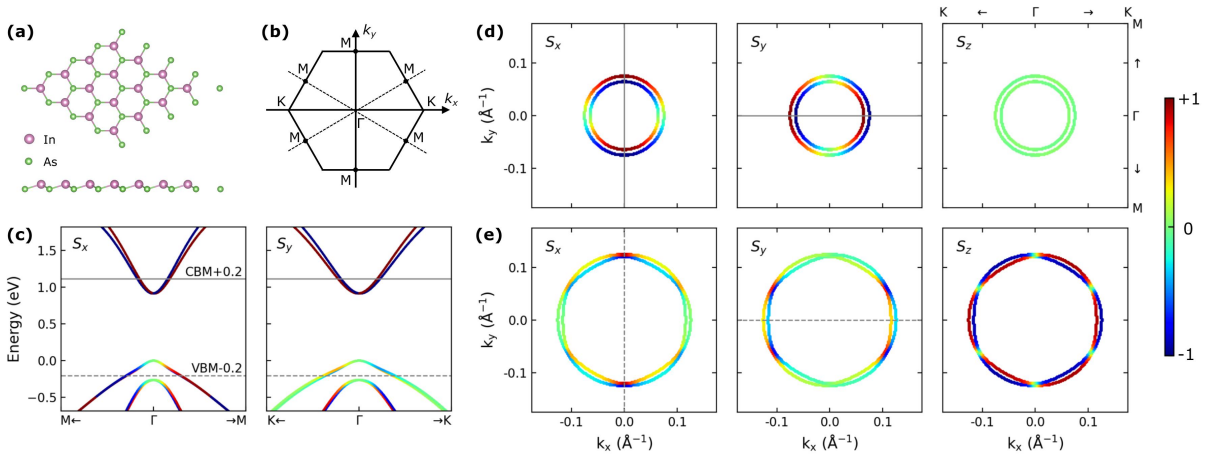


Figure 1: (a) Atomic structure of InAs monolayer (top view and side view). (b) Brillouin zone (BZ) and high-symmetry points. (c) Spin-resolved bands of S_x and S_y. Energy positions of CBM+0.2 eV and VBM-0.2 eV are marked by solid and dashed lines, respectively. (d) Spin textures in BZ at E = CBM+0.2 eV. (e) Spin textures in BZ at E = VBM-0.2 eV. The colorbar denotes the expectation values of spin operators.

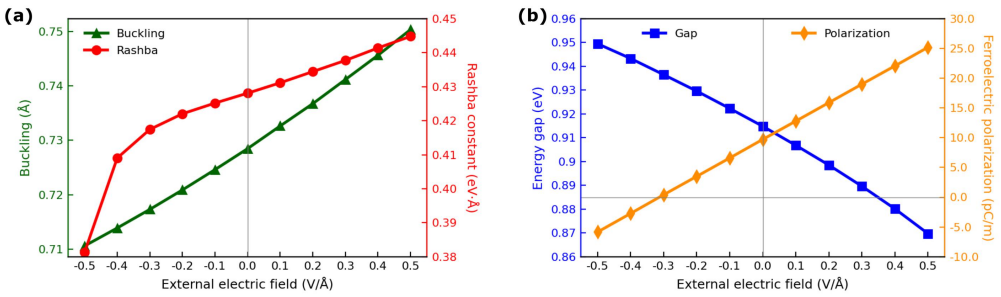


Figure 2: Tunabilities of InAs properties by EEFs: Buckling height, Rashba constant, energy gap, and ferroelectric polarization.

Ultrasensitive Dopamine Detection with Graphene Aptasensor Multitransistor Arrays

Pedro Alpuim[1,3]
Mafalda Abrantes[1,2,3], Diana Rodrigues[2], Telma Domingues[1,3], Patrícia Monteiro[2], Jérôme Borme[1], Luís Jacinto[2]

[1]*International Iberian Nanotechnology Laboratory, 4715-330, Braga, Portugal*
[2]*Life and Health Sciences Research Institute (ICVS), School of Medicine, University of Minho, 4710-057, Braga, Portugal*
[3]*Physics Centre of Minho and Porto Universities (CF-UM-UP), University of Minho, 4710-057, Braga, Portugal*
pedro.alpuim.us@inl.int

Dopamine is a neurotransmitter with critical roles in the human brain and body, and abnormal alterations of its levels underlie brain disorders such as Parkinson's Disease, Alzheimer's Disease, and substance addiction. Herein, we present a novel high-throughput biosensor based on graphene multitransistor arrays (gMTAs) functionalized with a selective aptamer for robust ultrasensitive dopamine detection. The miniaturized biosensor based on multiple electrolyte-gate graphene transistors in an array format was fabricated by high-yield reproducible and scalable methodologies optimized at the wafer level. Our previous works reported DNA detection down to the attomolar level [1] using DNA functionalization and protein detection on a picomolar range [2] using antibody functionalization. With these gMTA aptasensors, we present a record limit-of-detection of 1 aM (10^{-18} M) for dopamine in both undiluted phosphate-buffered saline (PBS) and dopamine-depleted brain homogenate samples spiked with dopamine. The gMTAs display wide sensing ranges in all physiological buffers, up to 100 µM (10^{-8} M), with a 22 mV/decade peak sensitivity in artificial cerebral spinal fluid (aCSF). Furthermore, we show that the gMTAs can detect minimal changes in dopamine concentrations in small working volume biological CSF samples obtained from a mouse model of Parkinson's Disease.

References

[1] Campos et al, ACS Sens, 4 (2019) 286-293.
[2] Fernandes et al., Appl. Surf. Science, 480 (2019) 709-716.

Figures

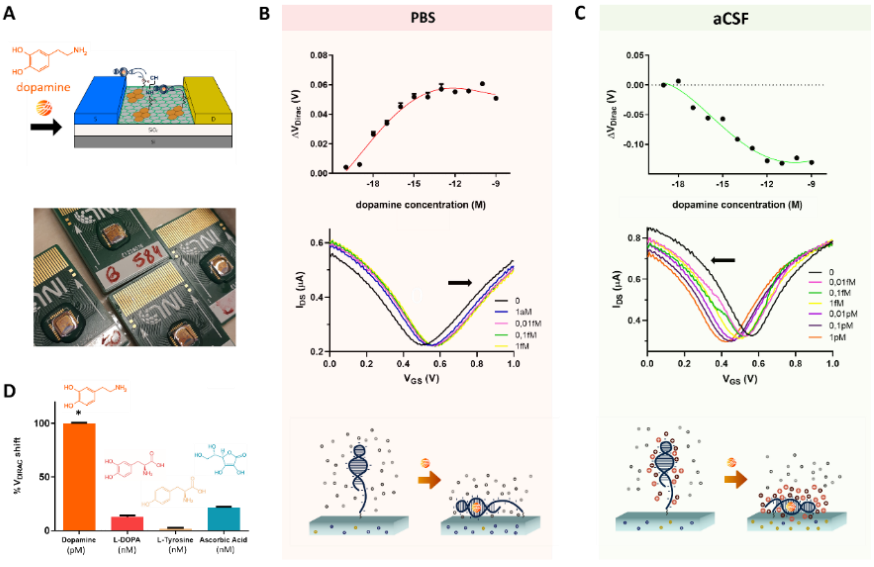


Figure 1: Dopamine detection *in vitro* with gMTAs. (A) Schematic illustration of aptamer structure reorientation close to an EG-gFET. Calibration curves in (B) PBS and (C) aCSF. (D) Comparative responses of gMTAs to 1 pM dopamine, 1 nM L-DOPA, 1nM L-tyrosine and 1 nM ascorbic acid in 1 × PBS.

Substrate Influence on the pH Response of Graphene-Based Field-Effect Transistors

David Kaiser[1], Christof Neumann[1], Zian Tang[1], Maria Küllmer[1], Daniel Hüger[1], Ugo Sassi[2], Matteo Bruna[2], Ana Ballestar[3], Alberto Garcia[4], Chuz Pérez-Roldán[4], Leopold Georgi[5], Thomas Weimann[6], and Andrey Turchanin[1,7] - *[1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany, [2]Nokia Bell Labs, CB3 0FA Cambridge, U.K., [3]Graphene Nanotech, 50018 Zaragoza, Spain, [4]IMB-CNM, 08193 Cerdanyola del Valles, Spain, [5]Research Center for Microperipheric Technologies, Technical University of Berlin, 13355 Berlin, Germany, [6]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany, [7]Jena Center for Soft Matter, 07743 Jena, Germany,* david.kaiser@uni-jena.de, andrey.turchanin@uni-jena.de

We studied the pH response of solution-gated graphene field-effect transistors (GFETs) microfabricated on SiO_2, poly(ethylene 2,6-naphthalate) (PEN) and SiC substrates. To this end, we employ graphene fabricated by (i) chemical vapor deposition (CVD), (ii) epitaxial graphene on SiC, and (iii) nanoporous graphene.[1] GFETs fabricated on PEN substrates and SiO_2 substrates using CVD graphene were also studied after functionalization with amino-terminated carbon nanomembranes (CNMs).[2] We characterize the shift of the transfer characteristic of the devices in a broad range of pH values from 2 – 12. It has been found that the pH response is enhanced by functionalization with NH_2-CNMs,[3] by increasing the surface number density of chargeable groups on the substrates, by increasing the number density of defects in graphene and by increasing the edge length to surface area ratio of the active device area. The obtained results are compared with model calculations that enable to study the substrate influence on the pH response and to correlate it with the defect number density in graphene obtained from the Raman spectroscopy.

References

[1] C. Neumann, D. Kaiser, M. J. Mohn, M. Füser, N.-E. Weber, O. Reimer, A. Gölzhäuser, T. Weimann, A. Terfort, U. Kaiser, A. Turchanin, ACS NANO 13 (2019) 7310-7322

[2] M. Woszczyna, A. Winter, M. Grothe, S. Wundrack, R. Stosch, T. Weimann, F. Ahlers, A. Turchanin, ADVANCED MATERIALS 26 (2014) 4831-4837

[3] D. Kaiser, Z. Tang, M. Küllmer, C. Neumann, A. Winter, R. Kahle, L. Georgi, T. Weimann, M. Siegmann, S. Gräfe, A. Centeno, A. Zurutuza, A. Turchanin, APPLIED PHYSICS REVIEWS 8 (2021) 031410

Figures

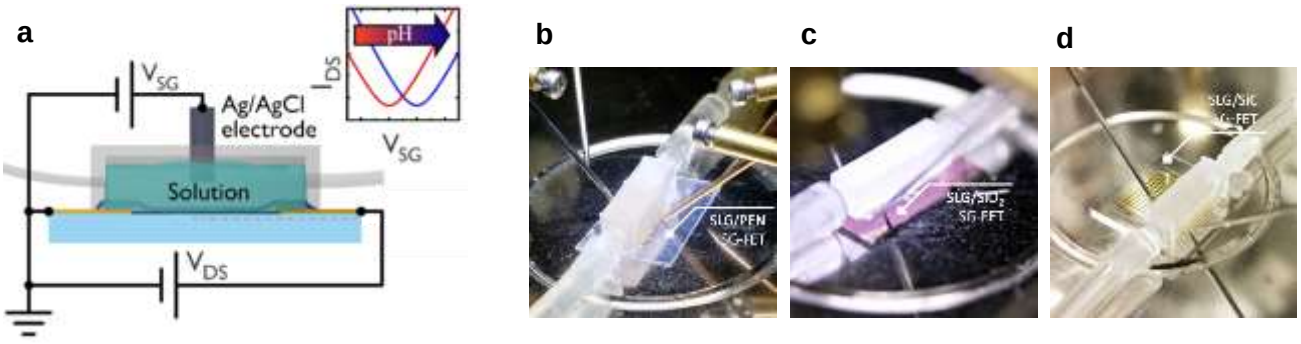


Figure 1: (a) Schematic diagram of the GFET device. (b) An image of the chip with an attached microfluidic channel on a CVD-SLG/PEN device. Probe needles are contacting the source and drain. (c, d) Similar images of GFET devices fabricated on SiO_2 and SiC substrates.

Improving amine-functionalised biosensors through understanding the bonding mechanisms for CVD-grown graphene

Elizabeth J. Legge[1]
Muhammad M. Ali,[3] Hina Y. Abbasi,[3] Benjamen Reed,[1] Barry Brennan,[1] Lidija Matjačić,[1] Zari Tehrani,[3] Vlad Stolojan,[2] S. Ravi P. Silva,[2] Owen J. Guy,[3,4] Andrew J. Pollard[1]
1. National Physical Laboratory, Teddington TW11 0LW, U.K
2. Advanced Technology Institute, University of Surrey, Guildford GU2 7XH, U.K
3. Centre for NanoHealth, College of Engineering, Swansea University, Swansea SA2 8PP, UK
4. Department of Chemistry, College of Science, Swansea University, Swansea, SA2 8PP, UK
elizabeth.legge@npl.co.uk

Due to graphene's desirable properties, such as the ease of chemical functionalisation, high electrical conductivity, and high surface area, graphene biosensors are a rapidly growing area of research. To achieve high selectivity, graphene must be functionalised with appropriate molecules, such as amine groups which are required to bind to antibodies then used for the detection of biomarkers. However, there are a range of possible methods to functionalise graphene with amine, and the optimal method is still unclear. Typically, covalent functionalisation is more durable, due to the greater bond strength, but this can disrupt the sp^2-hybridised carbon structure and thus degrade the electrical conductivity. Non-covalent functionalisation is expected to be less durable but maintains the sp^2 lattice and electrical conductivity. We have investigated the differences between a covalent functionalisation, with phenyl amine groups bound to graphene, and a non-covalent functionalisation, with poly(1,5-diaminonaphthalene) (pDAN) layers on graphene. The I_D/I_G ratio from the Raman spectra of graphene can be used as an indication of the level of disorder, and therefore can approximate the level of sp^3 defects due to molecules bound to the graphene. Consequentially, it is typically used to confirm the success of a functionalisation process. However, Bissett, M. A *et al*. [1] and Knirsch, K. C. *et al*. [2] both previously reported unexpected changes in the I_D/I_G, where the I_D/I_G increased with functionalisation, but decreased again after an external force, due to strain and a chemical process respectively. Greenwood, J. *et al*. [3] also reported changes in the Raman spectra after scanning tunnelling microscopy (STM) on functionalised highly oriented pyrolytic graphite (HOPG). The work presented here on amine-functionalised, chemical vapor deposition (CVD) graphene shows that while covalent functionalisation is usually the method of choice, it is not necessarily preferable over non-covalent alternatives. Removal of functional groups from CVD graphene with contact-mode atomic force microscopy (AFM) explains unexpected changes in the Raman spectra and suggests the durability of covalent functionalisation can be similar or worse than non-covalent functionalisation. Utilising a combination of imaging techniques, we demonstrate some imaging challenges and the importance of using different analytical techniques to investigate the physicochemical properties of biosensors. Our characterisation combines the use of contact-mode and tapping-mode AFM, Raman spectroscopy and time-of-flight secondary ion mass spectrometry (ToF-SIMS). We have also shown how different functionalisation processes affect the operation of a pH sensor, showing a higher sensitivity for the non-covalent process compared to the covalent process.

References

[1] M. A. Bissett, M. Tsuji, and H. Ago, J. Phys. Chem. C, 117 (2013) 3152
[2] K. C. Knirsch, R. A. Schäfer, F. Hauke, and A. Hirsch, Angew. Chem., Int. Ed., 55 (2016) 5861
[3] J. Greenwood, T. H. Phan, Y. Fujita, Z. Li, O. Ivasenko, W. Vanderlinden, H. Van Gorp, W. Frederickx, G. Lu, K. Tahara, Y. Tobe, H. Uji-I, S. F. L. Mertens, and S. De Feyter, ACS Nano, 9 (2015) 5520

Binding kinetics and biological recognition of nanobodies functionalized on graphene derivatives for immunosensing applications

Daniel Melendrez
Piramon Hampitak, Maria Iliut, Ben Spencer, Thomas Jowitt, Aravind Vijayaraghavan
University of Manchester, Oxford Road, Manchester, United Kingdom
daniel.melendrezarmada@manchester.ac.uk

The development of nanobodies for therapeutic and diagnostic applications has attracted the attention of a number of biomedical research groups due to their smaller size and ease of production on a large scale. They can selectively bind to a specific antigen like the conventional antibody but the size of nanobody molecule is much smaller, only at about 12–15 kDa while that of a common antibody is approximately 150–160 kDa. They are considered effective protein receptors because of their single antigen-binding site and fewer possible orientations compared to the conventional antibody, however, their bio-interface functionalization on solid platforms is still challenging. In this study, we have explored methods to functionalize nanobodies and graphene derivatives based on physical adsorption, amine crosslinking and streptavidin (SA)-biotin interaction. The graphene-based solid supports require functionalization with molecular receptors to promote specific binding to the target molecules. We have previously reported an effective method to obtain a film of denatured BSA (dBSA) on reduced graphene oxide (rGO) and its application in immunosensing [1,2]. We have also demonstrated the development and use of graphene-coated (G-) quartz crystal microbalance (QCM) sensor chips to study interactions between biomolecules and graphene surfaces [1], [3,4] and the application of G-QCM in clinical diagnostics [2]. The nanobody against lysozyme was used as a model protein pair. The QCM-D technique was used to monitor the adsorption of the nanobody on different surfaces, its biomolecular recognition and selectivity against other proteins and animal serum. rGO-biotBSA-SA was used as a sensing platform in this study (Figure 1). The kinetics dissociation (KD) factor was determined from the QCM-D results and compared with those from Surface Plasmon Resonance (SPR) for validation. This sensing surface exhibited good specificity and high sensitivity toward the target, with a detection limit of 0.5 µg/ml, and capable of detecting an analyte in serum media. The KD value obtained from this sensing platform is 545 nM which is comparable to the standard value from the SPR technique, validating its feasibility to be used as the basis of a highly selective and reliable immunosensing device.

References

[1] P. Hampitak et al., Carbon N. Y., vol. 165, 2020, pp. 317–327
[2] P. Hampitak et al., ACS Sensors, vol. 5, no. 11, 2020, pp. 3520–3532,
[3] D. A. Melendrez et al., Nanoscale, vol. 10, no. 5, 2018, pp. 2555–2567
[4] D. Meléndrez, et al., Anal. Chim. Acta, vol. 1156, 2021, p. 338329

Figures

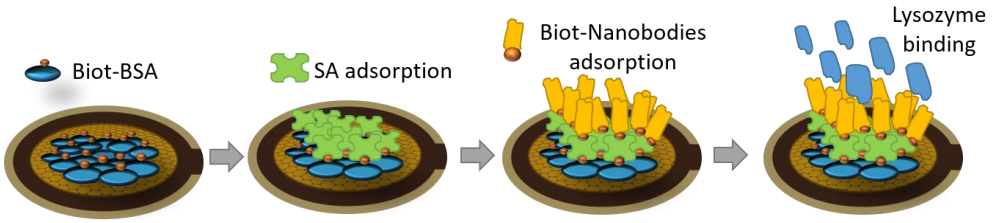


Figure 1: *Sensing surface preparation for quantifying lysozyme in cow serum. The gold electrode from a QCM crystal is coated with a thin layer of GO then thermally reduced. Injection sequences are shown.*

Biomolecules on graphene flatlands: Unique interactions and transduction at graphene-based field-effect biosensors

Vivek Pachauri[1]
D. Storelli[1], D. Khan[2], S. Leisten[1], H. Amiri[1], A. Nikookhesal[1], G. Figueroa-Miranda[2], A. Singh[1], X.T. Vu[1], A. Offenhäusser[2], D. Mayer[2], S. Ingebrandt[1]
1. Institute of Materials in Electrical Engineering 1, RWTH Aachen University, Sommerfeldstrasse 24, 52074 Aachen, Germany
2. Institute of Biological Information Processing, Bioelectronics (IBI-3), Forschungszentrum Jülich GmbH, Jülich, Germany
pachauri@iwe1.rwth-aachen.de

Use of graphene-based materials (GBMs) as transducers of biomolecular interactions has been at the forefront for development of future diagnostics applications. Availability of highest surface-area with respect to material volume and efficient charge-transport in GBMs while facilitate the efficient charge transduction, a variety of heterogeneities at such two-dimensional interfaces pose unique challenges for real-use as diagnostics solutions, especially towards fulfilling clinical requirements.[1,2]

In this work, we highlight such interfacial heterogeneities of GBMs deployed as field-effect based biosensors. Other than the substrate-interactions, influences from chemical surface-modification, biofunctionalization, critically influence the charge-carrier transport in such electrical devices. Over past years, our studies of graphene-based field-effect devices have focused on optimization of such two-dimensional bionanointerfaces and make effort towards detailed understanding of electrical transduction of dynamic biological interactions. In particular, we present an updated analytical model for such field-effect based bionanosystems that are able to detect and delineate changes in biomolecular characteristics such as surface charge and size. Specific examples of biomolecular systems include thickness changes in DNAs and DNA-protein interactions.

References

[1] V. Pachauri, S. Ingebrandt, Essays in Biochemistry *2016*, 60(1), 81-90
[2] S. Kumar, T. Kurkina, S. Ingebrandt, V. Pachauri*, Organic Bioelectronics for Life Science and Healthcare 2019, 56, 185-242

Figures

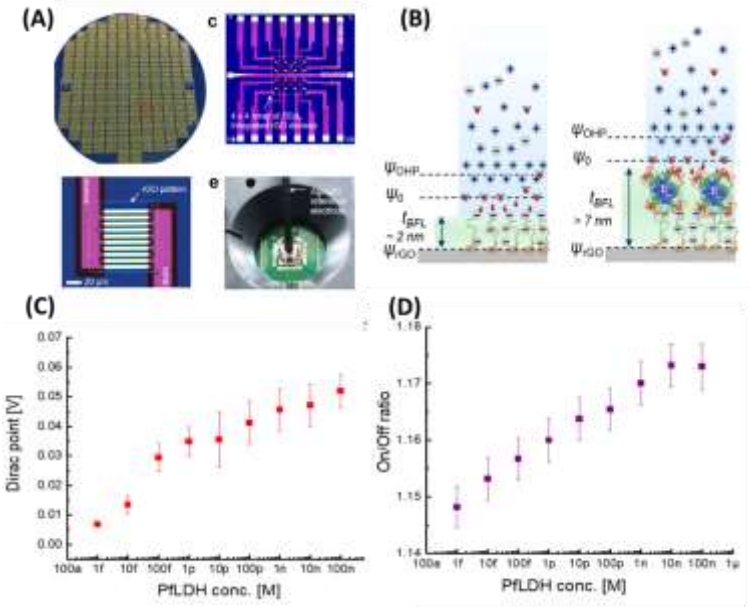


Figure 1: System integrated field-effect biosensors based on GBMs (A) deployed for monitoring of complex biomolecular interactions such as aptamers-proteins (B) display unique electrical transductions related to changes in charges (C) and sizes (D) at the interface.

Exotic Physics of Indium Selenide Based van der Waals Heterostructures

Nilanthy Balakrishnan[1]
Zakhar R. Kudrynskyi[2], David Buckley[3], Eli Castanon[3,4], Shihong Xie[2,5], Anubhab Dey[2], Wenjing Yan[2], Tom Vincent[3], Zakhar D. Kovalyuk[6], Oleg Kolosov[4], Olga Kazakova[3], Alexander Tzalenchuk[3], Oleg Makarovsky[2], Kaiyou Wang[5], Amalia Patanè[2]
[1]School of Chemical and Physical Sciences, Keele University, Keele, ST5 5BG, UK
[2]School of Physics and Astronomy, The University of Nottingham, Nottingham, NG7 2RD, UK
[3]National Physical Laboratory, Hampton Road, Teddington, TW11 0LW, UK
[4]Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK
[5]State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, People's Republic of China
[6] Institute for Problems of Materials Science, The National Academy of Sciences of Ukraine, Chernivtsi Branch, Chernivtsi 58001, Ukraine
n.balakrishnan@keele.ac.uk

The pressing demand for miniaturize devices can be fulfilled by two-dimensional (2D) semiconducting materials. Among the 2D semiconducting materials, indium selenide (InSe) compounds are attracting great attention due to their desirable electronic and optical properties [1-2]. InSe compounds can exist with different stoichiometries (e.g. InSe, In2Se3 and In4Se3) and polytype phases (α, β, γ, etc.), providing band gaps tuneable from the near-infrared to the visible range (1.2 - 2 eV) of the electromagnetic spectrum [2], a high electron mobility at room temperature (> 0.1 m2 /Vs) [1], room temperature ferroelectricity [3] and strong carrier correlations in atomically thin layers due to an inverted "Mexican hat" valence band 4].

Here, we review our recent work on In-Se based van der Waals heterostructures of interest for optoelectronics, thermoelectrics and nanoelectronics. Both InSe/GaSe and InSe/In_2O_3 heterojunctions exhibit room temperature electroluminescence and spectral response from the near-infrared to the visible and near-ultraviolet ranges. This demonstrates the technological potential of heterostructures based on InSe with an optical response over an extended wavelength range [5-6]. On the other hand, the nanoscale thermal properties of InSe layers shows an anomalous low and anisotropic thermal conductivity, which is smaller than that of low-κ dielectrics, such as silicon oxide [7]. The thermal response of free-standing InSe layers and layers supported by a substrate, reveals the role of interfacial thermal resistance, phonon scattering, and strain. These thermal properties are critical for future technologies, such as field-effect transistors that require efficient heat dissipation or thermoelectric energy conversion with both low thermal conductance and high electron mobility 2D materials, such as InSe. Furthermore, we report on the ferroelectric semiconductor α-In_2Se_3 embedded between two single-layer graphene electrodes. We show how the ferroelectric polarization of the In_2Se_3 layer can modulate the transmission of electrons across the graphene/In_2Se_3 interface, leading to memristive effects that are controlled by an applied voltages and/or by light [8].

References

[1] D. A. Bandurin, *et al*., Nat. Nanotechnol., (2017)**12**, 223-7.
[2] W. Huang, *et al*., Cryst. Eng. Comm., (2016) **18**, 3968-84.
[3] C. Zheng, *et al*., Sci. Adv., (2018) **4**, eaar7720.
[4] L. Debbichi, *et al*., J Phys Chem Lett, (2015) **6**, 3098-103.
[5] N. Balakrishnan, *et al*., Adv. Opt. Mater. (2015) **2**, 1064-9.
[6] N. Balakrishnan, *et al*., 2D Mater., (2017) **4**, 025043.
[7] D. Buckley, *et al*., Adv. Funct. Mater., *2020) **31**, 2008967.
[8] S. Xie, *et al*., 2D Mater., (2021) **8**, 045020.

Optoelectronic properties of encapsulated 2d-semiconductors

Artur Erbe[1]
Himani Arora[1], Tommaso Venanzi[2], Zahra Fekri[1], Phanish Chava[1], Yordan M. Georgiev[1], Kenji Watanabe[3], Takashi Taniguchi[3], Manfred Helm[1], James C. Hone[4]
[1]*Helmholtz-Zentrum Dresden-Rossendorf, Germany,* [2]*University of Rome Sapienza, Italy,* [3]*National Institute for Materials Science, Japan,* [4]*Columbia University, USA*
a.erbe@hzdr.de

Abstract

Two-dimensional semiconductors provide fascinating prospects for optoelectronics, because they combine charge transport with high mobility and tuneable optical gaps. Many of those materials are, however, sensitive to air and other environmental influences. Examples of such materials are InSe, GaSe, and black phosphorus (BP). Therefore, it is essential to encapsulate these materials in order to stabilise their properties for extended times. We have shown that the materials mentioned above are stable when encapsulated with thin layers of hexagonal boron nitride (hBN), and can, at the same time, be electrically contacted using via contacts created through the hBN-layers by dry etching. We show how the optical [1] and optoelectronic [2] properties of the semiconductor are affected by the presence or absence of the encapsulating material. We also demonstrate that we can operate the resulting structure as field-effect transistor (FET). FETs with BP as semiconducting material are ambipolar, making them candidates for reconfigurable transistors with high mobility.

References

[1] T. Venanzi, H. Arora, A. Erbe, A. Pashkin, S. Winnerl, M. Helm, and H. Schneider, *Exciton Localization in MoSe2 Monolayers Induced by Adsorbed Gas Molecules*, Appl.~Phys.~Lett. **114**, 172106 (2019).

[2] H. Arora, Y. Jung, T. Venanzi, K. Watanabe, T. Taniguchi, R. Hübner, H. Schneider, M. Helm, J. C. Hone, and A. Erbe, *Effective Hexagonal Boron Nitride Passivation of Few-Layered InSe and GaSe to Enhance Their Electronic and Optical Properties*, ACS Appl. Mater. Interfaces, **11** 43480 (2019).

Figures

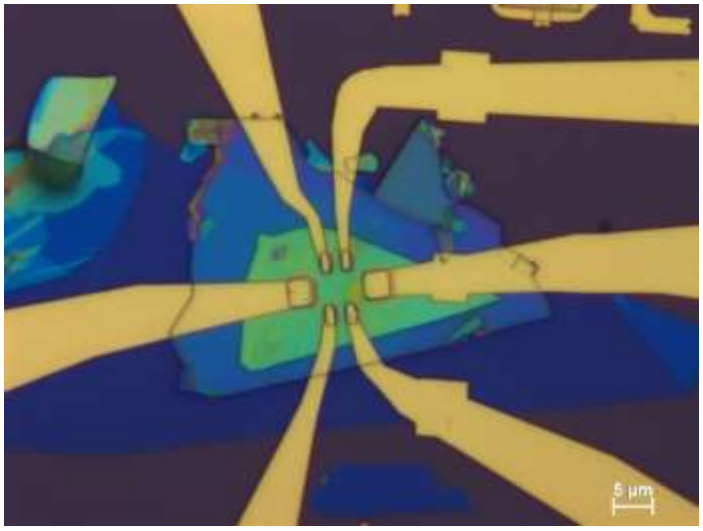


Figure 1BP flake contacted by via contacts in Hall-bar geometry

Collective modes and screened interactions in double layers of massless Dirac fermions

Tohid Farajollahpour[1, 2]
Andrea Secchi[3], Iacopo Torre[4], Frank H.L. Koppens[4, 5] and Marco Polini[2, 4, 1]
1) Istituto Italiano di Tecnologia, graphene Labs, Via Morego 30, I-16163 Genova, Italy
2) Dipartimento di Fisica dell'Università di Pisa, Largo Bruno Pontecorvo 3, I-56127 Pisa, Italy
3) Centro S3, CNR - Istituto di Nanoscienze, via G. Campi 213/A, I-41125 Modena, Italy
4) ICFO-Institut de Ciències Fotòniques, The Barcelona Institute of Science and Technology, Av. Carl Friedrich Gauss 3, 08860 Castelldefels (Barcelona), Spain
5) ICREA-Institució Catalana de Recerca i Estudis Avançats, Passeig Lluís Companys 23, 08010 Barcelona, Spain
Tohid@iit.it
Marco.Polini@unipi.it

We present a detailed theoretical study of collective modes and screened interactions in double layers of massless Dirac fermions with tunable Fermi velocities. By fixing the Fermi velocity of the carriers of one of the two layers to a reference value, we study the dependence of all the relevant response functions and their poles on the ratio between the Fermi velocity of the other layer and the reference value. We employ the random phase approximation to obtain all our results, finding in particular a compact analytical expression for the acoustic plasmon group velocity. We compare analytical results with numerical results for the loss function, finding excellent agreement. We also quantify the damping rate of acoustic modes, highlighting the role of a "pseudo gap" phase in which the acoustic plasmon lies inside the electron-hole continuum of the faster fermions, and outside the electron-hole continuum of the slow fermions. We finally illustrate the role of the acoustic plasmon in altering effective electron-electron interactions. We hope that this theoretical study will stimulate the experimental search of acoustic plasmons in systems of "slow" Dirac fermions, such as those that are hosted by twisted bilayer graphene.

Figure

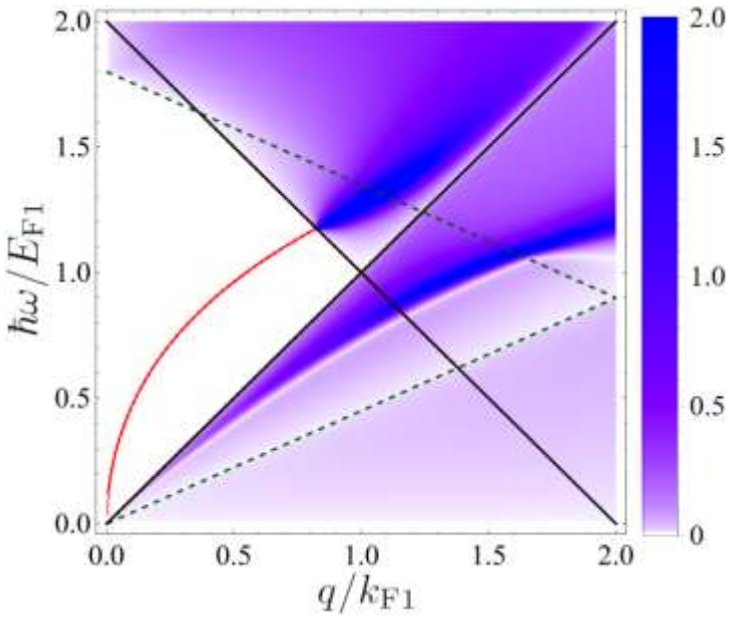


Figure 1: Optical and acoustic plasmon dispersions as functions of wave vector in a double layer system of graphene encapsulated by hexagonal Boron Nitride. The black solid lines illustrate the regions of reference layer while dashed dark green lines display the regions related to slow fermions. The acoustic plasmon lies inside the electron-hole continuum of the faster fermions, and outside the electron-hole continuum of the slow fermions.

References

[1] R. E. V. Profumo, R. Asgari, M. Polini, and A. H. Mac- Donald, Phys. Rev. B 85, (2012) 085443.
[2] G. E. Santoro and G. F. Giuliani, Phys. Rev. B 37, (1988) 937.
[3] G. Borghi, M. Polini, R. Asgari, and A. H. MacDonald, Phys. Rev. B 80, (2009) 241402.

Acknowledgment

This work was supported by the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 881603 - GrapheneCore3.

Growth, Intercalation and Tunnel Spectroscopy of Cobalt Nanodots Bellow Graphene on SiC(0001)

Yann GIRARD
S. Benbouabdellah, O. Chahib, C. Chacon, A.Bellec, V. Repain, J. Lagoute, Y. J. Dappe, Wei-Bin Su.
Université Paris Cité, CNRS, Laboratoire Matériaux et Phénomènes Quantiques, 75013 Paris, France.
yann.girard@u-paris.fr

The intercalation of cobalt between a graphene layer and the buffer layer on SiC(0001) leads to three different situations depending on the local atomic concentration: isolated atoms [1], clusters of a few atoms [2][3] and nanodots (see figure). STM images shows, on the one hand, that the clusters have a very narrow size distribution and a single atomic height and, on the other hand, that the nanodots have sizes of a few tens of nm and heights compatible with one to three cobalt planes covered by one graphene plane as evidenced on the figure by two typical "flower" defects of graphene [4]. These nanodots present moirés whose non-hexagonal symmetry is currently not understood. Spectroscopic measurements of conductance and work functions, see figure, confirm that graphene is n-doped without cobalt [5] and that it loses its doping progressively for an intercalation of isolated atoms to a quasi-neutrality for the nanodots, cobalt acting as a p-dopant. Correlatively, the work function increases from 4.25 eV for a cobalt-free graphene monolayer, a value comparable to that measured by ARPES [6], to 4.6 eV on the nanodots. The study of Image Potential States by STS shows that the asymmetry of the two first peaks seen on graphene is absent on nanodots. DFT calculations of the band structures of graphene multilayers on SiC confirm the opening of a gap at the K-point in the solid states for graphene bilayers and trilayers, which allows to compare the calculated densities of states with the experimental results and, although indirectly, to allow a more accurate interpretation of those results.

References

[1] T. Eelbo et al. Phys. Rev. B 87 (**2013**) 205443
[2] L.H. de Lima, R. Landers, A. de Siervo, Chem. Mater. 26 (**2014**) 4172
[3] Y. Zhang, H. Zhang, Y. Cai, J. Song, P. He, Nanotechnol. 28 (**2017**) 075701
[4] Q. Berrahal, et al. Carbon 170 (**2020**) 174
[5] J. Ristein, S. Mammadov, Th. Seyller, Phys. Rev. Lett. 108 (**2012**) 246104
[6] S. Mammadov et al., 2D Mater. 4 (**2017**) 015043

Figure

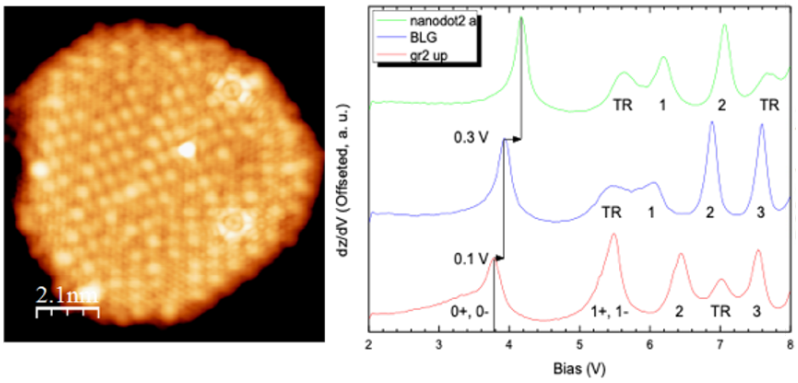


Figure : STM image of a 2D cobalt nanodot intercalated between a monolayer graphene and a buffer layer on SiC(0001). Spectroscopy of image potentials surface states revels a Co p-doping effect.

Non trivial doping evolution of electronic properties in an aliovalent transition metal dichalcogenide alloy.

Rishav Harsh[1]
Wen Wan[1], Darshana Wickramaratne[2], Paul Dreher[1], I. I. Mazin[3] and Miguel M. Ugeda[1,4,5]
[1]*Donostia International Physics Center, Paseo Manuel de Lardizabal, 4, Donostia-San Sebastian, Spain*
[2]*Center for Computational Materials Science, U.S. Naval Research Laboratory, Washington, DC 20375, USA*
[3]*Department of Physics and Astronomy, Quantum Science and Engineering Center, George Mason University, Fairfax, VA 22030, USA*
[4]*Centro de Física de Materiales (CSIC-UPV-EHU), Paseo Manuel de Lardizábal 5, 20018 San Sebastián, Spain.*
[5]*Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain.*
rishav.harsh@gmail.com

Transition metal dichalcogenides (TMDs) offer unprecedented versatility to engineer two dimensional (2D) materials with tailored properties to explore novel structural and electronic phase transitions. The possibility of substituting one of the atomic elements by different species has greatly expanded the potential of this family of 2D materials. So far, isovalent group VI TMD alloys (such as $Mo_\delta W_{1-\delta}S_2$, $WS_{2(1-\delta)}Se_{2\delta}$, etc.) have received most of the attention due to the possibility to tune the electronic and optical bandgaps[1,2]. Regarding aliovalent TMD alloys where TMs with different valences are involved, most efforts have focused on the dilute limit. In this talk, an experimental and theoretical investigation of the aliovalent TMD alloy $Nb_{1-\delta}Mo_\delta Se_2$ is presented[3]. We have successfully synthesized high-quality monolayers across the entire $0 < \delta < 1$ range, and examine the evolution of the atomic and electronic structure using low-temperature (0.34 – 4.2 K) STM/STS. Our measurements enable us to explore the effect of electron doping on the monolayer $NbSe_2$ and track its impact on the electronic bands. Particularly, the semiconductor to metallic transition, the robustness of charge density waves and evolution of superconductivity is discussed for this system.

References

[1] Zheng et.al., ACS Nano, 2014, 8,7, 7130-7137
[2] Mann et.al., Advanced Materials, 2014, 26, 9, 1399-1404
[3] Wan et.al., (article submitted)

Figures

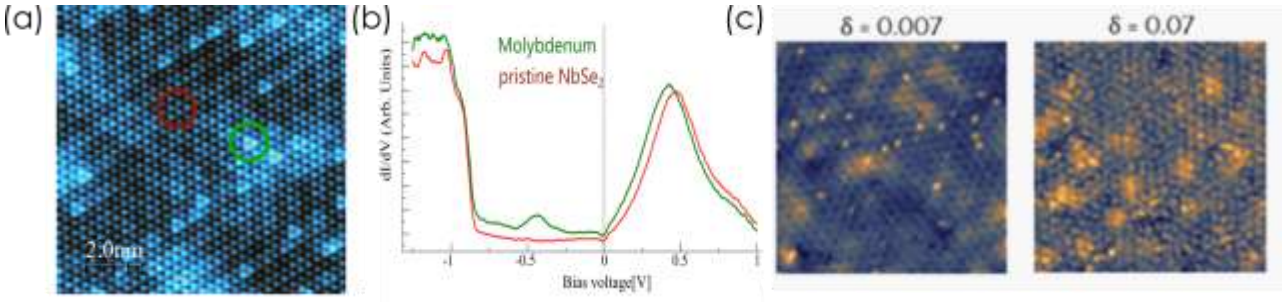


Figure 1: Identifying a Mo defect in $NbSe_2$ lattice by (a) STM topography and (b) the corresponding STS comparison. (c) High-resolution STM images showing charge density waves for different Mo concentrations (left shows for 0.7 % and right one for 7 % Mo doping)

Time-resolved Plasmons and Magneto-plasmons in Epitaxial Graphene

Jan Kunc[1]
Mykhailo Shestopalov[1], Bohdan Morzhuk[1], Václav Dědič[1], Vaisakh C. Paingad[2], Ivan Rychetský[2], Petr Kužel[2], Ivan Mohelský[3], Milan Orlita[1,3]
[1]*Charles University, Faculty of Mathematics and Physics, Institute of Physics, Ke Karlovu 5, CZ-121 16, Prague 2, Czech Republic*
[2]*Institute of Physics of the Academy of Sciences, Na Slovance 2, Prague 8, 18221, Czech Republic*
[3]*LNCMI-EMFL, CNRS UPR3228, Univ. Grenoble Alpes, Univ. Toulouse, Univ. Toulouse 3, INSA-T, Grenoble and Toulouse, France*
kunc@karlov.mff.cuni.cz

We present a magneto-optical and time-resolved terahertz spectroscopy study of plasmons in as-grown graphene[1] and lithographically defined nanoribbons. We compare magneto-plasmons in regular oxygen-etched, gold-protected, and gold-defined ribbons[2]. We experimentally show a discrepancy with theoretically predicted plasmon resonances. We explain the experimental observation within a core-shell model. The model considers a realistic lateral distribution of dielectric surroundings of graphene flakes and nanoribbons. A weak polarization dependence and high structural anisotropy of SiC substrate exclude the role of SiC step bunching as a primary source of translational symmetry breaking. We also show the temporal evolution of plasmon decay. The plasmon decay results in the formation of hot carriers, and we describe this process by a simple model allowing us to determine hot carriers' temperature and time evolution of energy dissipation.

References

[1] V. C. Paingad et al., Ultrafast Plasmon Thermalization in Epitaxial Graphene Probed by Time-Resolved THz Spectroscopy, Advanced Functional Materials 31, 2105763 (2021)
[2] M. M. Jadidi et al., Tunable Terahertz Hybrid Metal-Graphene Plasmons, Nano Letters 15, 7099 (2015).

Figures

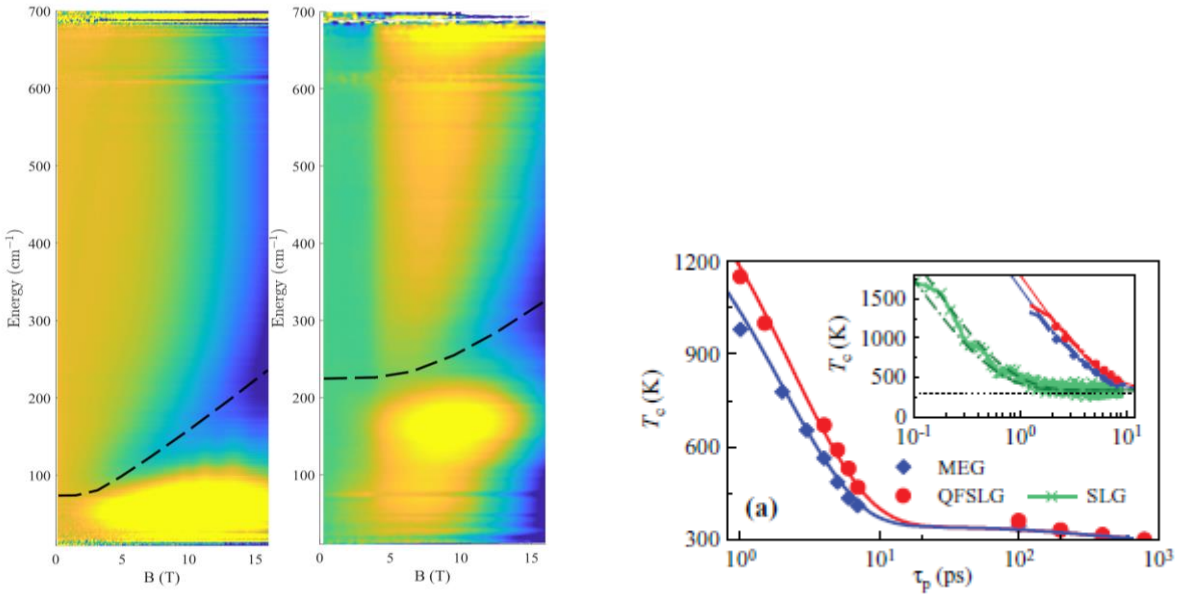


Figure 1: Magneto-plasmons in (left) 3000 nm and (middle) 350 nm wide graphene nanoribbons. (right) Temporal evolution of hot carriers' temperature caused by energy dissipation of decaying plasmon excitations[1].

Hot electron cooling dynamics in graphene/hBN van der Waals heterostructures

Jake Dudley Mehew[1]
Alexander Block,[1] Jaime Díez Mérida,[2] Rafael Luque Merino,[2] Dmitri K. Efetov,[2] and Klaas-Jan Tielrooij[1]
[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, 08193 Barcelona, Spain*
[2] *ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain*
Jake.mehew@icn2.cat

Van der Waals heterostructures allow for the layer by layer design of complex material systems in which new physics and novel device properties can be studied. Electronic and optoelectronic applications will benefit from these enhanced properties providing that the nature of heat flow at the nanoscale is well understood. [1,2,3,4]

In this work, we study hot electron cooling dynamics at pn-junctions electrostatically formed in heterostructures of mono- and bi-layer graphene encapsulated in hexagonal boron nitride (hBN). Using time-resolved photocurrent measurements, we find that the cooling time constant varies from 1-100 ps as we modify the number of graphene layers, Fermi level and lattice temperature.

These results are particularly relevant for applications in thermal management, photodetection and high speed electronics.

References

[1] Dong Sun et al, Nat. Nano., 7 (2012) 114
[2] Matt W. Graham et al, Nat. Physics, 9 (2013) 103
[3] Klaas-Jan Tielrooij et al, Nat. Nano., 13 (2018) 41
[4] Alexander Block et al, Nat. Nano., 16 (2021) 1195

Active Thermal Imaging for Carbon and Metal thin films

Giulia Mirabello[1]
Christoph Geers[2], Alke Fink[1], Mathias Bonmarin[3], Marco Lattuada[1]
[1] *University of Fribourg,* [2] *NanoLockin GmbH,* [3] *Zürich University of Applied Sciences*
giulia.mirabello@unifr.ch

A large variety of methods exists to analyze inorganic engineered (nano)materials in thin films. Many standard analyses can offer information on the film homogeneity and film thickness. However, techniques such as electron microscopies and atomic force microscopy are often not statistically significant because they allow investigating only a small portion of the sample, and often require a complex sample preparation (e.g., TEM lamella preparation with a focused ion beam) and highly specialized users. Moreover, measurements become unreliable when the film thickness is below tens of nm (e.g., interferometry) and above hundreds of µm. [1, 2] Ellipsometry can investigate very thin films, but requires complex models to interpret the results, while other commercially available spectroscopic instruments fail to investigate materials made of light elements such as carbon.[3]
Here, we present a new non-destructive technique based on lock-in-thermography (LIT) to determine the thickness and homogeneity of carbon and metal thin films. LIT measures and quantifies the heat produced by carbon-based nanomaterials exposed to amplitude-modulated light stimulation.[4, 5] This heat can be recorded with an infrared camera and is then processed by a specially developed LIT algorithm to yield 2D images, which can be used to analyzing the uniformity of samples.[6, 7] The presented model allows the quantitative determination of the film thickness. The great advantage of our novel approach is the fast, easy and accurate analysis of carbon thin films, without requiring complicated sample preparation. The approach was also validated with gold and platinum thin films of different thicknesses.

References

[1] SW Kim, GH Kim, Appl Opt., 28 (1999) 5968-5973
[2] T Jo, KR Kim, SR Kim, and HJ Pahk, J. Opt. Soc. Korea, 3 (2014) 236-243
[3] G Walter, E Berretti, M Innocenti, and A Lavacch, Mater. Proc., 1 (2020)
[4] K Jiang, DA Smith, A Pinchuk, J. Phys. Chem. C, 55 (2013) 27073–27080
[5] D Jaque, L Martínez Maestro et. al, Nanoscale, 6 (2016) 9494-9530
[6] L Steinmetz, J Bourquin, et. al, Nanoscale, 12 (2020) 17362
[7] L Steinmetz, C Geers et. al, J. Phys. Chem. C, 10 (2021) 5890-5896

Figures

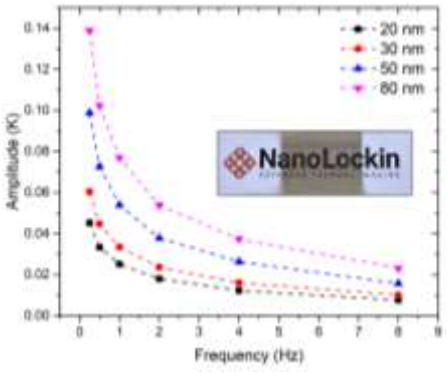


Figure 1: Graph of the measured temperature amplitude of different carbon deposited films as a function of the modulation frequency of the thermal stimulation. The inset shows a picture of a typical carbon films investigated in this work.

Self-organized, linear hydrocarbons as a major source of surface contamination on van der Waals materials

András Pálinkás[1]
György Kálvin[1], Konrád Kandrai[1], Gergely Németh[2], Miklós Németh[3], Áron Pekker[2], József S. Pap[3], Péter Petrik[1], Katalin Kamarás[2], Levente Tapasztó[1] and Péter Nemes-Incze[1]
[1]*Centre for Energy Research, Institute of Technical Physics and Materials Science, 1121 Budapest, Hungary*
[2]*Wigner Research Centre for Physics, 1121 Budapest, Hungary*
[3]*Centre for Energy Research, Institute for Energy Security and Environmental Safety, 1121 Budapest, Hungary*
andras.palinkas@ek-cer.hu

There is a rule of thumb in surface science which says: 'Once a freshly prepared, clean surface is brought out from UHV to open lab air, it becomes contaminated with water, hydrocarbons, other vapors, etc.' Here we show by complementary, high-resolution atomic force (PeakForce QNM and LFM) and scanning tunneling microscopy (STM) that after a few days of exposure to ambient air, a self-organized, crystalline lattice of molecules is formed on the surface of van der Waals (vdW) materials. The molecules self-organize into parallel stripes with 4 ± 1 nm periodicity on several, distinct surfaces: graphene, graphite, hBN, MoS_2. By low-temperature STM measurements, we have resolved the atomic structure of the molecules on graphite (see Fig1c) and in combination with infrared spectroscopy, we reveal that the molecules are linear, saturated hydrocarbons with a length of 20-24 atoms (see Fig2), most likely normal alkanes. We show a direct causal link between the self-organized stripe structure of the molecule layer and the well-known [1], but yet unexplained friction anisotropy domains measured on vdW materials (see Fig1a-b). Additionally, we found that the local orientation of the molecular layer can be switched on purpose between the three distinct zigzag crystal directions. Repeated scans along the desired direction by contact mode AFM enables the redrawing or "nano-patterning" [2] of the friction domains on vdW-materials. Beyond the manipulation of the molecular lattice, we show details of the growth dynamics and the controlled desorption through annealing. Our work is a major step towards understanding the origin of the ubiquitous hydrocarbon contamination on vdW crystals and its effects on their measured properties.

References

[1] Gallagher, P. et al. Nat. Commun. 7 (2016) 10745
[2] Verstraete, L. & De Feyter, S., Chem. Soc. Rev. 50 (2021) 5884–5897

Figures

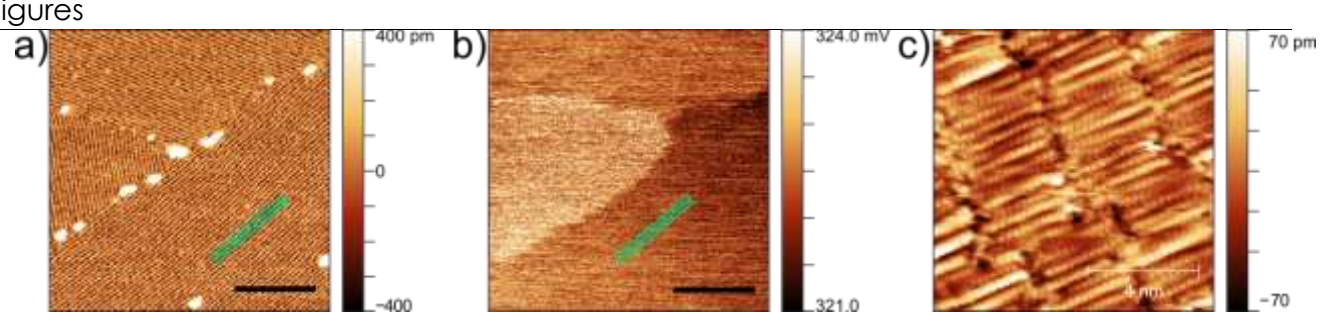


Figure 1: a) Parallel stripes of 4 nm periodicity on the surface of a graphene/hBN heterostructure (PeakForce AFM Topography). **b)** Friction force signal of the same region as in a). **c)** Low temperature STM image of the airborne monolayer on graphite.

Generation of graphene nano-sieves by ultrashort laser pulses

J. Parthenios
S. Katsiaounis[1,2], N. Chourdakis[1], J. Parthenios[1] and K. Papagelis[1,3]
[1]*Foundation of Research and Technology Hellas, Institute of Chemical Engineering Sciences, P.O. Box 1414, GR-26504 Patras (Greece)*
[2]*Department of Physics, University of Patras, GR-26504 Patras (Greece)*
[3]*School of Physics, Department of Solid-State Physics, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece*
jparthen@iceht.forth.gr, kpapag@physics.auth.gr

Femtosecond lasers have become an advanced tool in the field of micromachining due to their extensive use for the processing of advanced materials [1]. Their ultrashort light pulses combined with high peak powers offer unique advantages such as sub-micrometer spatial resolution, repeatability, non-contact processing and non-thermal heating of the affected area [2]. In this context, femtosecond laser illumination for patterning or engineering defects on graphene can be utilized for the fabrication of graphene nano-sieves.
In our experiments we irradiated monolayer CVD graphene on SiO_2 substrates, with low energy femtosecond laser pulses by varying: a) the laser fluence from 1.6 to 50.9 mJ/cm^2 at a constant exposure time of 20s and b) the irradiation time from 1 up to 500s at laser power of 4.8 mJ/cm^2. At each spot, three topographically distinct regions are clearly visible. The outer region is a non-irradiated area, the ring flatter area where only wrinkles are discriminated and the inner circular area (fig.1a) where the black spots correspond to the nanopores of a circular sieve with diameter of 1.3 μm.
Figure 1b illustrates three indicative Raman spectra in the range 1200 - 3000 cm^{-1} recorded at the locations denoted with the coloured circles in fig. 1a. G and 2D band characteristics and peaks associated with defected areas (D, D') are used to identify and distinguish the nanopore area. Therefore, we show how Raman microscopy in combination with AFM imaging can be utilized to quickly identify the graphene nano-sieve formed by ultrashort pulse irradiation.

References

[1] Gattass, R.R. and E. Mazur, Nature Photonics, 2 (2008) 219.
[2] Feng, N. and J. Yong, Frontiers in Chemistry, 8 (2020) 884.

Figures

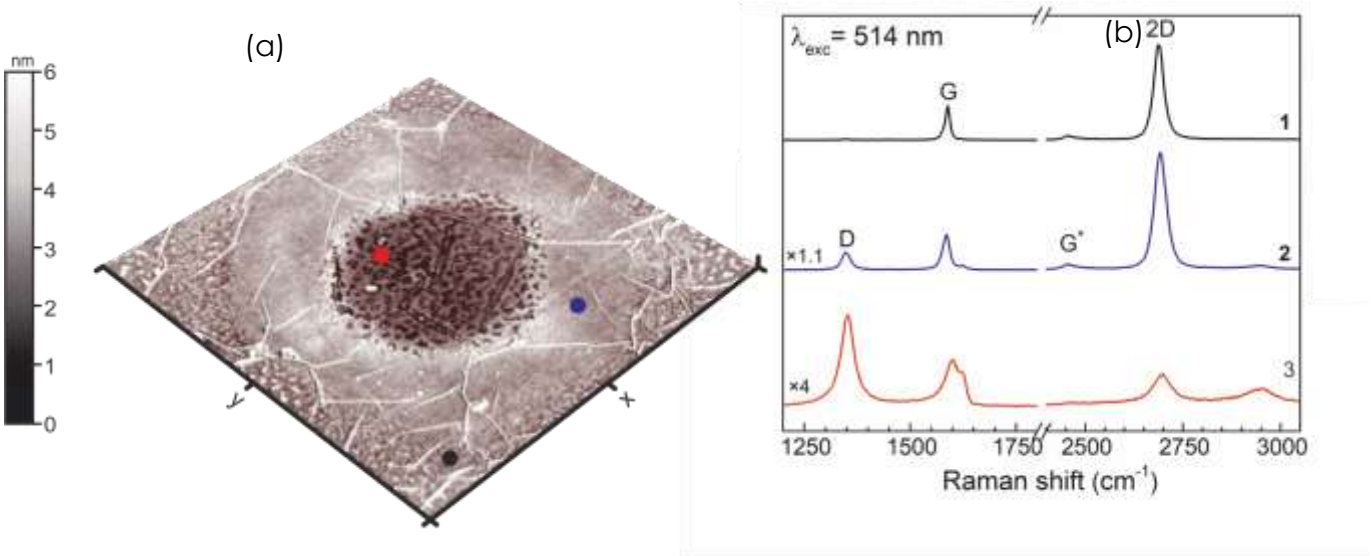


Figure 1: (a) A 3D topography AFM image (3x3 μm^2) of graphene at an irradiated spot. The black spots in the central area with diameter of 1.3 μm correspond to the created nanopores. (b) Raman spectra recorded at the locations denoted with the coloured circles in (a).

Plasmon Enhanced Optical Response of Metal-2D TMDC Hybrids for Nanophotonic Devices

Samit K Ray
Subhajit Jana and Rup K. Chowdhury
Department of Physics, Indian Institute of Technology Kharagpur
Kharagpur 721302, India
Email: physkr@phy.iitkgp.ac.in

Abstract :

Tunable light-matter couplings in dissimilar constituents (metal & semiconductors) play a leading role in the development of two-dimensional (2D) transition metal dichalcogenides (TMDCs) based quantum hybrids along with their applications in Si-compatible photonics. We shall present the superior broadband photodetection characteristics of few-layer MoS_2 and black phosphorus (BP) nanosheets integrated with metal nanoparticles (Au & Ag NPs) using vertical heterojunctions on Si platform. The hybrid Ag-NP:BP sample exhibits broadband absorption with a strong plasmonic peak around ~425 nm due to the localized surface plasmon resonance (LSPR) of Ag-NPs of average size ~6.0 nm. The quenching of photoluminescence intensity in plasmonic hybrid compared to the pristine sample ascertains the energy transfer from black phosphorus nanoflakes to Ag-NPs. The size-dependent optical response of BP nanostructure/Si state-of-art broadband (300–1600) photodiodes have been studied extensively. The tunable spectral responsivity with a peak value of ~3.2 A/W (@ ~440 nm, –5 V) for the Ag-BP/Si heterojunction device demonstrates the potential of plasmonic BPs hybrid for future nanophotonic devices [1]. On the other hand, the ultrafast time-domain results reveal a three hundred-fold enhancement in the lifetime of inter-band hot-electrons for Au/MoS_2 nanohybrids, over the pristine one. The real-time investigation of double Fano lineshapes is also demonstrated in Au nanodisk-MoS_2 hybrids. The time-domain double Fano build-up shown in Fig.1 starts at ~ 1.0 ps timescale, which sustains up to 5.0 ns [2]. The diverse ultrafast light-matter couplings for layered TMDCs and their plasmonic hybrids are attractive for next generation quantum photonic devices.

References

[1] S. Jana, S. Mukherjee, S. B.N. Bhaktha and S. K. Ray, ACS Appl. Mater. Interfaces, 14 (2022), 1699

[2] R. K Chowdhury, S.Mukherjee, S.N B Bhaktha and S.K.Ray, Physical Review B, 101 (2020), 245442

Figures

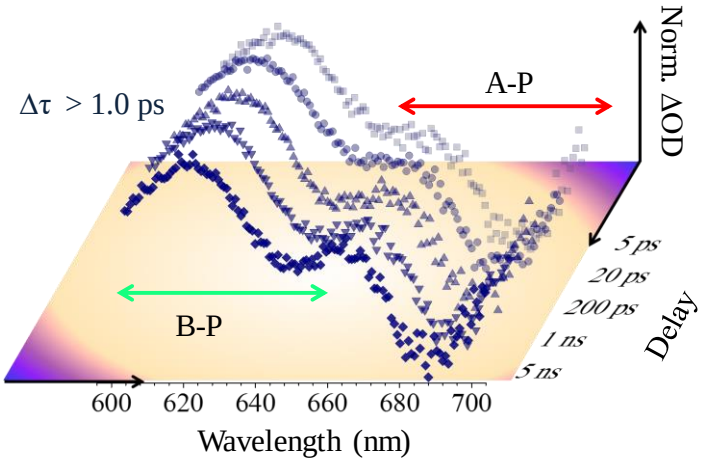


Figure 1: Normalized double Fano spectra of excitons for Δτ > 1.0 ps probe delay in Au-MoS_2 hybrids

Measuring van der Waals interactions of monolayer materials

Stanislav Tsoi
Saujan Sivaram, Matthew Rosenberger, Kathleen McCreary, Hsun-Jen Chuang, Berend T. Jonker
US Naval Research Laboratory, Washington, DC 20375, USA
Stanislav.tsoi@nrl.navy.mil

Van der Waals interactions play a major role in the science of monolayer materials, yet their measurement has received a limited attention. We exploit AFM to measure an attractive van der Waals (vdW) force acting on a sharp AFM tip from a composite sample consisting of a monolayer material supported on a thick substrate. The force is measured as a function of a separation between the tip and the monolayer/substrate stack in the range from 2–20 nm for graphene/silicon oxide, fluorinated graphene/silicon oxide, MoS_2/graphite and $MoSe_2$/graphite. The obtained results indicate that distinct contributions to the force from the monolayer and substrate can be distinguished by their different dependence on the separation, an inverse cubed for the former and inverse square for the latter. Thus, van der Waals interaction for different monolayer materials is determined and compared to the traditional bulk materials. Further, we demonstrate that the monolayer materials screen van der Waals interactions of the underlying substrate, with full screening in graphene/silicon oxide and partial screening in fluorinated graphene/silicon oxide, MoS_2/graphite and $MoSe_2$/graphite.

Breakdown of Universal Scaling Nanometer-Sized Bubbles in Graphene

Renan Villarreal[1]
Zviadi Zarkua[1], Pin-Cheng Lin[1], Fahim Faraji[2,3], Nasim Hassani[4], Harsh Bana[1], Victor Schinckus[1], Maya N. Nair[5], Hung-Chieh Tsai[6,7], Manuel Auge[8], Felix Junge[8], Hans Hofsass[8], Stefan De Gendt[6,7], Steven De Feyter[9], Steven Brems[6], Harriet Åhlgren[10], Erik C. Neyts[2], Lucian Covaci[3], François M. Peeters[3], Mehdi Neek-Amal[4], Lino M. C. Pereira[1]
[1]*Quantum Solid State Physics, KU Leuven, 3001 Leuven, Belgium*
[2]*Research group PLASMANT, Universiteit Antwerpen, 2610 Antwerpen, Belgium*
[3]*Department Natuurkunde, Universiteit Antwerpen, 2610 Antwerpen, Belgium*
[4]*Department of Physics, Shahid Rajaee Teacher Training University, 16875-16 Lavizan, Tehran, Iran*
[5]*CUNY Advanced Science Research Center, 85 St. Nicholas Terrace, New York, US*
[6]*imec vzw (Interuniversitair Micro-Electronica Centrum), 3001 Leuven, Belgium*
[7]*Division of Molecular Design and Synthesis, KU Leuven, 3001 Leuven, Belgium*
[8]*Institute of Physics, University of Göttingen, 37077 Göttingen, Germany*
[9]*Division of Molecular Imaging and Photonics, KU Leuven, 3001 Leuven, Belgium*
[10]*Faculty of Physics, University of Vienna, 1090 Vienna, Austria*
Renan.Villarreal@kuleuven.be

Owing to its unrivalled elasticity and strength, graphene can hold matter at extreme pressures in the form of bubbles with dimensions down to the nanometer scale. These bubbles offer new opportunities to explore physics and chemistry and under the extreme conditions that both graphene and the trapped matter are subject to. While previous research has mostly dealt with bubbles with a radius of few nm and larger, the sub-nanometer regime remains largely unexplored. Here, we report the formation of graphene nanobubbles with radius of the order of 1 nm, which are produced using ultralow energy implantation of noble gas ions (He, Ne and Ar) into graphene grown on a Pt (111) surface [1]. We show that the universal scaling of the aspect ratio (height over radius), which has previously been established for larger bubbles (with radius of few nm and higher), breaks down when the bubble radius approaches 1 nm, as the bubble height converges to a minimum value corresponding to one atomic monolayer. Moreover, we observe that the bubble stability and aspect ratio depend on the substrate onto which the graphene is grown and on trapped element. We discuss these dependencies in terms of the role of the atomic compressibility of the noble gases as well as of the adhesion energies between the three constituents: graphene, substrate and noble gas atoms. The high strain (of the order of 10%) induced in graphene by the trapped atoms and the high van der Waals pressure (of the order of tens of GPa) inside the bubbles illustrate the unique characteristics of this sub-nanometer bubble regime, compared to the previously studied (larger) nanobubbles. We also discuss prospects to explore our approach (based on ultralow energy ion implantation) in the context of inducing periodic pseudomagnetic fields and flat bands in graphene.

References

[1] R. Villarreal, P.-C. Lin, F. Faraji, N. Hassani, H. Bana, Z. Zarkua, M. N. Nair, H.-C. Tsai, M. Auge, F. Junge, H. Hofsaess, S. De Gendt, S. De Feyter, S. Brems, E.H. Åhlgren, E.C. Neyts, L. Covaci, F.M. Peeters, M. Neek-Amal, L.M.C. Pereira, Nano Letters 21, 8103-8110 (2021).

Figures

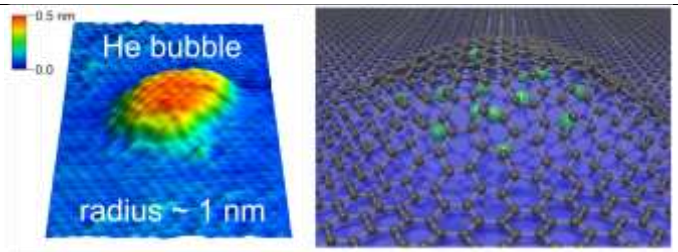


Figure 1: STM topography of a He bubble in graphene on Pt(111) and 3D atomic model.

Breakdown of dipolar blueshift at low-temperatures indicating quantum correlations in exciton ensembles in WSe_2-$MoSe_2$ hetero-bilayer

Nihit Saigal[1]
Torsten Stiehm[1], Hendrik Lambers[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], K. Watanabe[3], T. Taniguchi[3], Alexander W. Holleitner[2] and Ursula Wurstbauer[1]
[1] *Institute of Physics, University of Münster, 48149 Münster, Germany*
[2] *Walter Schottky Institut und Physik Department, TU Munich, Am Coulombwall 4a, 85748 Garching, Germany*
[3] *National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan*
nsaigal@uni-muenster.de

Atomistic van der Waals hetero-bilayers are ideal systems to study the (quantum-) phase diagram of excitons including Bose-Einstein condensation due to large exciton binding energies, an interfacial dipole moment, an in-plane optical dipole and long lifetimes [1-3]. Light emission and electron energy-loss spectroscopy showed first evidence of excitonic many-body states in such two-dimensional materials [4,5]. Pure optical studies, the most obvious way to access the phase diagram of photogenerated excitons have been elusive. We observe several criticalities in photogenerated exciton ensembles hosted in $MoSe_2$–WSe_2 hetero-bilayers with respect to photoluminescence intensity, linewidth, and temporal coherence pointing towards the transition to a coherent many-body quantum state, consistent with the predicted critical degeneracy temperature [6]. Most intriguing, the density dependent dipolar blueshift breaks down at millikelvin temperatures over at least 5 orders of magnitude of the excitation fluence indicating transition to a quantum liquid phase [7]. For this state, the estimated occupation is approximately 100%. The phenomena stay robust till above 10 Kelvin [6,7].

We gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) via Projects WU 637/4 and HO3324/9 and the priority program PP2244.

References

[1] B. Miller, et al. Nano Letters 17, 5229 (2017). (2017).
[2] J. Kiemle, et al. Phys. Rev. B 101, 121404(R) (2020).
[3] L. Sigl, et al. Phys. Rev. B 105, 035417 (2022).
[4] A. Kogar, et al. Science 358, 1314 (2017).
[5] Z.Wang, et al. Nature 574, 76 (2019).
[6] L. Sigl, et al. Physical Review Research 2, 042044(R) (2020).
[7] T. Stiehm et al, in preparation. (2022).

Figures

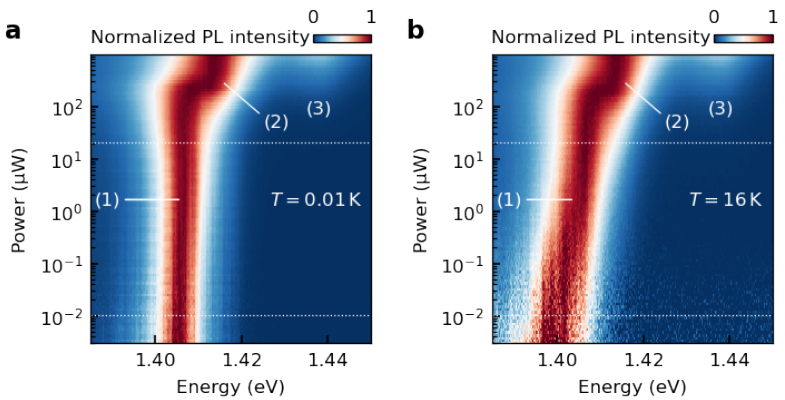


Figure 1: Excitation power dependent photoluminescence (PL) of interlayer excitons (IX) of a $MoSe_2$-$WeSe_2$ hetero bilayer. (a) IX PL obtained under continuous wave (cw) excitation at 1.704 eV as a function of excitation power at 10 mK displaying the breakdown of exciton blue sift of peak (1). (b) IX PL as in (a) for T = 16 K clearly showing a significant dipolar shift for peak (1).

Long-term reliable filament formation in 2D material-based synaptic memristor by inserting active metal reservoir

Wonbae Ahn[1]
Han Beom Jeong[2], Jungyeop Oh[1], Jun-Hwe Cha[1], Hu Young Jeong[3], and Sung-Yool Choi[1*]
[1]*School of Electrical Engineering, Graphene/2D Materials Research Center, Center for Advanced Materials Discovery towards 3D Displays, KAIST, 291, Daehakro, Yuseong-gu, Daejeon, South Korea*
[2]*Materials Science and Engineering, KAIST, 291, Daehakro, Yuseong-gu, Daejeon, South Korea*
[3]*Graduation School of Semiconductor Materials and Devices Engineering, UNIST, 50, UNIST-gil, Eonyang-eup, Ulju-gun, Ulsan, South Korea*
solbaestar@kaist.ac.kr

Abstract

This low diffusion energy barrier through multi-vacancies in 2D materials leads to the advantages of low switching voltage and excellent synaptic characteristics but also leads to the disadvantages of short retention characteristics. Herein, we suggest the new approach to form a robust copper filament that has excellent retention characteristics by inserting the copper reservoir. MoS_2 and Al_2O_3 are used as the switching layer and the copper reservoir, respectively. The fabricated Cu/Ti/MoS_2/Al_2O_3/Au device exhibits low switching voltage (<0.5 V), wide dynamic range (>12), and great switching uniformity (σ/μ ~ 0.07). Additionally, the linear potentiation/depression curve (a_P=0.31 and a_D=-1.01) is achieved. Most importantly, this device has excellent multistate retention characteristics over 10^4 s in the switching conductance range. The recognition rate of deep neural network (DNN) simulation is over 93% and the same recognition rate is maintained for 10 years.

References

[1] Xu R, et al., Nano letters, 19 (2019) 2411.

Figures

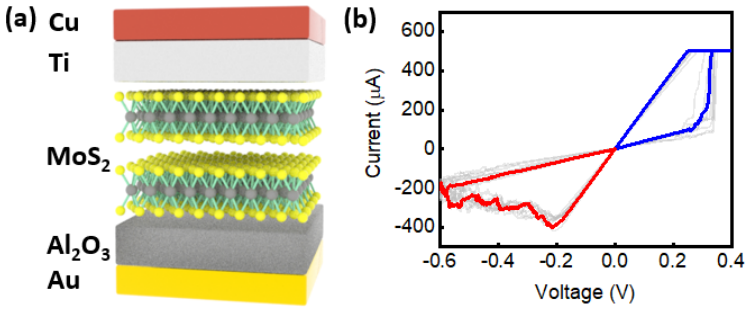


Figure 1: a) Schematic illustration of the Cu/Ti/MoS_2/Al_2O_3/Au device. b) I-V curves of 10 DC sweep

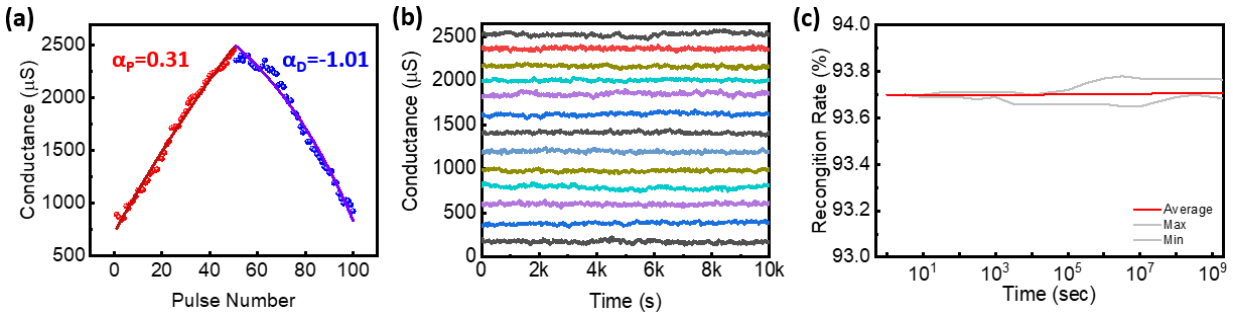


Figure 2: a) Potentiation/depression curve of the device. b) Retention characteristics of the device in the switching range. c) MNIST data recognition rate of DNN simulation for the 10 years.

Functionalized NbS_2-based solid-state electrolyte for flexible supercapacitors

Ahmad Bagheri[a,b]
Sebastiano Bellani,[c] Hossein Beydaghi,[c] Matilde Eredia,[c] Gabriele Bianca,[a,d] Marilena I. Zappia,[c] Elisa Mantero,[c] Zdenek Sofer,[e] and Francesco Bonaccorso[c]
[a] *Graphene Labs, Istituto Italiano di Tecnologia, via Morego 30, 16163 Genoa, Italy*
[b] *Faculty of Chemistry and Food Chemistry and Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Dresden 01062, Germany*
[c] *BeDimensional SpA, Lungotorrente Secca 30R, 16163 Genoa, Italy*
[d] *Dipartimento di Chimica e Chimica Industriale, Università degli Studi di Genova, via Dodecaneso 31, 16146 Genoa, Italy*
[e] *Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic*
Ahmad.bagheri@iit.it

Highly efficient and durable flexible solid-state supercapacitors (FSSSCs) are emerging as low-cost devices for portable and wearable electronics because of the elimination of leakage of toxic/corrosive liquid electrolytes and their capability to withstand elevated mechanical stresses [1,2]. Nevertheless, the spread of FSSSCs requires the development of durable and highly conductive solid-state electrolytes, whose electrochemical characteristics must be competitive with those of traditional liquid electrolytes [3,4]. Here, we propose a novel composite solid-state electrolyte prepared by incorporating metallic two-dimensional (2D) group-V transition metal dichalcogenides (TMDs), namely liquid-phase exfoliated functionalized niobium disulfide (f-NbS_2) nanoflakes, into sulfonated poly(ether ether ketone) (SPEEK) polymeric matrix [5]. The terminal sulfonate groups in f-NbS_2 nanoflakes interact with the sulfonic acid groups of SPEEK by forming a robust hydrogen bonding network [6]. Consequently, the composite solid-state electrolyte is mechanically/chemically stable even at the degree of sulfonation of SPEEK as high as 70.2%, at which the mechanical strength is 38.3 MPa and the proton conductivity is maximized to 94.35 mS cm^{-2} at room temperature. Beyond the intrinsic properties of the solid-state electrolyte, the performance of FSSSC is strongly determined by the electrical connection between electrode materials and the electrolyte. In this context, the binders, used in the electrode material formulation to produce mechanically robust electrodes, must guarantee a close contact between the solid-state electrolyte and electrode active materials for effective double-layer formation [7]. To elucidate the importance of the interaction between the electrode materials (including active materials and binders) and the solid-state electrolyte, solid-state supercapacitors were produced using either SPEEK or polyvinylidene fluoride as proton-conducting and non-conducting binders, respectively. The use of our solid-state electrolyte in combination with proton-conducting SPEEK binder results in a solid-state supercapacitor with a specific capacitance of 115.724 F g^{-1} at 0.02 A g^{-1}, optimal rate capability (75.94 F g^{-1} at 10 A g^{-1}), and electrochemical stability over galvanostatic charge/discharge cycling.

References

[1] W. A. Haider, *et al.*, ACS Cent. Sci. 2020, 6, 1901.
[2] V. Romano, *et al.*, ChemPlusChem 2019, 84, 882.
[3] N. Joseph, P. M. Shafi, A. C. Bose, Energy and Fuels 2020, 34, 6558.
[4] W. K. Chee, *et al.*, J. Phys. Chem. C 2016, 120, 4153.
[5] H. Beydaghi, *et al.*, J. Mater. Chem. A 2021, 9, 6368.
[6] H. Beydaghi, *et al.*, Nanoscale 2022 DOI: 10.1039/d1nr07872k.
[7] H. E. Nsude, *et al.*, J. Nanoparticle Res. 2020, 22, 1.

"This project has received funding from the European Union's Horizon 2020 MSCA-ITN ULTIMATE project under grant agreement No. 813036"

Cross-field optoelectronic modulation *via* inter-coupled ferroelectricity in 2D In_2Se_3

Debopriya Dutta, Subhrajit Mukherjee, Michael Uzhansky, Elad Koren
Nanoscale Electronic Materials and Devices Laboratory, Faculty of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa, 3200003, Israel
debopriyad@campus.technion.ac.il

Abstract -
Ferroelectricity in two-dimensional (2D) materials has been at the forefront of recent research owing to its potential application in low powered non-volatile phase change memory, energy harvesting, strain tuned electronics, artificial brain and neuromorphic sensors. Among the 2D materials exhibiting ferroelectricity in room temperature, a-In_2Se_3 stands out owing to the presence of both in-plane (IP) and out-of-plane (OOP) dipole polarizations[1]. In addition, the ability to modulate IP by switching OOP and vice versa owing to their intercoupled nature makes it a promising material for multimodal memory and optoelectronic applications. Herein, we experimentally demonstrate the cross-field modulation of opto- and electronic properties in a-In_2Se_3 based field effect devices[2]. Gate dependent surface potential measurements using Kelvin Probe Force Microscopy (KPFM) were extensively used in In_2Se_3 based devices to directly reveal the bi-directional dipole modulation. Electric field calculations obtained from the surface potential studies also show hysteretic behavior of the dipoles following high gate voltage pulses. Also, to explore the consequence of the hysteretic change in the in-plane electrical field, photoresponse measurements following high gate pulses were performed exhibiting its functionality as a non-volatile memory switch. The multi-level photoresponse characteristics for different gate polarities in the fabricated photodetectors show a potential for their implementation and integration into non-volatile memory and electro-optical applications.

References

[1] Cui, C., Hu, W., Yan, X. et al. Nano Letters 18 (2018), 1253-1258.
[2] Dutta, D., Mukherjee, S., Uzhansky, M. et al. npj 2D Mater Appl 5 (2021), 81.

Figures

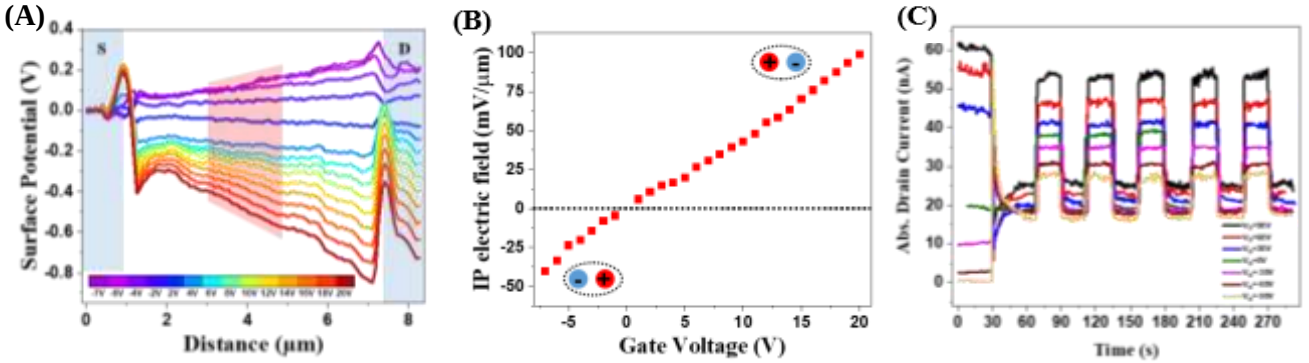


Figure 1: (A) Surface potential profiles across a-In_2Se_3 channel for various gate biases ranging from VG= -7 V to VG= 20 V. The semi-transparent blue boxes indicate the source and the drain positions. **(B)** Effective IP electric field calculated from a section of the line profiles away from electrodes (marked by semi-transparent red quadrilateral) in Fig. 1(A) as a function of applied gate voltage. **(C)** Temporal response of photocurrent in a-In_2Se_3 for various gate pulses. Gate pulses were applied for 30s after which the gate was withdrawn. The measurements were performed with zero applied gate potential and drain voltage of -2 V thereafter.

Converting paper into laser-induced graphene for physical and biochemical sensors

Bohdan Kulyk[1,2]
Beatriz F. R. Silva[1], Alexandre F. Carvalho[1], Marina Matos[3], Paula Barbosa[4], António J. S. Fernandes[1], Ana V. Girão[5], Jonas Deuermeier[2], Sónia O. Pereira[1], Nuno F. Santos[1], Dmitry V. Evtuguin[3], Filipe M. L. Figueiredo[4], Elvira Fortunato[2], Florinda M. Costa[1]
[1]i3N, Department of Physics, University of Aveiro, Campus Universitário de Santiago, 3810-193, Aveiro, Portugal. [2]i3N/CENIMAT, Department of Materials Science and CEMOP/UNINOVA, NOVA School of Science and Technology, NOVA University Lisbon, Campus de Caparica, 2829-516, Caparica, Portugal. [3]CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal. [4]CICECO – Aveiro Institute of Materials, Department of Physics, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal. [5]CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.
bkulyk@ua.pt

Laser-induced graphene (LIG), a porous, conductive, and flexible graphene foam produced by direct conversion of a wide range of carbon-containing materials by laser irradiation, has been gaining notoriety due to its ease of fabrication and broad applicability in fields such as energy storage and generation, transduction, electrocatalysis, water treatment, de-icing, antifouling, and biomedicine. Particularly appealing is the synthesis of this material from paper, a biodegradable, flexible and low-cost substrate. Here, we describe the formation of this paper-LIG using affordable IR (10.6 µm) and UV (355 nm) lasers and present several applications of this material (Figure 1). In particular, we demonstrate precise patterning of conductive paths onto fire-retardant treated filter paper for strain and bending sensing,[1] discuss the synthesis process under UV irradiation for humidity and temperature sensors [2] and introduce the synthesis of LIG from xylan, a widely available and underutilized biopolymer by-product of biorefineries.[3] Lastly, we take full advantage of the unique mix of features of paper-LIG, such as large surface area, porosity, good electrochemical performance and affordability, to present disposable uric acid biosensors capable of quantification of this clinically relevant analyte in real human urine samples. Overall, we provide an overview of the unique characteristics and vast capabilities of paper-LIG, highlighting its applicability in the field of low-cost and environmentally friendly sensing.

References

[1] Bohdan Kulyk, Beatriz F. R. Silva, Alexandre F. Carvalho, Sara Silvestre, António J. S. Fernandes, Rodrigo Martins, Elvira Fortunato, and Florinda M. Costa, ACS Applied Materials & Interfaces, 13(8) (2021) 10210-10221
[2] Bohdan Kulyk, Beatriz F. R. Silva, Alexandre F. Carvalho, Paula Barbosa, Ana V. Girão, Jonas Deuermeier, António J. S. Fernandes, Filipe M. L. Figueiredo, Elvira Fortunato, and Florinda M. Costa, Advanced Materials Technologies, (2022) 2101311
[3] Bohdan Kulyk, Marina Matos, Beatriz F.R. Silva, Alexandre F. Carvalho, António J. S. Fernandes, Dmitry V. Evtuguin, Elvira Fortunato, and Florinda M. Costa, Diamond and Related Materials, 123 (2022) 108855

Figures

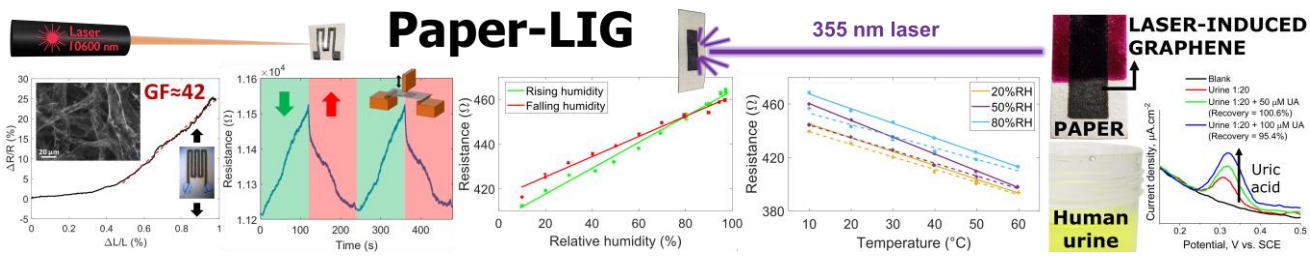


Figure 1: Different applications of paper-LIG.

Growth of selfstanding h-BN crystals: hunting for crystal defects and contamination

Camille MAESTRE[1,2]
Bérangère TOURY[1], Philippe STEYER[2], Vincent GARNIER[2], Catherine JOURNET[1]
[1]*Laboratoire des Multimatériaux et Interfaces, UMR CNRS 5615, Univ Lyon, Université Claude Bernard Lyon 1, F-69622 Villeurbanne, France*
[2]*Univ Lyon, INSA Lyon, Université Claude Bernard Lyon 1, CNRS, MATEIS, UMR5510, 69621 Villeurbanne, France*
camille.maestre@univ-lyon1.fr

Whether used as a substrate or as an active layer, high quality 2D hexagonal boron nitride (hBN) holds great promise for future research applications, especially in optoelectronics. Vapor-phase processes can achieve large scale coverage, but selfstanding hexagonal boron nitride crystals provide exfoliated nanosheets (BNNS) of unrivalled purity and crystal quality which are still preferred for demanding applications. In order to obtain high quality and large size BNNSs, we propose a synthesis route coupling the Polymer Derived Ceramics (PDCs) process with a sintering step. [1,2] The hBN obtained by this method has already demonstrated a very high crystalline quality attested by a Raman FWHM value of 7.6 cm^{-1}, one of the best reported in literature. [1] Our study aims at understanding the mechanisms of hBN crystal growth and the generation of crystalline defects in order to better control the synthesis and to provide hBN with the desired quality. X-ray tomography (Figure 1a) provide insights into nucleation and growth orientation. To search for defects in the crystal, its optical and electrical properties are explored (see Figure 1b and c). BNNSs exfoliated from these crystals have been used to fabricate metal-hBN-metal capacitor devices to measure the dielectric constant and the breakdown electric field of hBN, which were found to be 3.136 and 0.64 $V.nm^{-1}$ respectively [3], i.e very close to the theoretical values. Such routine functional measurements allow the assessment of the overall crystal quality. These BNNSs have also been used to encapsulate Transition Metal Dichalcogenides (TMDs) tested by optical spectroscopy. The photoluminescence widths of WSe_2 and $MoSe_2$ neutral exciton lines at 4K were measured within the 2-3 meV range [2] which is comparable to the results obtained with the highest quality hBN. All these results demonstrate that the BNNSs are relevant for future electronic and opto-electronic applications.

References

[1] Y. Li, V. Garnier, C. Journet, J. Barjon, A. Loiseau, I. Stenger, A. Plaud, B. Toury, P. Steyer, Nanotechnology, 30 (2019) 035604
[2] C. Maestre, Y. Li et al., submitted (arXiv:2201.07673).
[3] A. Pierret, B. Plaçais , et al., accepted (arXiv:2201.05826).

Figures

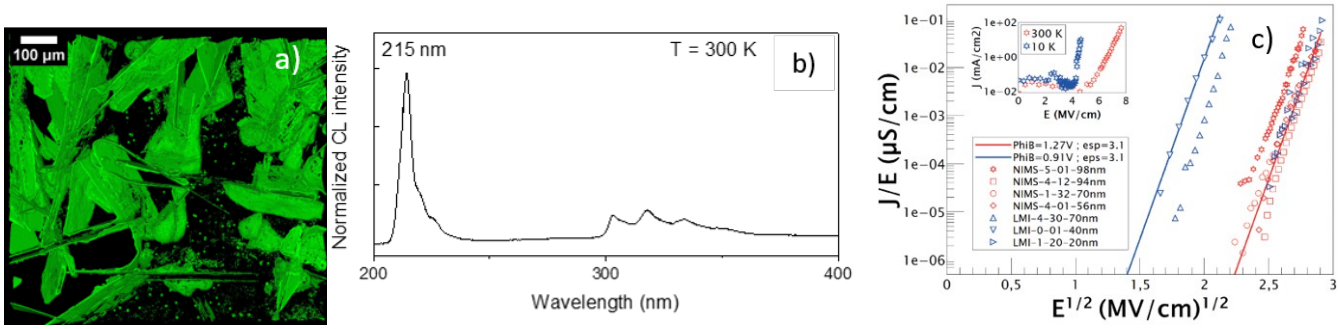


Figure 1: (a) X-ray tomography 3D extracted view of entangled crystals inside the as-obtained ingot; (b) Cathodoluminescence measurement of a PDC hBN crystal [2]; (c) Frenkel-Pool plot of the high field hBN conductivity, exfoliated crystals from LMI and NIMS [3].

Tuneable electrohydrodynamics of graphene oxide vortex rings

Kaiwen Nie
Yizhen Shao, Maria Iliut, Finn Box, Dai Luan, Yuan Shen, Weimiao Wang, Ingo Dierking and Aravind Vijayaraghavan
The University of Manchester, Oxford Road, Manchester, UK
Contact Email: aravind@manchester.ac.uk

The vortex ring (VR) effect occurs when fluid droplets impact on another fluid, where the toroidal flow emerges within the impacting droplet due to viscous friction, resulting in a wide variety of flow-induced morphologies [1]. Here, this effect was used to generate 3-dimensional assemblies of graphene oxide (GO) flakes [2]. In order to stabilise various axially symmetric shapes, the cationic aqueous surfactant system (cetyltrimethylammonium bromide, CTAB) was utilised, which could interact with GO flakes who showed negative-charged in water. Then, GO hydrogel and aerogel particles with sphere, donut and jellyfish shapes could be obtained which all with a core-shell structure were featuring a shell of aligned GO flakes. The mechanism of this can be controlled by the competing influence of impact forces, viscous friction and graphene-fluid electrostatic interactions. Also, these GO particles have rich porous structure on their shell. In this fashion, these particles can be used in the water purification [3].

References

[1] Ji San Lee et al., Nature Communications, 6 (2015) 8187.
[2] Duo An et al., Nature Communications, 7 (2016) 12401.
[3] Yizhen Shao et al., Paper Submitted (2022).

Figures

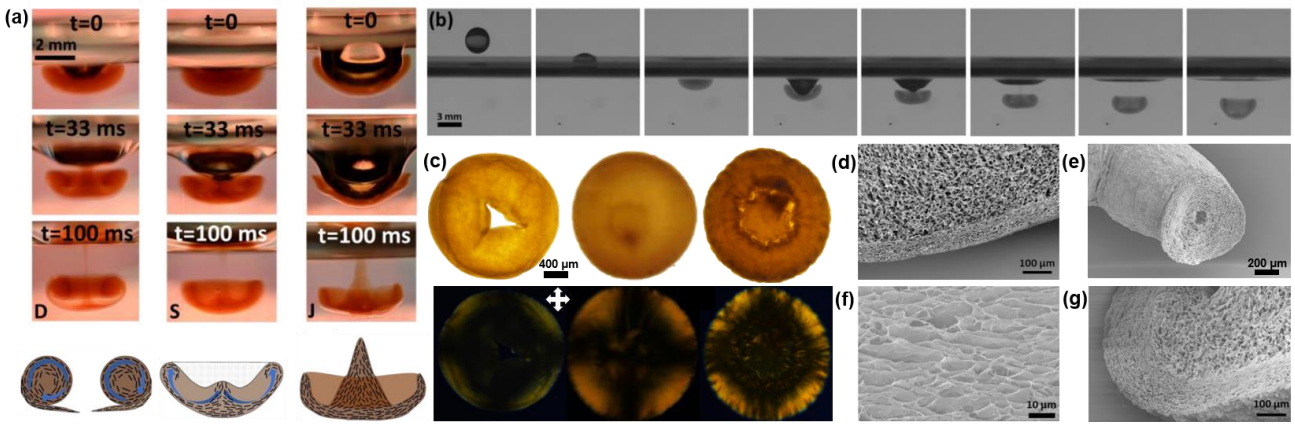


Figure 1: (a) Resting stages of GO-VRs formed by GO with donut, sphere and jellyfish shapes. (b) High-speed photographic images of a GO droplet penetrating CTAB solution and the formation of a vortex ring. (c) Microscopic and polarised optical microscopic images. (d)-(g) Core-shell structure.

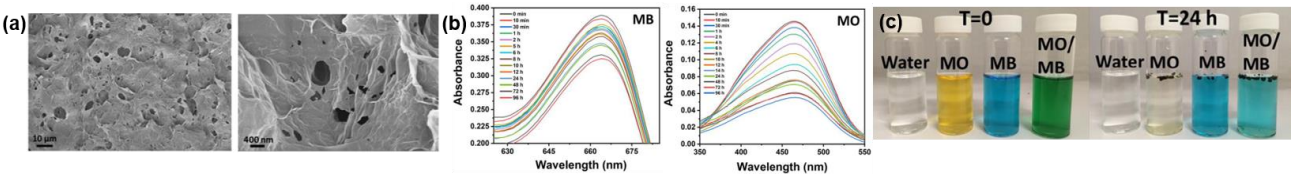


Figure 2: (a) Porous structure of GO aerogel particles. (b)-(c) UV-vis spectra and color change for the adsorption test at different time for methyl orange and methyl blue respectively.

Stable Al_2O_3 encapsulation of MoS_2-FETs Enabled by CVD grown h-BN

Agata Piacentini[1,2]
Damiano Marian[3], *Daniel S. Schneider*[1,2], *Enrique González Marín*[4], *Zhenyu Wang*[5], *Martin Otto*[1], *Bárbara Canto*[1], *Aleksandra Radenovic*[5], *Andras Kis*[5], *Gianluca Fiori*[3], *Max C. Lemme*[1,2], *and Daniel Neumaier*[1,6]
[1]*AMO GmbH, Otto-Blumenthal-Str. 25, 52074 Aachen, Germany*
[2] *RWTH Aachen University, Otto-Blumenthal-Straße 2, 52074 Aachen, Germany*
[3] *Università di Pisa, Via Girolamo Caruso 16, 56122 Pisa, Italy*
[4] *University of Granada, Avenida de la Fuente Nueva S/N, 18071 Granada, Spain*
[5] *École Polytechnique Fédérale de Lausanne (EPFL), Lausanne 1015, Switzerland*
[6] *Bergische Universität Wuppertal, Lise-Meitner-Straße 13, 42119 Wuppertal, Germany*
piacentini@amo.de

Two-dimensional materials have attracted massive attention especially for their potential as an alternative in ultra-scaled FET and for flexible electronic applications. Molybdenum disulfide (MoS_2) is the most widely studied transition metal dichalcogenides because of its high carrier mobility compared to ultra-thin silicon FETs and its specific optoelectronic properties, but the electrical performance is strongly affected by the environment and dielectric interfaces, often leading to large hysteresis in MoS_2-based devices [1]. Encapsulation layer like aluminium oxide (Al_2O_3) is widely used in (opto)-electronics. At the same time, it leads to detrimental charge transfer n-doping to MoS_2 [2]. Here, we report a scalable encapsulation approach for MoS_2 FETs where hexagonal boron nitride (h-BN) monolayers are employed as a barrier layer in-between each of the Al_2O_3 and MoS_2 interfaces (Fig. 1a and b). These devices exhibit a significant reduction of charge transfer when compared to structures without h-BN (Fig. 1c and d). This has been confirmed by ab-initio Density Functional Theory calculations. In addition, the devices with h-BN layers show very low hysteresis even under ambient operating conditions [3].

References

[1] Late, Dattatray J., et al. ACS nano 6.6 (2012): 5635-5641.
[2] Na, Junhong, et al. Nanoscale 6.1 (2014): 433-441.
[3] Piacentini, Agata et al. Unpublished manuscript (2022).

Figures

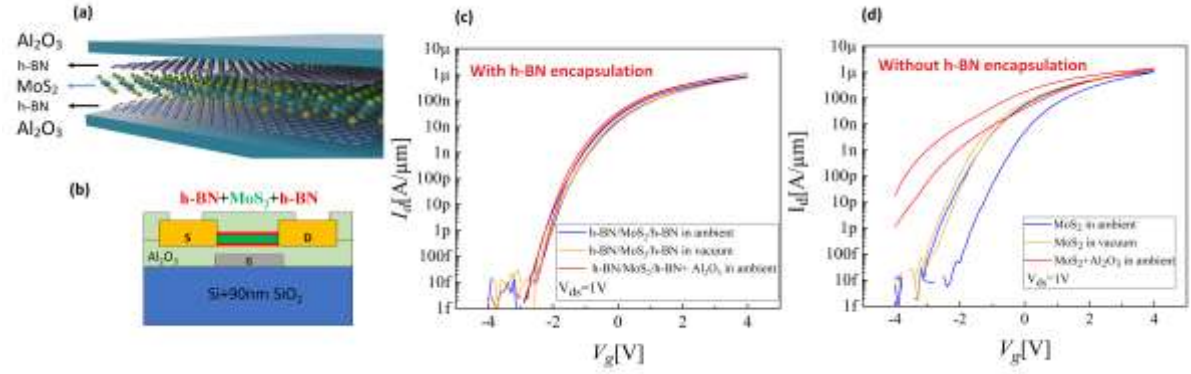


Figure 1: (a) Schematic of the channel material stack and (b) cross sections of the used FET structure. Electrical characterisation of a FET (c) with h-BN encapsulation and (d) without h-BN encapsulation in different conditions.

Acknowledgment: EU (881603, 829035, 863258), DFG (LE 2440/7-1 and LE 2440/8-1) BMBF (16ES1134)

Synthesis and water dispersion of two-dimensional layered double hydroxides

Marco Piccinni[a,b]
Sebastiano Bellani[c], *Gabriele Bianca*[a,b], *Diego Colombara*[b], *and Francesco Bonaccorso*[a,c]
[a] *Istituto Italiano di Tecnologia, Graphene Labs, via Morego 30, Genoa, Italy.*
[b] *Dipartimento di Chimica e Chimica Industriale, Università degli Studi di Genova, via Dodecaneso 31, 16146 Genoa, Italy.*
[c] *BeDimensional Spa., via Lungotorrente Secca 3D, 16163 Genova, Italy.*
marco.piccini@iit.it

Layered double hydroxides (LDHs) are a class of anionic clays consisting of positive charged brucite-like layers spaced by water molecules and counterbalancing anions [1]. In particular, LDHs based on the first row of transition metals have recently drawn attention due to their (electro)photocatalytic properties [2]. Differently from other layered materials (*e.g.*, graphite, hexagonal boron nitride, transition metal mono-di-chalcogenides, MXenes, …) [3,4,5], LDH layers are held together by the electrostatic forces between layers and anions amid them and a dense network of hydrogen bonds that involves interlayered water molecules and hydroxyl terminations on layer surfaces [1]. In our work, we propose an environmentally friendly synthesis procedure able to produce two-dimensional LDH materials. The formation of single layer nanosheets is confirmed by X-ray diffraction and atomic force microscopy analysis [6]. Lastly, we focus on the characterization of the optical and electrochemical properties of the nickel-iron LDH.

References

[1] Cavani et al., Catalysis Today, 11, 2 (1991) 173-301.
[2] Q. Wang and D. O'Hare, Chem. Rev. 112, 7 (2012) 4124-4155.
[3] F. Bonaccorso et al., Adv. Mater., 28 (2016) 6136-6166.
[4] A. C. Ferrari, F. Bonaccorso et al., Nanoscale 7, 11 (2015), 4598-4810.
[5] S. Bellani et al., Chem Soc. Rev. 50, (2021)11870-11965
[6] M. Piccinni et al., Inorg. Chem., (2022) doi: 10.1021/acs.inorgchem.1c03485

Figures

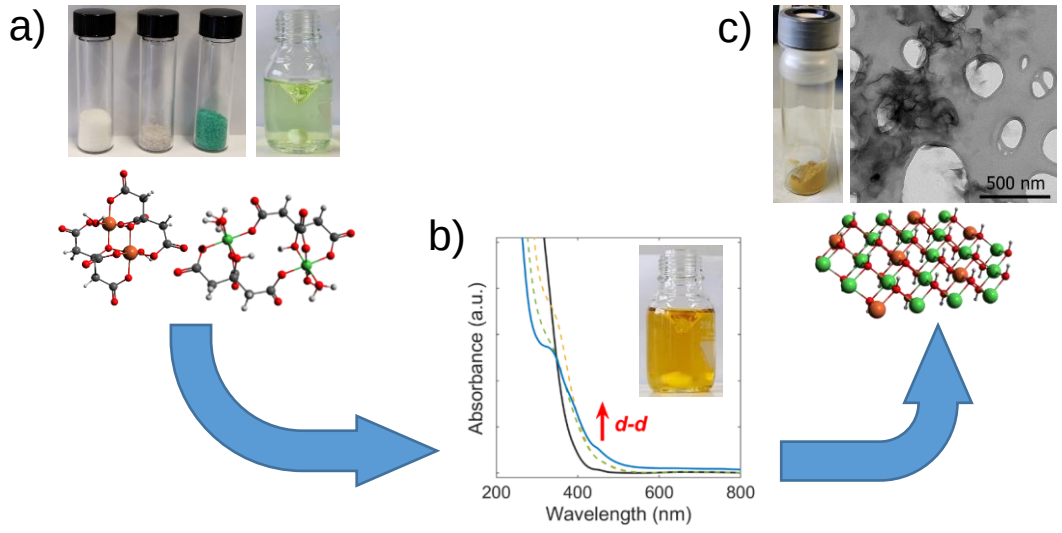


Figure 1: Synthesis process of LDHs. a) Nickel and iron citrate coordination compounds. b) The polymerization of citrate coordination compounds lead to an absorbance increase of d-d transitions. c) The nanostructured LDH product is collected and characterized.

Zero-Bias Power Detector Circuits based on MoS_2 Field Effect Transistors on Wafer-Scale Flexible Substrates

Eros Reato[1,2]

Paula Palacios[3], Burkay Uzlu[1,2], Mohamed Saeed[3], Annika Grundmann[4], Zhenyu Wang[5], Daniel S. Schneider[1,2], Zhenxing Wang[1], Michael Heuken[6], Holger Kalisch[4], Andrei Vescan[4], Alexandra Radenovic[5], Andras Kis[5], Daniel Neumaier[7], Renato Negra[3] and Max C. Lemme[1,2]

[1]*AMO GmbH;* [2]*Chair of Electronic Devices, RWTH Aachen University, Otto-Blumenthal-Strasse 25, 52074 Aachen, Germany*

[3]*Chair of High Frequency Electronics, RWTH Aachen University, Aachen, Germany*

[4]*Compound Semiconductor Technology, RWTH Aachen University, Aachen, Germany*

[5]*School of Engineering, EPFL, Lausanne, Switzerland*

[6]*AIXTRON SE, Herzogenrath, Germany*

[7]*Bergische Universität Wuppertal, Wuppertal, Germany*

reato@amo.de

This contribution discusses the design, fabrication, and characterization of wafer-scale, zero-bias power detectors based on two-dimensional MoS_2 field effect transistors (FETs) on a flexible Polyamide (PI) substrate [1]. The performance of two CVD-MoS_2 samples (monolayer and multilayer), grown with different processes, is analyzed and compared starting from material growth, through device fabrication and characterization steps to the circuit level. By relying on the nonlinearity of the channel conductivity, the operation frequency of the circuit is between 12 and 18 GHz, with a demonstrated voltage responsivity of 45 V/W at 18 GHz for the monolayer MoS_2 and 104 V/W at 16 GHz for the multilayer. The measured dynamic range exceeds 30 dB, outperforming other semiconductor technologies like CMOS circuits [2] and GaAs Schottky diodes [3]. In addition, since the circuits operate without DC bias, they also have zero DC power consumption. These results make them the best performing power detectors fabricated on flexible substrate reported to date. The concept could be extended to future generations of flexible 2D microwave circuits [4].

References

[1] E. Reato, P. Palacios *et al.*, *Advanced Materials*, Jan. 2022, Accepted Article, p. 2108469, doi: 10.1002/adma.202108469.

[2] K. Kim and Y. Kwon, *IEEE Microwave and Wireless Components Letters*, Sep. 2013, vol. 23, no. 9, pp. 498–500, doi: 10.1109/LMWC.2013.2274994.

[3] M. Hrobak *et al.*, *2013 European Microwave Conference*, Oct. 2013, pp. 179–182. doi: 10.23919/EuMC.2013.6686620.

[4] M. Saeed *et al.*, *Advanced Materials*, Dec. 2021, Accepted Article, p. 2108473, doi: 10.1002/adma.202108473.

Figures

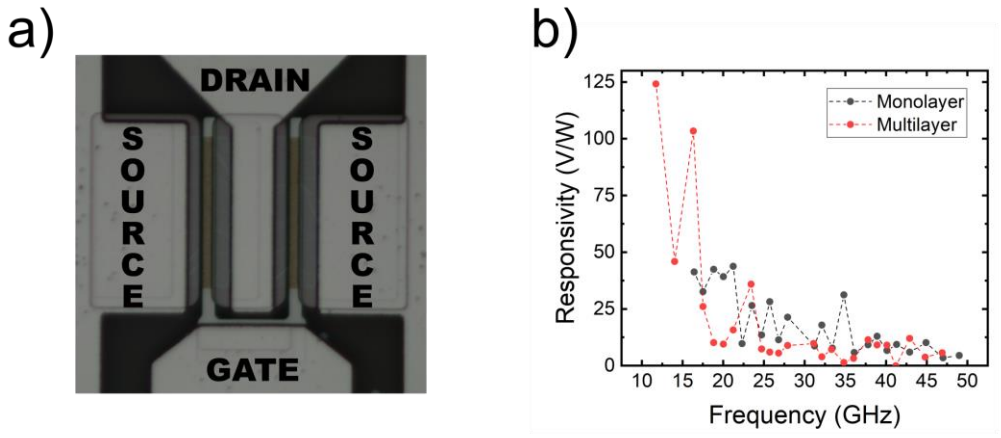


Figure 1: a) Optical micrograph of one of the fabricated MoS_2 devices, the channel dimensions are 5 x 60 µm. b) Comparison in responsivity of the two power detector circuits.

Tuning colloidal tungsten dichalcogenide nanomonolayers bandgap by controlling their size and composition

Ashkan Shahmanesh
Benoit Mahler
Institut Lumière Matière, UMR5306 - UCBL – CNRS 10 rue Ada Byron, Lyon, France
Ashkan.shahmanesh@univ-lyon1.fr

Group 6 transition metal dichalcogenides are a promising family of materials with a tunable bandgap, a stable and a metastable phase, and a large surface area in the form of monolayers, which makes them an exceptional choice for different applications such as electronics, optoelectronics, and electrocatalysts. Bandgap tailoring is achievable by reducing the size of the material to monolayer thickness or by alloying[1]. Engineering the crystal structure of transition metal dichalcogenides is crucial for controlling the electronic and optoelectronic properties of these materials. Here, we report a colloidal protocol to produce size-controlled and well-dispersed nanomonolayers (NMLs) of 1T'-WS_2 and 1T'-WSSe in the size range 10-70 nm, and we investigate the phase transformation into the 2H structure on the different sizes. TEM and STEM images demonstrate the well-dispersed monodisperse nanomonolayers of 1T'-WS_2 and 1T'-WSSe (changing the reaction parameters causes a change in the mean size). Figure 1a and c show the low magnification STEM images of well-dispersed 1T'-WS_2 NMLs, and b and d demonstrate high magnification ones. X-ray photoemission spectroscopy and X-ray diffraction confirm the phase transformation from 1T' to 2H. UV-vis spectroscopy supports the phase change and exhibits the bandgap change either by alloying or by controlling the mean size (Figure 1e and f). Hypsochromic shift happens by reducing the size of nanosheets due to quantum confinement. In conclusion, we developed a new colloidal protocol to produce size-controlled and well-dispersed NMLs of semi-metallic WS_2 and WSSe, then change the structure to semiconducting and investigate the bandgap change due to the change in diameters and composition.

References

[1] Shahmanesh, Ashkan, et al. "2D Monolayer of the 1T'Phase of Alloyed WSSe from Colloidal Synthesis." *The Journal of Physical Chemistry C* 125.20 (2021): 11058-11065.
[2] Sokolikova, Maria S., and Cecilia Mattevi. "Direct synthesis of metastable phases of 2D transition metal dichalcogenides." Chemical Society Reviews 49.12 (2020): 3952-3980.

Figures

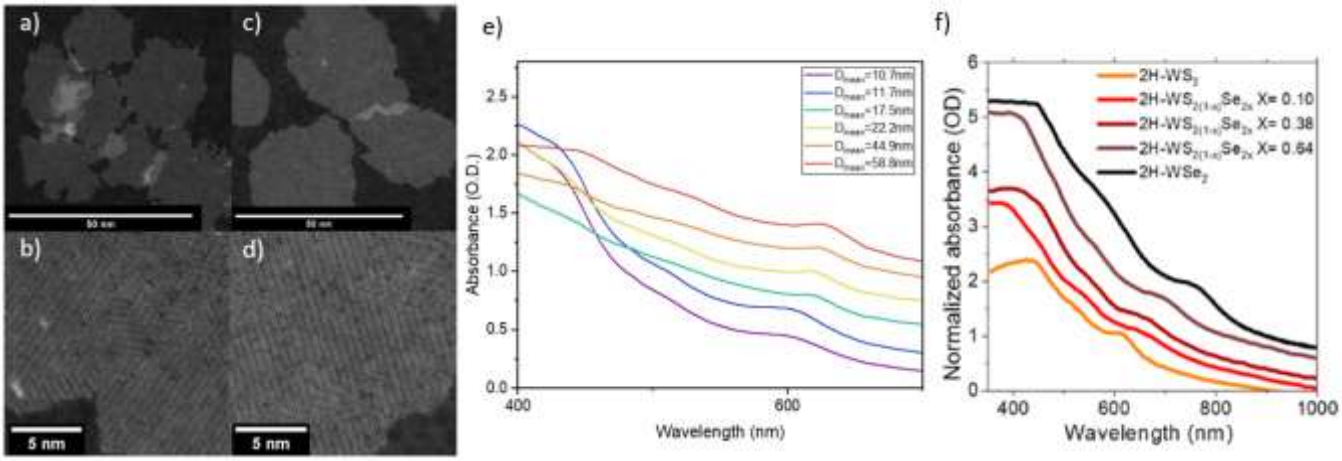


Figure 1: HAADF-STEM image of monolayers of 1T'-WS_2 with different mean sizes: a,b) 22.2 nm, c,d) 58.8nm. e) Absorption spectra of different sizes 2H-WS_2. F) Absorption spectra of 1T'-WSSe with different selenium content.

Generating extreme electric fields in 2D materials by dual ionic gating

Benjamin I. Weintrub
Yu-Ling Hsieh, Jan N. Kirchhof, and Kirill I. Bolotin
Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany
weintrbi@zedat.fu-berlin.de

We demonstrate a new type of dual gate transistor to induce record electric fields through two-dimensional materials (2DMs). At the heart of this device is a 2DM suspended between two volumes of ionic liquid (IL) with independently controlled potentials. The potential difference between the ILs falls across an ultrathin layer consisting of the 2DM and the electrical double layers above and below it, thereby producing an intense electric field across the 2DM. We determine the field strength via i) electrical transport measurements and ii) direct measurements of electrochemical potentials of the ILs using semiconducting 2DM, WSe_2. The field strength across a bilayer WSe_2 sample reaches ~2.5 V/nm, the largest static electric field through the bulk of any electronic device to date. Our approach grants access to previously-inaccessible phenomena occurring in ultrastrong electric fields.

Figures

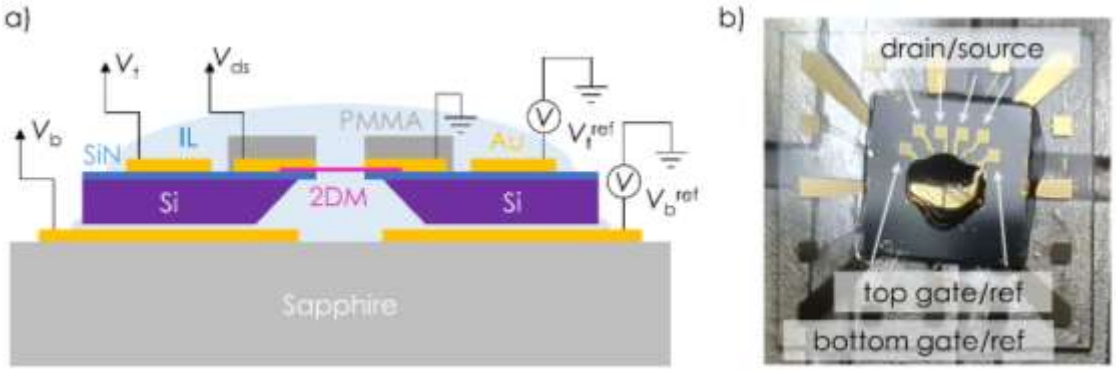


Figure 1 Dual ionic liquid gate device and measurement overview. a) Side-view cartoon of the device and measurement scheme. **b)** Photograph of a device just before measurement.

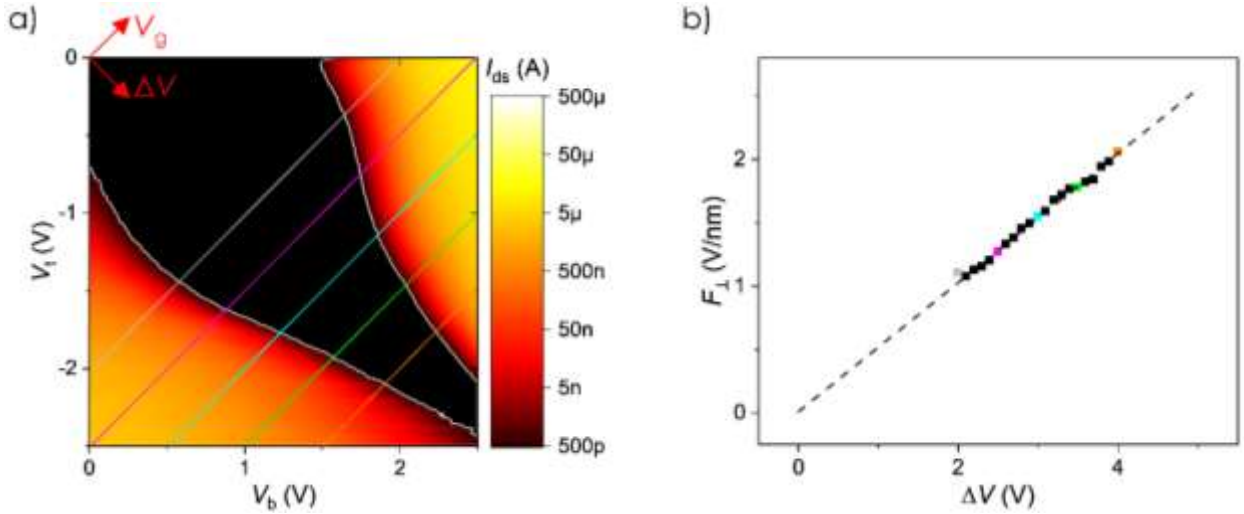


Figure 2 Transport measurement of dual ionically-gated bilayer WSe_2. a) Map of I_{ds} vs. (V_b, V_t) for bilayer WSe_2. As the perpendicular electric field, $F_\perp$ (controlled by $\Delta V = V_b - V_t$), increases, the bandgap shrinks. Each colored line represents constant ΔV from 2 V (gray) to 4 V (orange). **b)** Calculated $F_\perp$ vs. ΔV from the map in *a*). The field should depend linearly on ΔV, so we form a fit to the data (dashed line). The colored dots correspond to the lines of constant ΔV in *a*). The largest ΔV we apply in the map is 5 V, where the fit shows that we reach a perpendicular field of ~2.5 V/nm.

Bond defects in graphene created by ultralow energy ion implantation

Presenting Author: Zviadi Zarkua[1]

Co-Authors: Renan Villarreal[1], Pin-Cheng Lin[1], Zviadi Zarkua[1], Harsh Bana[1], Hung-Chieh Tsai[2,3], Manuel Auge[4], Felix Junge[4], Hans Hofs¨ass[4], Ezequiel Tosi[5], Paolo Lacovig[5], Silvano Lizzit[5], Steven De Feyter[3], Stefan De Gendt[2,3], Steven Brems[2], E. Harriet ˚Ahlgren[6], and Lino M. C. Pereira[1]

[1]Quantum Solid State Physics, KU Leuven, 3001 Leuven, Belgium
[2]imec vzw (Interuniversitair Micro-Electronica Centrum), 3001 Leuven, Belgium
[3] Department of Chemistry, Division of Molecular Imaging and Photonics, KULeuven,3001Leuven, Belgium
[4] Institute of Physics, University of Gottingen, 37077 Gottingen, Germany
[5] Elettra Sincrotrone Trieste, Strada Statale 14 km 163.5, 34149 Trieste, Italy
[6] Faculty of Physics, University of Vienna, 1090 Vienna, Austria
Contact@E-mail: zviadi.zarkua@kuleuvenbe, renan.villarreal@kuleuven.be, lino.pereira@kuleuven.be

Ultralow energy (ULE) ion implantation is increasingly being applied to the modification of 2D materials, in particular, for substitutional doping and intercalation of graphene[1][2]. Implantation-induced defects, whether desired or not, have a strong impact on the properties of graphene[3]. While significant research has been devoted to vacancy-related defects, disorder induced by ion irradiation in the ULE limit, that is, for energies below the vacancy-formation threshold, remains poorly understood. Here, we focus on that regime and report the formation of defects resulting from the breaking of C-C sp2 bonds and formation of C-substrate bonds (figure 1). The bond defect density is found to increase with increasing energy and atomic number of the implanted element [figure 2]. These findings significantly advance our understanding of disorder induced in graphene by ULE ion implantation, while simultaneously revealing the potential for exploiting such bond defects for physical or chemical functionalization. In particular, these bond defects can be generated with a high degree of selectivity, since they occur in the low-energy limit (at least down to 15 eV), significantly below the energies required to form stable vacancies.

References

[1] Lin P C, Villarreal R, Achilli S, Bana H, Nair M N, Tejeda A, Verguts K, De Gendt S, Auge M,Hofs ¨ass H et al. (2021) ACS Nano 15 5449–5458.
[2] Villarreal R, Lin P C, Faraji F, Hassani N, Bana H, Zarkua Z, Nair M N, Tsai H C, Auge M, Junge F et al. (2021) Nano Letters 21 8103–8110.
[3] Wei Y, Wu J, Yin H, Shi X, Yang R and Dresselhaus M (2012) Nature materials 11 759–763

Figures

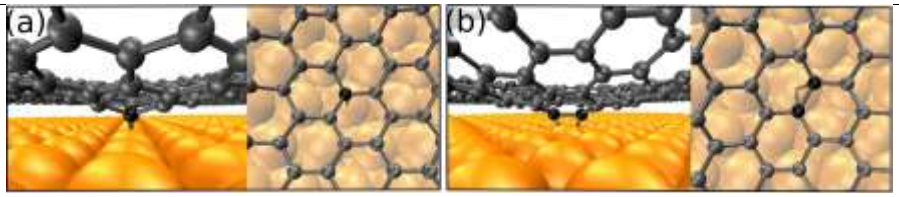


Figure 1: Snapshots of MD simulations after ion impact depicting the bond defects formed when the C-C sp2 bonds (grey) are broken and the displaced C atoms (black) form new bonds with the Pt surface (orange). Examples with side and top view of (a) one and (b) two bond defects.

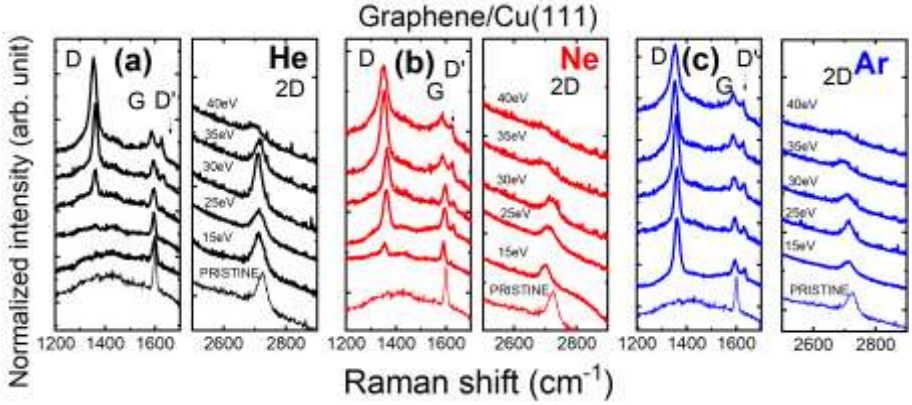


Figure 2: Raman spectra for Gr/Cu, pristine and implanted with He, Ne and Ar, for implantation energies between 15 eV and 40 eV. The implantation energies and the positions of the D, G, D' and 2D bands of graphene are indicated (D band corresponds to defective Graphene).

Ordered arrays of quantum emitters from hydrogen-filled TMDC domes

Salvatore Cianci[a]
Elena Blundo[a], Giorgio Pettinari[b], Antonio Polimeni[a], Marco Felici[a]
a Physics Department, Sapienza University of Rome, Piazzale Aldo Moro 2, 00185, Rome Italy
b Institute for Photonics and Nanotechnologies, National Research Council, 00156, Rome Italy
salvatore.cianci@uniroma1.it

Abstract

Single-photon emitters (SPEs) have recently attracted a lot of attention from the 2D crystals community [1]. Monolayer-thick hydrogen-filled TMDC domes [2] (Fig. 1a) are presented as a new system for the formation of SPEs. The size and position of the domes is accurately controlled via the application of an H-opaque mask on the bulk crystal, prior to hydrogen irradiation [2]. Notably, capping of the domes with few-layer hexagonal boron nitride (h-BN) is sufficient to prevent their deflation at cryogenic temperatures, due to the condensation of H_2 (Fig.1 b). Second-order autocorrelation measurements confirm the single-photon nature of the domes' photoluminescence (PL) emission that appears at low temperatures (Fig. 1 c). This system provides a new method to create ordered arrays of site-controlled SPEs, without the need for the etching of the substrate, and with the exciting perspective of coupling the quantum emitters with the nano-mechanical resonator represented by the dome's membrane [3,4].

References

[1] S. I. Azzam et al., Appl. Phys. Lett., 118 (2021) 240502
[2] D. Tedeschi et al., Adv. Mater, 31 (2019) 1903795
[3] M. Munsch et al., Nat. Commun. 8 (2017) 76
[4] A. Castellanos-Gomez et al., Adv. Mater., 25 (2013) 6719

Figures

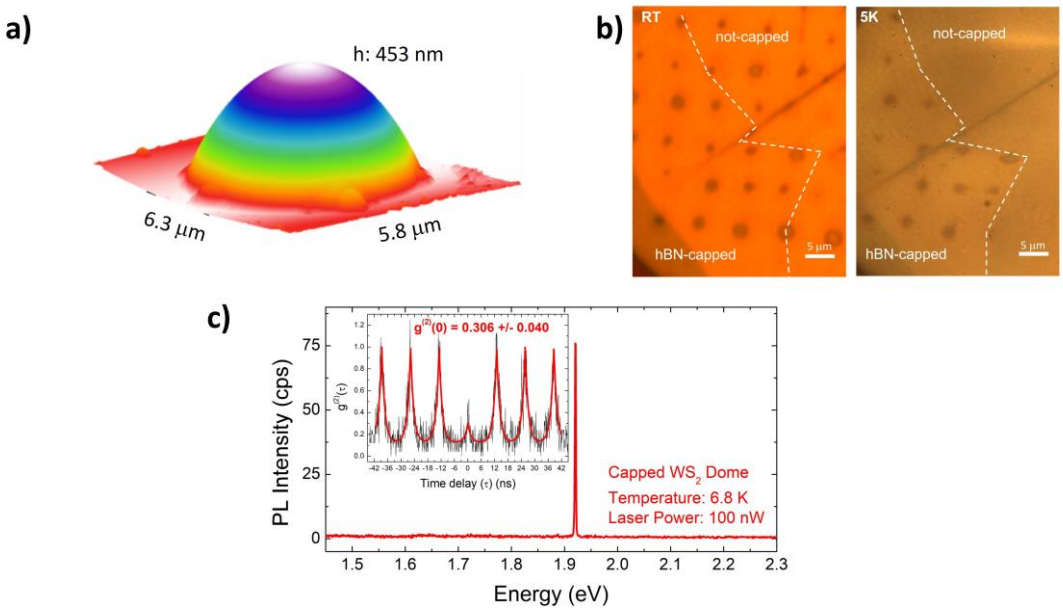


Figure 1: a) AFM image of a hydrogen-filled WS_2 dome, showing its spherical shape. b) Optical images of an ordered array of WS_2 domes capped with h-BN at RT and at 5 K. Only the domes capped with h-BN do not deflate at low temperature. Scalebar, 5 µm. c) PL spectrum at 6.8 K of a WS_2 dome capped with h-BN. The inset shows the second-order autocorrelation function, $g^{(2)}(\tau)$, proving the single-photon nature of the emission.

Spin and valley degrees of freedom in a bilayer graphene quantum point contact: Zeeman splitting and interaction effects [1]

Vanessa Gall
Rainer Kraft, Igor V. Gornyi, Romain Danneau
KIT, TKM, 76131 Karlsruhe, Germany
vanessa.gall2@kit.edu

We present a study on the lifting of degeneracy of the size-quantized energy levels in an electrostatically defined quantum point contact in bilayer graphene by the application of in-plane magnetic fields. We observe a Zeeman spin splitting of the first three subbands, characterized by effective Landè g-factors that are enhanced by confinement and interactions. In the gate-voltage dependence of the conductance, a shoulder-like feature below the lowest subband appears, which we identify as a 0.7 anomaly stemming from the interaction-induced lifting of the band degeneracy. We employ a phenomenological model of the 0.7 anomaly to the gate-defined channel in bilayer graphene subject to in-plane magnetic field. Based on the qualitative theoretical predictions for the conductance evolution with increasing magnetic field, we conclude that the assumption of an effective spontaneous spin splitting [2] is capable of describing our observations, while the valley degree of freedom remains degenerate [1].

References

[1] V. Gall, R. Kraft, I. V. Gornyi, R. Danneau, arXiv 2108.10098 (2022)
[2] H. Bruus, V. V. Cheianov, and K. Flensberg, Physica E: Low-dimensional Systems and Nanostructures 10, 97 (2001)

Figures

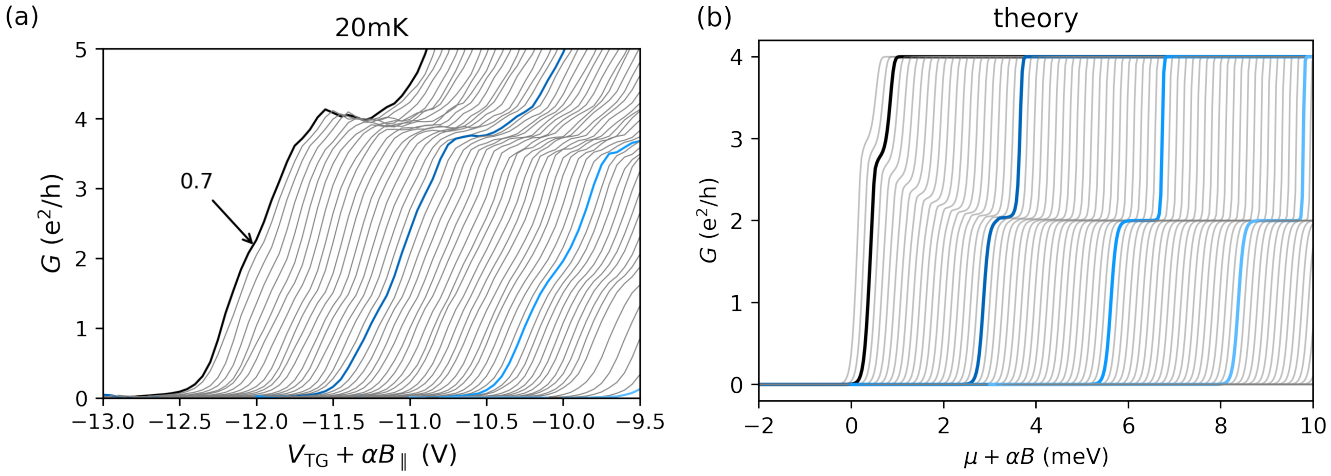


Figure 1: (a) Measured differential conductance G as a function of top-gate voltage V_{TG} for in-plane magnetic fields B between 0.2T (black line) and 6T (light blue line) with horizontal shifts. (b) Differential conductance obtained from the extension of the phenomenological model [2] to four subbands, assuming an effective spontaneous spin splitting. Colored lines correspond to the same magnetic fields as in (a). Figures taken from [1].

Spin lifetime in bilayer graphene quantum dots

Rebekka Garreis[1*]
L. M. Gächter[1*], J. D. Gerber[1], M. Ruckriegel[1], C. Tong[1], B. Kratochwil[1],
F. K. de Vries[1], A. Kurzmann[1,2], K. Watanabe[3], T. Taniguchi[3], T. Ihn[1], K. Ensslin[1], W. W. Huang[1]
[1]*ETH Zürich, Otto-Stern-Weg 1, 8093 Zürich, Switzerland*
[2]*2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany*
[3]*National Institute for Material Science, 1-1 Namiki, Tsukuba 30-0044, Japan*
[*]*These authors contributed equally*
garreisr@ethz.ch

Graphene is a promising candidate for future nano-electronic devices including building blocks for quantum information processing. Reasons are the expected long spin lifetimes and high carrier mobilities. So far, these spin lifetimes could only be estimated with a lower bound experimentally [1,2].

Here, we use bilayer graphene and its electrostatically induced band gap to fabricate a fully gate-defined device with quantum dots, where one is used as a charge detector [3]. The Coulomb resonances in the detecting dot are sensitive to individual charging events on another quantum dot nearby. The potential change due to single-electron charging causes a step-like change in the current through the charge detector which matches in signal to noise ratio the traditional semiconductors Si and GaAs. This high-quality detection signal allows us to confirm and investigate the dynamics of last electron\hole quantum dots. Furthermore, we can tune the tunnel barriers individually, such that the tunnel rates get low enough for time resolved measurements.

We apply the Elzerman single shot readout technique [4] to investigate the spin excited state of the first electron in our QD and find spin relaxation times of up to 30ms.

References

[1] L. Banszerus, K. Hecker, S. Möller, E. Icking, et al., arXiv:2110.13051 (2021)
[2] L. M. Gächter, R. Garreis, J. D. Gerber, C. Tong, et al., arXiv:2112.12091 (2021)
[3] A. Kurzmann, H. Overweg, M. Eich, et al., Nano Lett. 19, 8 (2019) 5216-522
[4] J. M. Elzerman, R. Hanson, L. H. Willems van Beveren, et al., Nature 430, 431 (2004)

Figures

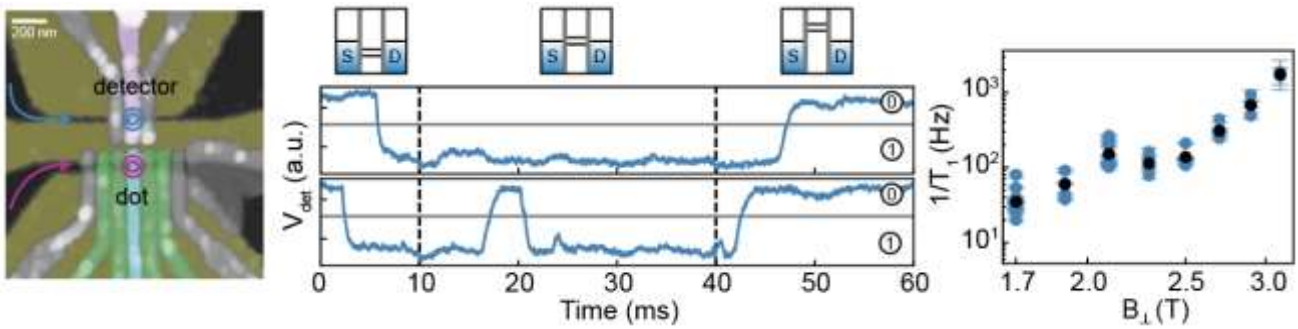


Figure 1: Left: False color atomic force micrograph of the gate structure used to for the quantum dots. Middle: Two exemplary time traces, where the lower one shows the signature 'blip' of an electron tunnelling out of the excited state and back in the ground state. Right: Magnetic field dependence of the measured spin relaxation time.

Viscous Point Contacts in Magnetic Field in Graphene and GaAs

Lev V. Ginzburg[1]
Yuze Wu[1], Marc P. Röösli[1], Pedro Rosso Gomez[1], Rebekka Garreis[1], Chuyao Tong[1], Veronika Stara[2], Carolin Gold[1], Hiske Overweg[1], Christian Reichl[1], Matthias Berl[1], Takashi Taniguchi[3], Kenji Watanabe[4], Werner Wegsheider[1], Thomas Ihn[1], Klaus Ensslin[1]
[1]*Solid State Physics Laboratory, ETH Zürich, CH-8093 Zürich, Switzerland*
[2]*CEITEC - Central European Institute of Technology, Brno University of Technology, Purkyňova 123, 612 00 Brno, Czech Republic*
[3]*International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
[4]*Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan*
glev@phys.ethz.ch

Abstract

In clean electron systems where the electron-electron mean-free path is much shorter than both the characteristic sample size and the transport mean-free path, electron transport is similar to viscous flow of a classical fluid [1]. Signatures of viscous electron transport have been observed in different materials, including graphene [2] and GaAs [3]. One of these signatures is the so-called superballistic flow, or the conductance of the point contact exceeding the ballistic (Sharvin) limit due to the collective movement of electrons [2, 4]. We investigate carrier transport through point contacts in graphene and GaAs as a function of magnetic field perpendicular to the plane of the system at different temperatures. A peak of the magnetoconductance is observed in both materials around zero magnetic field (see Figure). This peak is pronounced at elevated temperatures (~100 K for graphene, ~10 K for GaAs) and disappears at low temperatures. We interpret this peak as arising from the suppression of superballistic flow with magnetic field. We propose a scaling analysis based on hydrodynamics that makes predictions that agree with the observations.

References

[1] R. N. Gurzhi, JETP Lett. **17**, 521 (1963)
[2] R. Krishna Kumar, D. A. Bandurin, F. M. D. Pellegrino, Y. Cao, A. Principi, H. Guo, G. H. Auton, M. Ben Shalom, L. A. Ponomarenko, G. Falkovich, K. Watanabe, T. Taniguchi, I. V. Grigorieva, L. S. Levitov, M. Polini, and A. K. Geim, Nature Physics **13**, 1182 (2017)
[3] M. J. M. de Jong and L. W. Molenkamp, Phys. Rev. B **51**, 13389 (1995)
[4] H. Guo, E. Ilseven, G. Falkovich, and L. S. Levitov, PNAS **114**, 3068 (2017)

Figures

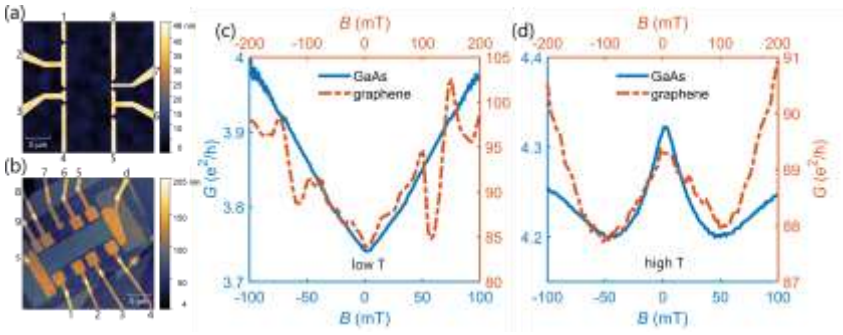


Figure 1: (a) and (b): AFM images of the GaAs and graphene devices. (c) Point contact conductance at low temperatures (0.3 K for GaAs, 4.2 K for graphene). (d) Point contact conductance at high temperatures (5 K for GaAs, 120 K for graphene).

Direct observation of ultraclean tunable band gaps in bilayer

E. Icking[1,2]
L. Banszerus[1,2], F. Wörtche[1], F. Volmer[1], P. Schmidt[1,2], C. Steiner[1,2], S. Engels[1,2], J. Hesselmann[1], M. Goldsche[1,2], K. Watanabe[3], T. Taniguchi[4], C. Volk[1,2], B. Beschoten[1] and C. Stampfer[1,2]
[1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany, EU
[2]Peter Grünberg Insitute (PGI-9), Forschungszentrum Jülich, Germany, EU
[3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan
[4]International Center for Materials Nanoarchitectonics,National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan
icking@physik.rwth-aachen.de

Controlling both the charge carrier density and the band gap of a semiconductor opens the doors to a wide range of applications, including, e.g., highly-tunable transistors, photodetectors, and lasers. Bernal-stacked bilayer graphene is a unique van-der-Waals material that enables the opening and tuning a band gap by applying an out-of-plane electric field [1]. While the first evidence of the tunable gap was found ten years ago [2], it took until recently to fabricate sufficiently clean heterostructures in which the electrostatically induced gap could be used to fully suppress transport or confine charge carriers [3].
Here, we present a detailed study of the tunable band gap in bilayer graphene using temperature-activated transport and finite-bias spectroscopy measurements. The high sensitivity of the latter method allows comparing different gate materials and device technologies, which directly affects the disorder potential in bilayer graphene. We show that graphite-gated bilayer graphene displays extremely low disorder and shows as good as no subgap states resulting in ultraclean tunable band gaps up to 120 meV. The size of the band gaps is in good agreement with theory and allows complete current suppression enabling a wide range of semiconductor applications.

References

[1] E. McCann, M. Koshino, Rep. Prog. Phys. 76 (2013) 056503
[2] J.B. Oostings *et al.,* Nature Materials, 7 (2008) 151
[3] H. Overweg *et al.*, Nano Lett., 8 (2018) 553

Figures

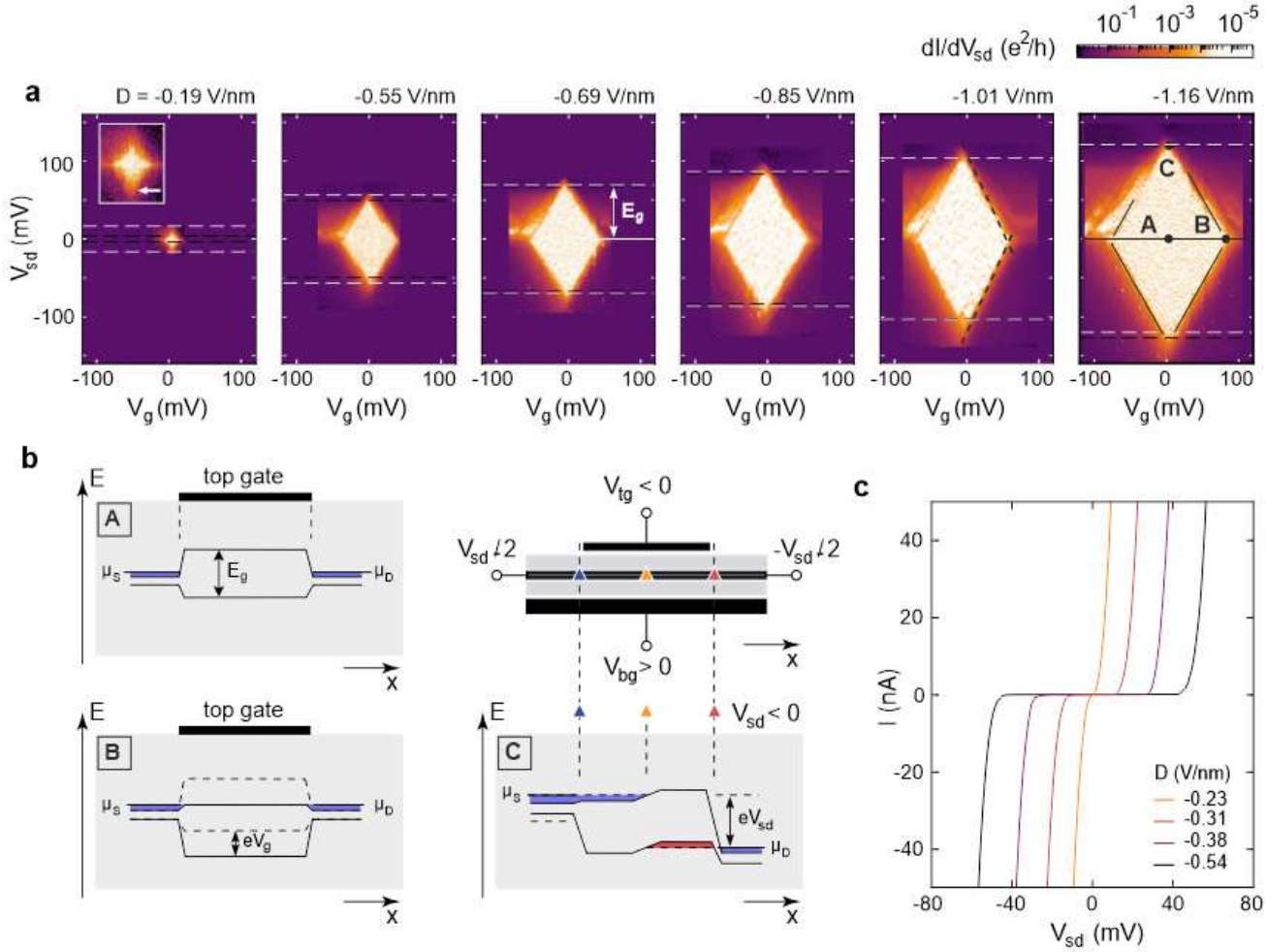


Figure 1: (a) Colour plot of the differential conductance dI/dV_{sd} of a Gr/hBN/BLG device, measured at T = 50 mK as a function of V_{sd} and V_g for different displacement fields (see labels). The white dashed lines denote the band gap predicted theory, the black dashed lines the effective band gap E^{eff}_g. The inset shows a magnification for displacement field D=−0.19 V/nm. Even at small displacement fields, the area of suppressed differential conductance presents a pronounced diamond shape. (b) Schematic representation of the various transport regimes at the points denoted as A, B, C in the rightmost diamond in panel (a). At $V_{sd} = 0$, the presence of the band gap strongly suppresses transport in the double-gated region (A). Transport is re-established either by changing the chemical potential in the double-gated region using the effective gate voltage V_g (B) or by applying a sufficiently large source-drain voltage V_{sd}, which changes the effective potential at the edges of the double-gated BLG, introducing charge carriers and forming a p-n junction. (c) I-V-characteristic of the Gr/hBN/BLG device for different values of D at constant V_g. The device shows a clear diode-like behaviour, with no appreciable sub-threshold current.

QUANTUM TRANSPORT IN STRAINED GRAPHENE BARRIERS

R. Kerjouan[1]
M. Rosticher[1], A. Pierret[1], M.-B. Martin[2], D. Dolfi[2], K. Watanabe[3], T. Taniguchi[3], S. Dhillon[1], B. Plaçais[1], M. Görbig[4] and J. Mangeney[1]
[1] *Laboratoire de Physique de l'Ecole normale supérieure, ENS, Paris, France*
[2] *Thales Research and Technology, Palaiseau, France*
[3] *National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan*
[4] *Laboratoire de Physique des Solides, CNRS, Université Paris-Sud, Orsay, France.*
romaine.kerjouan@phys.ens.fr

Strain provides a powerful tool to tailor the scalar and vector potentials which Dirac fermions undergo in graphene. This gave rise to new phenomena at the nanoscale such as giant pseudo-magnetic fields and valley polarization [1]. Here, we unveil the effect of deformation on the quantum transport across a barrier of strained graphene. We transfer a high-mobility exfoliated graphene flake covered by a thin hBN layer on a nanostructured hBN substrate. The Top-hBN layer and the graphene conform to the substrate, creating periodic strain-induced barriers for electrons over a length of 10 µm (Fig. 1. a) and b)). Using low-bias transport measurements, we observe the emergence of a broad satellite resistance peak at positive energy, in contrast with unstrained graphene [2] (Fig. 1 c) and d)). We show that this experimental trend is quantitatively described by the reduced transmission probabilities of ballistic electrons through a strain barrier that can be described by low-energy Hamiltonian of graphene modified by a scalar potential and a pseudo-vector potential (Fig 1 e)) [3]. Our results demonstrates that corrugated van der Waals heterostructures is a promising platform for strain engineering with a view to applications and fundamental physics.

References

[1] Hsu, C.-C. *et al.*, Sci. Adv., **6** : eaat9488 (2020)
[2] Huang, P. *et al.*, Nat Commun **11,** 863 (2020)
[3] McRae, A.C. *et al.*, Phys. Rev. Appl. **11**, 054019 (2019)

Figures

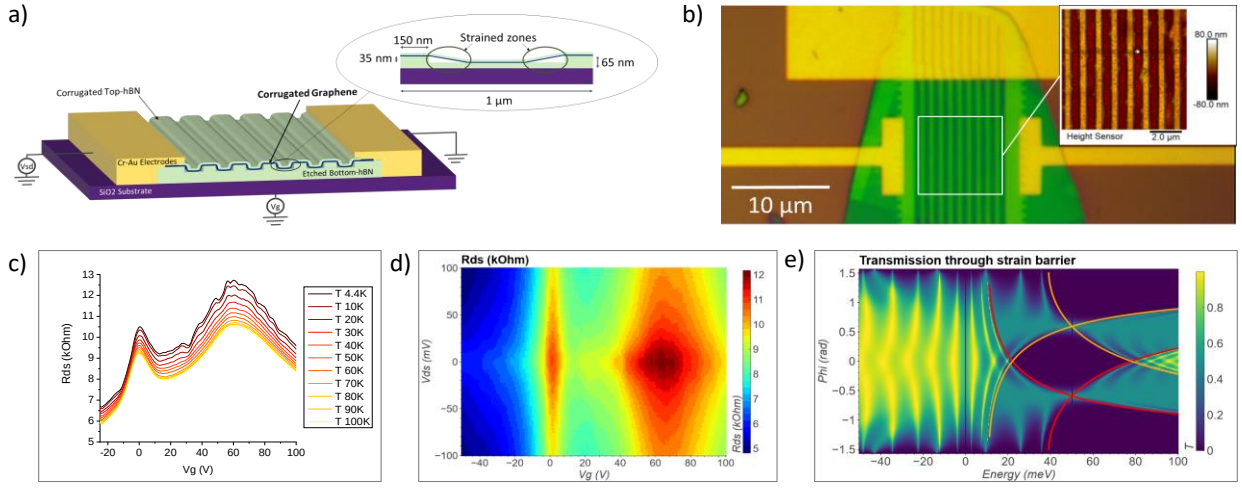


Figure 1: a) – Principle: Schematic view of the corrugated hBN/graphene/hBN device b) – Fabrication: Optical image of an encapsulated corrugated graphene. Inset: an AFM image of the corrugation c) R_{ds} as a function of Vg at zero-biais for different temperatures. d) Map of differential resistance R_{ds} as a function of the gate voltage V_g and of the bias voltage V_{ds} at T = 4.4 K. e) – Theory: Transmission probability through a 150nm long strain barrier with uniaxial strain ε= 2% in the zigzag direction as a function of the electron energy E and the incidence angle on the barrier φ. Red lines correspond to the limits of authorized incident angles for valley K and the orange ones for valley K'

Nonlinear Magneto-Transport in $MoTe_2$

Anna Carolina Marx Goncalves
Tian Liu, Bart J. van Wees and Marcos H. D. Guimaraes
Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, Groningen 9747 AG, The Netherlands
a.c.marx.goncalves@rug.nl

Molybdenum Ditelluride ($MoTe_2$) is a semimetallic transition-metal dichalcogenide (TMD) that can be found in two different structural phases, differing in the layer stacking angle: the monoclinic β-$MoTe_2$ and the orthorhombic γ-$MoTe_2$. A phase change from γ to β is expected in bulk $MoTe_2$ at a temperature of around 240 K [1]. To probe if this structural phase-change also happens in few-layer crystals and to understand its impact the on the band structure of this material, we perform temperature-dependent magentoresistance measurements on mechanically exfoliated few-layer γ-$MoTe_2$. We verify that the amplitude of the second-harmonic resistance signal scales with the strength of the magnetic field. This is consistent with the bilinear magnetoelectric resistance (BMR) effect, as reported before for WTe_2[2] and Bi_2Se_3[3]. The BMR effect is an important tool to explore the spin-dependent band structure of a material. Our results show a sinusoidal behaviour of the second-harmonic resistance signal as a function of the magnetic field angle, indicating an in-plane spin component consistent with a Rashba-like system (Fig 1). Moreover, we observe a sign change between 150 and 300 K, indicating a possible effect from a structural phase transition.

References

[1] HP Hughes and RH Friend, J. Phys. C: Solid State Phys., 11 (1978) L103
[2] P He, CH Hsu, S Shi et al, Nat. Comm., 10 (2019) 1290
[3] P He, SS-L Zhang, D Zhu et al, Nat. Phys., 14 (2018) 495

Figures

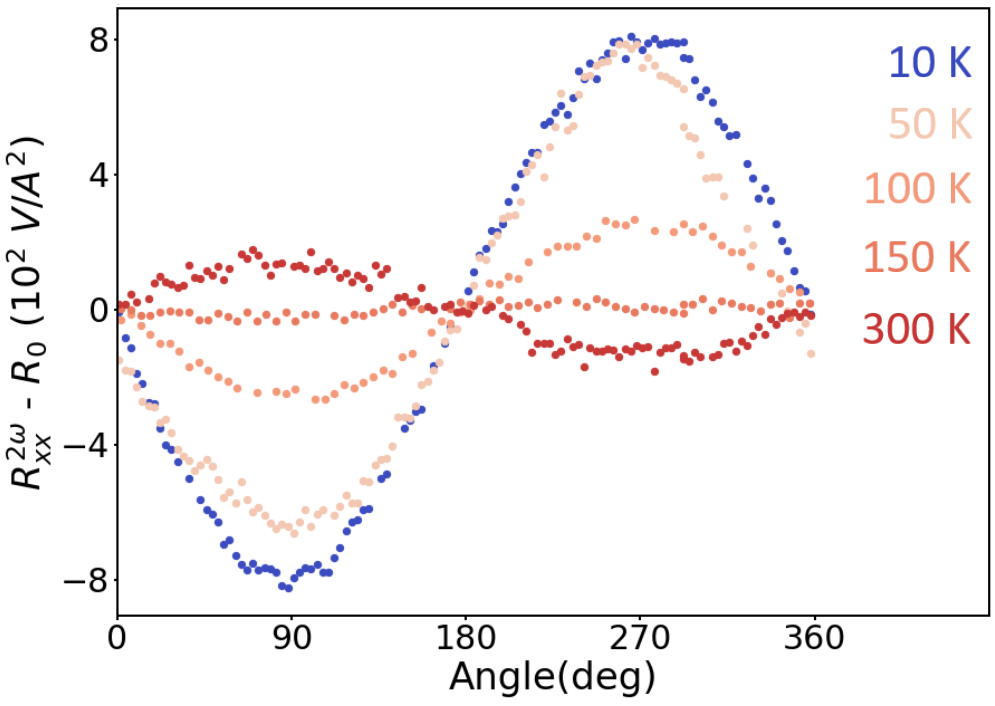


Figure 1: Second harmonic resistance measurement as a function of temperature in few-layer MoTe2.

Spin transport in edge-disordered graphene nanoribbons using machine learning

Méric M. Kucukbas†, Stephen R. Power ‡

†: *School of Physics, Trinity College Dublin, Dublin 2, Ireland.*
(kucukbam@tcd.ie)

‡: *School of Physical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland.*
(Stephen.r.power@dcu.ie)

Graphene nanoribbons (GNRs) have emerged as particularly attractive building blocks for nanodevices. At the nanoscopic scale, geometrical effects can critically affect electronic, magnetic, and transport properties. For example, zigzag-edged graphene nanoribbons (ZGNRs) can display spin-polarized edge states, which have very promising applications in future spintronics [1,2]. Despite impressive advances in fabrication techniques, it is an ongoing challenge to produce and control the desired transport properties in GNR devices. Therefore, characterising the effects of realistic disorders on device behaviour remains crucially important.

Theoretical predictions of spin properties, usually calculated using a time-consuming self-consistent (SC) procedure, can be intractable in computational resources required to deal with realistic system size. Machine learning (ML) techniques have been employed in various fields, such as consumer recommendation systems, protein folding and chemistry [3], to exploit patterns in data and make predictions. In this work, we address ML techniques to accurately estimate the magnetic moment profiles for arbitrarily large and disordered systems. Alongside conventional techniques, developing a neural network tool that accurately estimates the magnetic profile for large and disordered GNRs, we have conducted a thorough analysis on how the edge disorder impacts the robustness of spin-currents in GNRs. The robustness of spin-currents in ZGNRs is highly intertwined with the edge roughness profile at low energies. Whereas spin current is persistent in smooth-edged ribbons due to the absence of back-scattering possibilities, short-ranged scatterers in rough-edged profiles curtail the establishment of edge spin-polarised currents. Our results highlight how ML, by predicting quickly and accurately moment profiles for realistic systems, complements conventional transport techniques to study magnetism and spin transport in 2D materials.

References

[1] Fujita et al., J. Phys. Soc. Jpn. 65, 1920–1923 (1996)
[2] Son Y. et al., *Nature* 444, 347–349 (2006)
[3] Rupp M., IJQC, 115.10.1002/qua.24954. (2015)

Figures

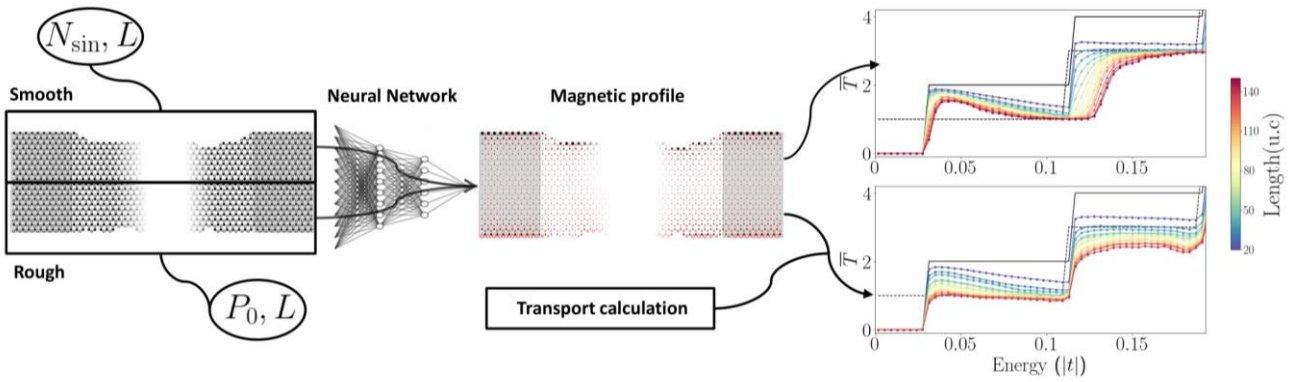


Figure 1: Workflow for the study of spin transport on disordered ribbons. We start by generating a large amount of configurations with different disorder profiles. The previously trained NN then accurately predicts the magnetic profile of the ribbons. This information allows to obtain the spin-polarised transmissions and to state the average behaviours of spin-currents according to the disorder profile.

Waveguide-Integrated Multilayer Platinum Diselenide Infrared Photodetectors

Shayan Parhizkar[1,2]
Maximilian Prechtl[3], Anna Lena Giesecke[2], Stephan Suckow[2], Sophia Wahl[4], Sebastian Lukas[1], Oliver Hartwig[3], Nour Negm[1,2], Arne Quellmalz[5], Kristinn Gylfason[5], Daniel Schall[2], Matthias Wuttig[4], Georg S. Duesberg[3], and Max C. Lemme[1,2]
[1]*Chair of Electronic Devices, RWTH Aachen University, 52074 Aachen, Germany*
[2]*AMO GmbH, Advanced Microelectronic Center Aachen, 52074 Aachen, Germany*
[3]*Institute of Physics, Faculty of Electrical Engineering and Information Technology (EIT 2) and Center for Integrated Sensor Systems, University of the Bundeswehr Munich, 85577 Neubiberg, Germany*
[4]*Institute of Physics IA, RWTH Aachen University, 52074 Aachen, Germany*
[5]*Division of Micro and Nanosystems, School of Electrical Engineering and Computer Science, KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden*
Parhizkar@amo.de

We demonstrate the use of layered platinum diselenide ($PtSe_2$) as an integrated infrared (IR) photodetector on Si photonic waveguides for the wavelength 1550 nm with high responsivity [1]. Our $PtSe_2$ photodetectors can be synthesized directly on photonic waveguides at CMOS-compatible temperatures using thermally assisted conversion (TAC) [2]. We have fabricated waveguide integrated $PtSe_2$ detectors using direct growth and conventional wet transfer, and we have studied the device performance and material quality of both approaches through analytical, electrical, and optical characterization.
The device schematic is shown in Fig. 1a. A responsivity of 11 mA/W was achieved for a directly grown $PtSe_2$ photodetector, with a fast response time of 8.4 µs. Our Fourier-transform infrared (FTIR) measurements indicate that $PtSe_2$ is also suitable for photodetection in the mid-IR regime, which expands its applications to broader fields such as gas detection, on-chip spectroscopy, or imaging. Our results show that multilayered $PtSe_2$ is a promising candidate for high-responsivity optoelectronic applications in commercial semiconductor technology platforms. This also includes silicon nitride (SiN) or other photonic platforms, as the direct TAC growth does not require any crystalline surfaces [3], in contrast to epitaxial processes.

References

[1] S. Parhizkar *et al.*, *ACS Photonics*, Mar. 2022
[2] C. Yim *et al.*, *ACS Nano*, Oct. 2016, vol. 10, no. 10, pp. 9550–9558
[3] M. Prechtl *et al.*, *Advanced Functional Materials*, Nov. 2021, vol. 31, no. 46, p. 2103936S

Figures

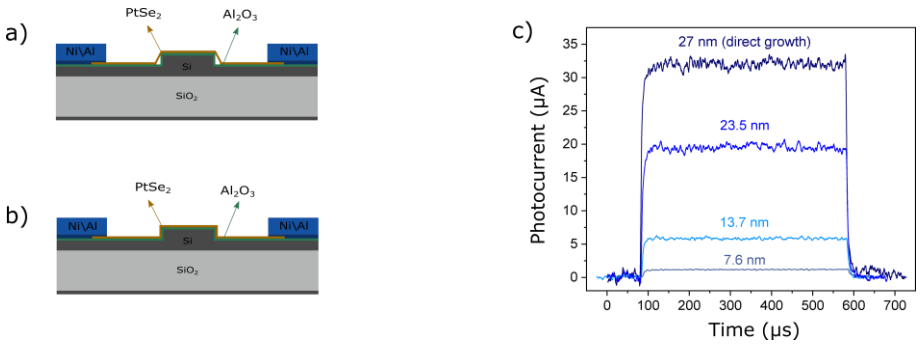


Figure 1: (a,b) Schematic cross sections of transferred and directly grown $PtSe_2$ detectors on the waveguides. (c) time resolved measurements of various $PtSe_2$ photodetectors. 27 nm thick $PtSe_2$ is grown directly on the waveguide using TAC and the other $PtSe_2$ films are integrated onto the waveguide using wet transfer.

Selective and Conformal Deposition of Layered 2D $PtSe_2$

Maximilian Prechtl
Shayan Parhizkar, Oliver Hartwig, Kangho Lee, Josef Biba, Tanja Stimpel-Lindner, Farzan Gity, Andreas Schels, Jens Bolten, Stephan Suckow, Anna Lena Giesecke, Max C. Lemme and Georg S. Duesberg
University of federal armed forces of Germany, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany
Maximilian.prechtl@unibw.de

2D $PtSe_2$ is continuing to attract considerable research interest due to its semi-metallic to semi-conducting transition at reduced thicknesses [1,2]. Here, we present method for conformal and selective deposition of $PtSe_2$ at back end of line compatible temperatures, enabling new fabrication routes through controlled patterned synthesis [3].
Platinum deposited by area selective atomic layer deposition is converted to $PtSe_2$ via thermal assisted conversion (Figure 1) [4]. The growth is described for a variety substrates and morphologies, including conformally on 3D topography, and is characterized by Raman, spatially resolved X-ray photoelectron spectroscopy, scanning and tunnelling electron microscopy. Furthermore, the fabrication of a 3D highly sensitive ammonia sensor and a fully integrated infrared-photodetector on silicon photonic waveguides demonstrate the versatility of this approach.

References

[1] L. Zeng et. al, NPG Asia Mater 10 (2018) 352–362.
[2] L. Ansari et. al., npj 2D Mater Appl 3 (2019) 1–8.
[3] M. Prechtl et. al, Adv Funct Materials 31 (2021) 2103936.
[4] C. Yim et. al, ACS nano 10 (2016) 9550–9558.

Figures

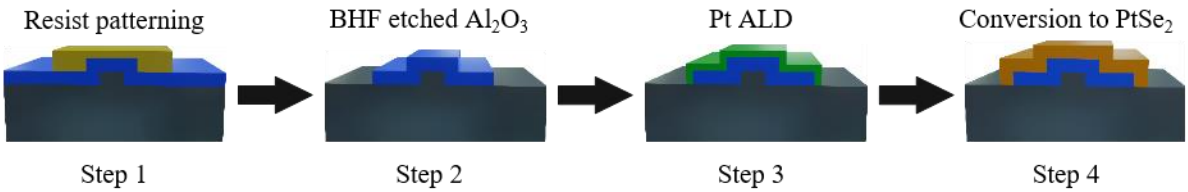


Figure 1: Process flow for selective and conformal deposition of $PtSe_2$. Al_2O_3 deposited by atomic layer deposition on silicon photonic waveguide structures is patterned using electron beam lithgraphy (Step 1). After buffered hydrofluoric acid (BHF) etching using the resist as hard mask (Step 2) Pt is selectively and conformally deposited (Step 3) and finally converted to $PtSe_2$ (Step 4).

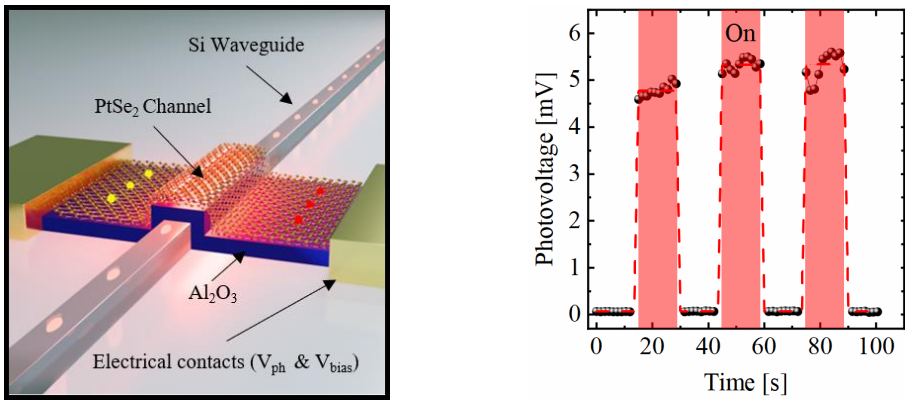


Figure 2: Left: Schematic of a fully integrated IR-photodetector using selectively and conformally deposited $PtSe_2$ as the active sensing material. Right: Time resolved photoresponse under pulsed excitation.

Impact of sapphire surface preparation on the MOCVD of epitaxial MoS_2 thin films

C. M. Schaefer[1]
A. T. Hoang[2], J. Caicedo Roque[1], A. Pérez-Tomás[1], J. Santiso[1], J.-H. Ahn[2], J. A. Garrido[1,3]
[1]*Catalan Institute of Nanoscience & Nanotechnology (ICN2), CSIC and BIST, Bellaterra, Spain*
[2]*Yonsei University, Seoul, Republic of Korea*
[3]*Catalan Institution for Research and Advanced Studies (ICREA), Barcelona, Spain*
christian.schafer@icn2.cat

In view of potential commercialization and mass production of electronic-grade transition metal dichalcogenides (TMDs) for next-generation semiconductor applications, metal-organic vapor deposition (MOCVD) is a promising fabrication method to meet the demand of wafer-scale homogenous TMD thin films. [1] In this context, sapphire (a-Al_2O_3) is an industrially important and widely available substrate enabling TMD epitaxy due to its crystallographic compatibility, and its stability in harsh growth conditions. Recent studies have highlighted controlled Al_2O_3 surface step topography to be key for edge-guided, unidirectional domain nucleation as a route towards single-crystalline TMDs, e.g. by using Al_2O_3 wafers with custom-manufactured miscut, [2] or by process control during MOCVD. [1] Moreover, Al_2O_3 surface reconstruction with Al-rich termination has been found to impact heteroepitaxial TMD registry. [3] However, optimal sapphire engineering for TMD epitaxy remains elusive due to case-specific, and complex interplay between surface and synthesis conditions, and the applied precursor chemistry. [4]

In this work, we investigate the MOCVD of epitaxial MoS_2 thin films grown from $Mo(CO)_6$ and dimethyl sulfide $(CH_3)_2S$ on distinct Al_2O_3 surfaces, employing in-depth characterization via atomic force microscopy (AFM), reflection high-energy electron diffraction (RHEED), grazing incidence X-ray diffraction (GIXRD), and Raman and X-ray photoelectron spectroscopy (XPS). We compare Al_2O_3(0001) substrates with standard ±0.2° and unconventionally low ±0.05° miscut angles after thermal annealing (1050-1200°C), resulting in atomically-smooth, stepped surfaces with defined step shape and terrace width. Additionally, we control sapphire termination in O_2- and H_2-annealing atmosphere, and obtain (1×1) and Al-rich $\left(\sqrt{31} \times \sqrt{31}\right)R9°$ reconstruction, respectively. While MOCVD on O_2-annealed sapphire yields uniform, triangular MoS_2 domains, MOCVD on H_2-annealed, ragged-stepped surface shows disturbed domains and increased carbon incorporation, as detected by Raman and XPS analyses, possibly induced by the Al-rich sapphire surface chemistry. This is further supported by AFM images showing non-uniform, mosaic terrace phase contrast on H_2-annealed sapphire, suggesting surface-selective MoS_2 domain nucleation, which sheds light on the importance of sapphire surface condition in organic chalcogen-source TMD epitaxy. Best results of commensurate domain growth were achieved on 1200°-O_2-annealed, 0.05°-miscut, straight-stepped Al_2O_3(0001), revealing a preferential $[11\bar{2}0]MoS_2(0001)//[11\bar{2}0]Al_2O_3(0001)$ epitaxial relationship in RHEED, and showing low, in-plane rotational twist below 2° in GIXRD Φ-scans.

This work provides fundamental understanding of large-scale synthesis of single-crystal 2D semiconductors from low-cost, low toxicity organic precursors on commercial substrates, which is highly relevant for their successful integration into industrial applications.

This work has received funding from the European Union's Horizon 2020 research & innovation program under grant agreement No. 732032 (BrainCom). We also acknowledge funding from the Generalitat de Catalunya (2017 SGR 1426). The ICN2 is supported by the Severo Ochoa Centres of Excellence programme, funded by the Spanish Research Agency (AEI, grant no. SEV-2017-0706). CMS acknowledges funding from ICN2's mobility program.

References

[1] Chubarov, M. et al., ACS Nano, 15, 2 (2021) 2532–2541
[2] Li, T. et al., Nat. Nanotechnol., 16, (2021) 1201–1207
[3] Mortelmans, W., et al., Nanotechnology, 30, (2019) 10
[4] Schaefer, C. et al., Chem. Mater., 33 (2021), 4474-4487

The Electroluminescence of Graphene/hBN transistors

Aurélien Schmitt[1]
Loubnan Abou-Hamdan[2,3], Marin Tharrault[1], David Mele[1], Aurélie Pierret[1], Michael Rosticher[1], Valentina Krachmalnicoff[2], Patrick Bouchon[3], Kenji Watanabe[4], Takashi Taniguchi[4], Christophe Voisin[1], Bernard Plaçais[1], Yannick de Wilde[2] and Emmanuel Baudin[1]
[1]*Laboratoire de Physique de l'Ecole Normale Supérieure, 24 rue Lhomond, 75005 Paris*
[2]*Institut Langevin, ESPCI Paris, Université PSL, CNRS, 1 rue Jussieu, F-75005 Paris, France*
[3]*DOTA, ONERA, Université Paris-Saclay, F-91123 Palaiseau, France*
[4]*Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan*
aurelien.schmitt@phys.ens.fr

In this talk, I will present our recent discovery of graphene's electroluminescence in the mid-infrared spectral range. Electroluminescence is the phenomenon by which a material emits light in response to the passage of an electrical current. In solids, it is the prerogative of semiconductors and related organic materials, and it results from the radiative recombination of electrons and holes. The semi-metallic nature of graphene a priori forbids electroluminescence. Nonetheless, electroluminescence is possible, because (i) of the remarkable inefficiency of the non-radiative carrier relaxation in graphene, and (ii) thanks to an original carrier injection mechanism specific to 2D semimetals: the Zener-Klein (ZK) tunnel conductance [1].
We study high mobility graphene field-effect transistors at room temperature and ambient conditions. These transistors consist of a monolayer graphene flake encapsulated in a hexagonal Boron nitride (hBN) insulator. When subjected to a large bias, we observe the appearance of a sharp emission peak at a photon energy of 190 meV (1532 cm^{-1}) in the far-field radiation spectrum of the transistor (see Fig. 1 (a)). Using a series of test experiments, we show the electroluminescent nature of this emission [2]. Using mid-infrared micro-spectroscopy, we observe both the blackbody radiation from the SiO_2 substrate – from which we deduce the out-of-plane cooling power- and the electroluminescent signal originating from the scattering of confined hyperbolic phonon-polaritons [3,4] of hBN (Fig. 1, panels (a) and (b)).

References

[1] W. Yang et al, Nature Nanotechnol. 2018, Vol. 13, 47
[2] A. Schmitt et al, *in preparation* (2022)
[3] K. Tielrooij et al, Nature Nanotechnol. 2018, Vol. 13, 41
[4] E. Baudin et al, Adv. Funct. Mater. 2020, Vol. 30, 8, p. 1904783

Figures

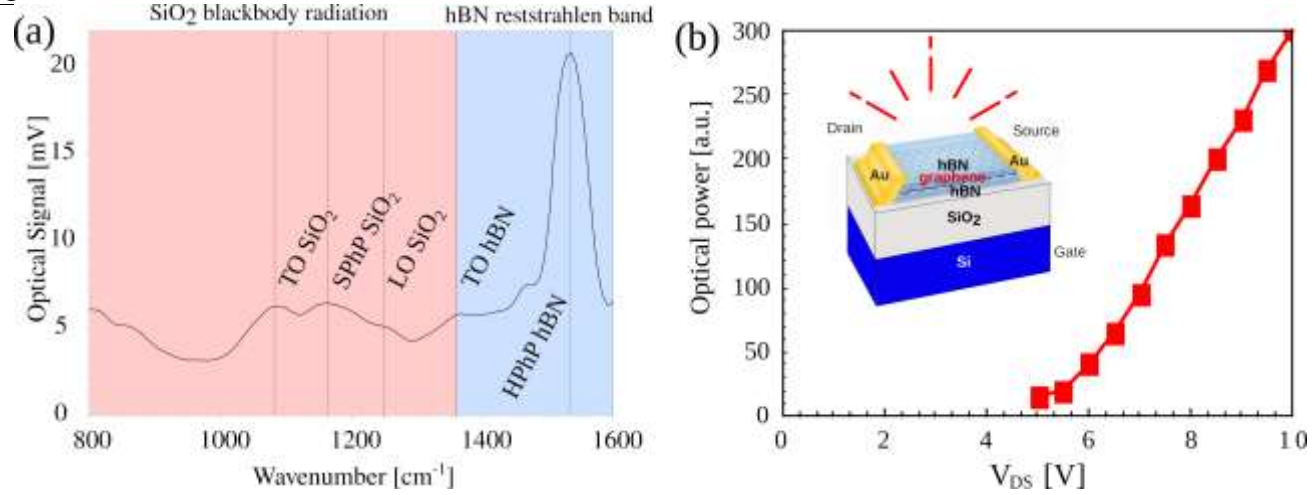


Figure 1: a) Mid-infrared emission spectrum of a graphene transistor, showing the blackbody radiation from the SiO_2 substrate and the electroluminescent signal from hBN. b) Integrated optical intensity as a function of bias voltage, revealing the electroluminescent threshold due to interband carrier injection.

MOCVD of Fully-Coalesced WS_2 Monolayers and W/WS_2 Heterostructures

Songyao Tang[1]
Annika Grundmann[1], Hleb Fiadziushkin[1], Zhaodong Wang[2], Susanne Hoffmann-Eifert[2], Amir Ghiami[1], Michael Heuken[1,3], Andrei Vescan[1], Holger Kalisch[1]
1. Compound Semiconductor Technology, RWTH Aachen University, Sommerfeldstraße 18, 52074 Aachen, Germany
2. PGI-7&10 and JARA-FIT, Forschungszentrum Jülich GmbH, Wilhelm Johnen Straße, 52428 Jülich, Germany
3. AIXTRON SE, Dornkaulstraße 2, 52134 Herzogenrath, Germany
tang@cst.rwth-aachen.de

Abstract

MOCVD has evolved as mainstream technique for large-scale production of 2D TMDC (transition metal dichalcogenide) materials. Despite fruitful works reporting on the successful synthesis of various types of TMDC with excellent performance in prototype devices, details of growth processes are not fully unveiled yet. For instance, as the coalescence of a monolayer (ML) is approaching, the probability of premature bilayer (BL) nucleation and growth will inevitably be rising. This phenomenon can be attributed to the limited supply of adatoms to lateral growth due to their finite migration length on top of ML domains. In order to fine-tune ML growth of 2D WS_2 films and suppress BL nucleation, a novel two-step migration-enhanced (ME) MOCVD process is introduced, which involves: (i) a nucleation stage at 700 °C and (ii) a lateral-growth stage at 820 °C with the W precursor ramped down to 25% of its initial flux.
All experiments were carried out on (0001)-oriented sapphire substrates in an AIXTRON CCS reactor in 7×2" geometry equipped with LayTec in-situ monitoring and surface temperature control. Pure H_2 was employed as the carrier gas, and $W(CO)_6$ and DTBS (di-tert butyl sulphide) were selected as metalorganic precursors. Prior to growth start, sapphire was H_2-desorbed at 1050 °C. 20 hPa was chosen as the reactor pressure during deposition to avoid parasitic C incorporation. With W adatoms being the growth-limiting species, a high S/W molar ratio (>6,000) was implemented.
By initializing the nucleation at 700 °C, a nucleation density of WS_2 as high as ~140 μm^{-2} can be achieved after 15 min, with a typical size of ML triangles ≤50 nm and a total ML coverage of ~24%. To suppress further ML nucleation, the lateral-growth stage is initiated by a temperature ramp of +70 K with +10 K/min. Simultaneously, the $W(CO)_6$ flux is ramped down (-75% over 144 min), aiming at reducing the arrival rate of W adatoms and thus increasing their migration length on the surface of the already-formed ML domains. By analysing the morphology, an estimate about the migration length on the coalesced ML can be concluded to be ≤100 nm. A fully-coalesced ML (>99%) with small BL coverage (<20%) can be obtained within 3 hours.
In the second part of the study, we present an alternative approach to the direct fabrication of metallic electrodes and conductive/reflective interlayers for TMDC devices by MOCVD and demonstrate the growth of both W films and W/WS_2 heterostructures. The underlying W thin film is deposited on sapphire via the decomposition of $W(CO)_6$ at 700 °C for 1 h (deposition rate roughly 5-10 nm/h). In the first experiment, a W/WS_2 heterostructure is synthesized via introducing both $W(CO)_6$ and DTBS into the reactor at 580 °C after W deposition in the same growth run. As indicated by Raman measurements and XPS (X-ray photoemission spectroscopy), the formation of a W/WS_2 heterostructure can be confirmed although the top WS_2 film still exhibits a similar nanocrystalline morphology as W. Although further optimization and characterization are required and ongoing, this study demonstrates the applicability of MOCVD to a large-scale fabrication of TMDC films and heterostructures for novel 2D devices.

Strain-tuning of the optoelectronic and spin properties of 2D crystals

Elena Blundo[1]
P.E. Faria Jr[2], A. Surrente[1], G. Pettinari[3], M.A. Prosnikov[4], K. Olkowska-Pucko[5], K. Zollner[2], T. Woźniak[6], A. Chaves[7], T. Kazimierczuk[5], M. Felici[1], A. Babinski[5], M.R. Molas[5], P.M.C. Christianen[4], J. Fabian[2], A. Polimeni[1]
1. Sapienza University of Rome, Physics Department, P.le Aldo Moro 2, 00185, Rome, Italy.
2. Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany.
3. Institute for Photonics and Nanotechnologies, National Research Council, 00156 Rome, Italy.
4. High Field Magnet Laboratory, Radboud University, 6525 ED Nijmegen, The Netherlands.
5. Institute of Experimental Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland.
6. Wrocław University of Science and Technology, 50-370 Wrocław, Poland.
7. Departamento de Fisica, Universidade Federal do Ceará, 60455-900 Fortaleza, Ceará, Brazil.
elena.blundo@uniroma1.it

Within the variegated family of two-dimensional crystals, semiconducting transition-metal dichalcogenides (TMDs) show alluring optoelectronic and spin properties in the monolayer (ML) limit, featuring a direct bandgap which results in an efficient visible/near-infrared light emission, and a strong spin-orbit coupling. Furthermore, these materials display exceptional flexibility and robustness and can be subjected to remarkable strains.
Here, we present a novel technique to induce controllable strain-fields in TMDs and study their effects. By hydrogen irradiation treatments, we induce the formation of hydrogen-filled nano- or micro- bubbles with single-layer-thickness, acting as efficient light emitters (Fig. 1(a-b)) [1]. These stable and robust nano- and micro-bubbles host complex strain fields, that cause dramatic changes in the TMD electronic properties. Photoluminescence steady-state and time-resolved studies highlight the occurrence of a strain-induced direct-to-indirect bandgap crossover (Fig. 1(c)) [2]. Magneto-optical experiments and ab-initio calculations allow us to achieve information on the spin and valley properties of k-space direct and indirect excitons. Indeed, a dramatic reduction of the exciton gyromagnetic (g-)factor is observed under high strains (Fig. 1(d)) and explained in terms of intriguing hybridisation mechanisms between the two exciton species. Our results reveal the potential of strain in tuning not only the emission energy of excitons in TMDs, but also their g-factor.

References

[1] D. Tedeschi, E. Blundo, M. Felici, G. Pettinari, B. Liu, T. Yildrim, E. Petroni, C. Zhang, Y. Zhu, S. Sennato, Y. Lu, A. Polimeni, Adv. Mater., 31 (2019), 1903795.
[2] E. Blundo, M Felici, T. Yildirim, G. Pettinari, D. Tedeschi, A. Miriametro, B. Liu, W. Ma, Y. Lu, A. Polimeni, Phys. Rev. Res., 2 (2020), 012024.

Figures

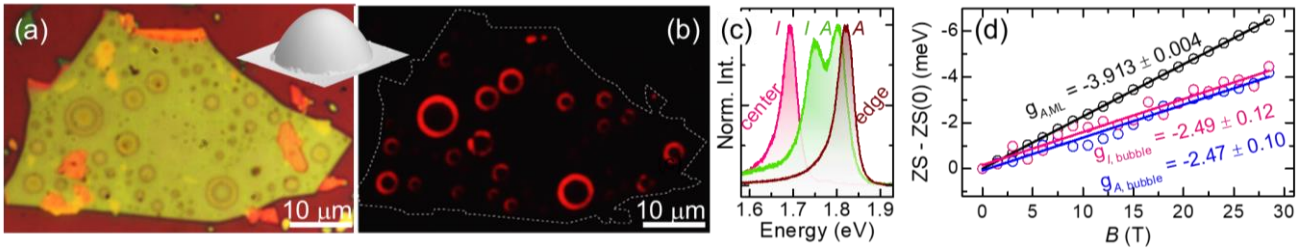


Figure 1: (a-b) Optical image of a WS_2 flake with micro-bubbles (a) and image of the luminescence measured from the same area (b) [2]. Inset: Atomic-force microscopy image of a bubble. (c) Typical spectra acquired while going from the edge of a bubble to its centre. At the edge the total strain ε_{tot} is ~2% and the direct *A* exciton dominates, while at the centre ε_{tot} ~4% and the indirect *I* exciton dominates. (d) Zeeman splitting (ZS) for increasing the magnetic field (up to 28.5 T) for an unstrained WS_2 ML (*A* exciton) and two WS_2 bubbles whose spectrum was dominated by *A* and *I* excitons.

Hubbard model for spin-1 Haldane chains

G. Catarina
J. Fernández-Rossier
International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal
goncalo.catarina@inl.int

The Haldane phase [1] for antiferromagnetic spin-1 chains is a celebrated topological state of matter, featuring gapped excitations and fractional spin-1/2 edge states. Here [2], we provide numerical evidence that this phase can be realized with a Hubbard model at half filling, where each s=1 spin is stored in a four-site fermionic structure (Fig. 1). We find that the noninteracting limit of our proposed model describes a one-dimensional (1D) topological insulator, and we conjecture it to be adiabatically connected to the Haldane phase. Our work opens a way to engineer spin-1 Haldane chains, as well as other spin networks, through a variety of physical systems that are being explored for quantum simulation of the Hubbard model [3,4]. We also show that our proposed Hubbard model accurately describes the observation of fractionalization in nanographene triangulene chains [5].

References

[1] F. D. M. Haldane, Phys. Rev. Lett., 50 (1983) 1153.
[2] **G. Catarina**, J. Fernández-Rossier, Phys. Rev. B, 105 (2022) L081116.
[3] T. Hensgens, T. Fujita, L. Janssen, X. Li, C. J. Van Diepen, C. Reichl, W. Wegscheider, S. Das Sarma, L. M. K. Vandersypen, Nature, 548 (2017) 70.
[4] A. Mazurenko, C. S. Chiu, G. Ji, M. F. Parsons, M. Kanász-Nagy, R. Schmidt, F. Grusdt, E. Demler, D. Greif, M. Greiner, Nature, 545 (2017) 462.
[5] S. Mishra, **G. Catarina**, F. Wu, R. Ortiz, D. Jacob, K. Eimre, J. Ma, C. A. Pignedoli, X. Feng, P. Ruffieux, J. Fernández-Rossier, R. Fasel, Nature, 598 (2021) 287.

Figures

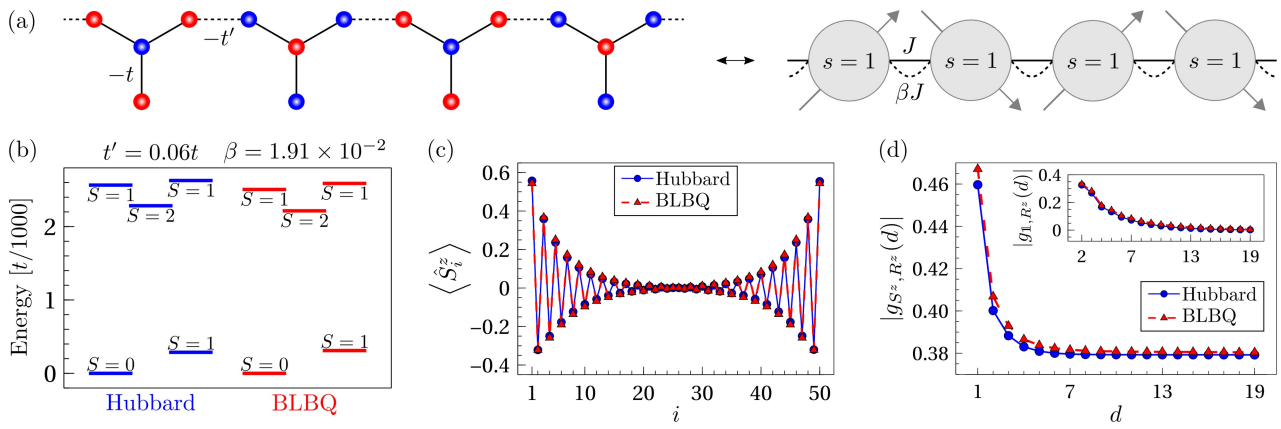


Figure 1: (a) Sketch of the general mapping between a 1D Hubbard lattice, with hoppings t and t', and an antiferromagnetic spin-1 chain, with bilinear (J) and biquadratic (βJ) exchange couplings (BLBQ model), where N four-site fermionic structures are mapped into N s=1 spins. (b) Comparison between the lowest-energy levels of N=10 four-site Hubbard and spin-1 BLBQ chains, with the corresponding total spin S indicated. Hubbard model results were obtained at half filling, for a Hubbard repulsion U=t, with t'=0.06t. BLBQ model parameters J=2.51×10^{-3}t and β=1.91×10^{-2} were fixed by matching the low-energy spectra of N=2 chains. (c) Average magnetization and (d) string order parameters, obtained for the lowest-energy state with $|S,S_z\rangle$=$|1,+1\rangle$ of N=50 four-site Hubbard and spin-1 BLBQ chains, using the same model parameters as in (b). The agreement between both models is apparent. The observation of spin-1/2 edge fractionalization (c), vanishing pure-string (d, inset) and nonvanishing spin-string (d) correlators are indicative of the spin-1 Haldane phase.

Re-entrant correlated insulator at 2π magnetic flux in magic-angle twisted bilayer graphene

Ipsita Das
Cheng Shen, Alexandre Jaoui, Jonah Herzog-Arbeitman, Aaron Chew, Chang-Woo Cho, Kenji Watanabe, Takashi Taniguchi, Benjamin A. Piot, B. Andrei Bernevig & Dmitri K. Efetov
ICFO - Institut de Ciencies Fotoniques, Castelldefels, 08860, Spain
ipsita.das@icfo.eu

The discovery of flat bands with non-trivial band topology in magic angle twisted bilayer graphene (MATBG) has provided a unique platform to study strongly correlated phenomena including superconductivity [1, 2], correlated insulators [3], Chern insulators [4] and magnetism. A fundamental feature of the MATBG, so far unexplored, is its high magnetic field Hofstadter spectrum. We report on a detailed magneto-transport study of a MATBG device in external magnetic fields of up to B = 31 T, corresponding to one magnetic flux quantum per moiré unit cell Φ_0. At Φ_0, we observe a re-entrant correlated insulator at a flat band filling factor of ν = +2, and interaction-driven Fermi surface reconstructions at other fillings, which are identified by new sets of Landau levels originating from these. These experimental observations are supplemented by theoretical work that predicts a new set of 8 well-isolated flat bands at Φ_0, of comparable band width but with different topology than in zero field [5]. Overall, our magneto-transport data reveals a qualitatively new Hofstadter spectrum in MATBG, which arises due to the strong electronic correlations in the re-entrant flat bands.

References

[1] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, *Nature*, **556**, (2018) 43.
[2] X. Lu, P. Stepanov, W. Yang, M. Xie, M. A. Aamir, I. Das, C. Urgell, K. Watanabe, T. Taniguchi, G. Zhang, et al., *Nature*, **574**, (2019) 653.
[3] Y. Cao, V. Fatemi, A. Demir, S. Fang, S. L. Tomarken, J. Y. Luo, J. D. Sanchez-Yamagishi, K. Watanabe, T. Taniguchi, E. Kaxiras, et al., *Nature* **556**, (2018) 80
[4] I. Das, X. Lu, J. Herzog-Arbeitman, Z. Song, K. Watanabe, T. Taniguchi, B. A. Bernevig and D. K. Efetov, *Nat. Phys.*, **17**, (2021) 710–714.
[5] J. Herzog-Arbeitman, A. Chew, D. K. Efetov, and B. A. Bernevig, Magnetic Bloch theorem and re-entrant flat bands in twisted bilayer graphene at 2π flux, To be published.

Figure

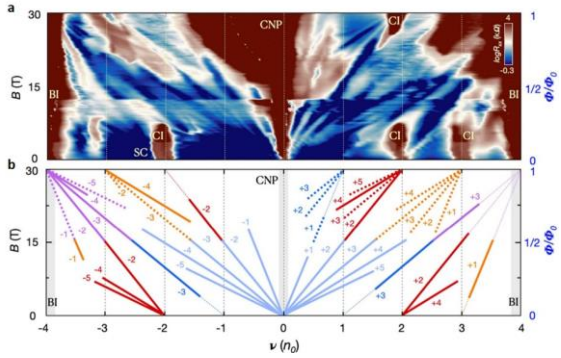


Figure 1: a) shows the colour plot of R_{xx} as a function of B and ν, for the full magnetic phase space from B = 0 T to B = 31 T and ν from -4 to 4. **b)** Schematics of all the LL gaps emerging from different fillings of the band from both zero magnetic field and one flux quantum of the moiré unit cell Φ_0. Different colours correspond to the new set of LL and reconstruction of Fermi surface.

Generalized Hamiltonian for Kekulé graphene and the emergence of valley-cooperative Klein tunnelling

Santiago Galván y García
Thomas Stegmann and Yonatan Betancur-Ocampo
Instituto de Ciencias Físicas, Universidad Nacional Autónoma de México
stegmann@icf.unam.mx, santiagogyg@icf.unam.mx

We introduce a generalized Hamiltonian describing not only all topological phases observed experimentally in Kekulé graphene (KekGr) but predicting also new ones. These phases show features like a quadratic band crossing point, valley splitting, or the crossing of conduction bands, typically induced by Rashba spin-orbit interactions or Zeeman fields. The electrons in KekGr behave as Dirac fermions and follow pseudo-relativistic dispersion relations with Fermi velocities, rest masses, and valley-dependent self-gating. Transitions between the topological phases can be induced by tuning these parameters. The model is applied to study the current flow in KekGr pn junctions evidencing a novel cooperative transport phenomenon, where Klein tunneling goes along with a valley flip. These junctions act as perfect filters and polarizers of massive Dirac fermions, which are the essential devices for valleytronics. The plethora of different topological phases in KekGr may also help to establish phenomena from spintronics.

Figures

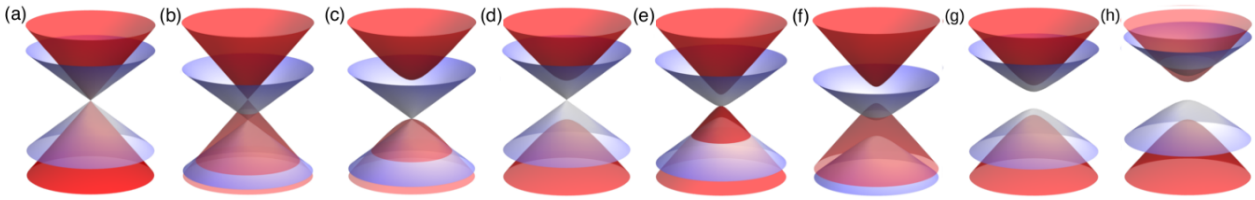


Figure 1: Topological phases of Kekulé graphene (KekGr). (a) and (b) Massless Dirac fermions in both valleys. (c) and (d) Chiral symmetry breaking in a single valley, where electrons behave as massless and massive Dirac fermions. (e) and (f) Quadratic band crossing point and valley-orbit coupling, respectively. (g) Zeeman-like effect. (h) Crossing of conduction bands.

References

[1] Santiago Galván y García, Thomas Stegmann and Yonatan Betancur-Ocampo, Generalized Hamiltonnian for Kekulé graphene and the emergence of valley-cooperative Klein tunneling, arXiv: 2111:06001

Towards large-scale conductance simulations of twisted bilayer graphene: the CAP-Chebyshev method

Santiago Giménez de Castro
Dario Andrés Bahamon Ardila
Universidade Presbiteriana Mackenzie, R. da Consolação, 930, São Paulo, Brazil
santiago.gdc@gmail.com

Realistic conductance simulations of real space twisted bilayer graphene (TBG) devices remains a demanding task. Specifically, the impact of moiré supercells on charge carrier transport requires giant system sizes to be considered. Near the magic angle, a single supercell reaches a size of about 15nm; ~10^4 cells are often needed to reach the experimentally relevant diffusive regime. Here, we develop a large-scale linear-response simulation ("CAP-Chebyshev") framework, combining Chebyshev approximation theory with a complex absorbing potential (CAP), to efficiently account for semi-infinite contacts [1-4]. Our method is benchmarked in a large 2-terminal 100nm x 100nm TBG model system containing 2.3x10^6 atomic orbitals. Exactly at the magic angle 1.24° , the conductance exhibits a peak at the charge neutrality point [Fig. 1] - evidence of a strong interlayer coupling state and a flat band supermetallic phase [5]. Finally, our framework is used to investigate the impact of twist-angle disorder on a 50nm x 50nm magic angle TBG device.

References

[1] Zheyong Fan, José H. Garcia, et. al., Physics Reports, Volume 903, 2021, Pages [1-69], DOI: 10.1016/j.physrep.2020.12.001.
[2] Simão M. João, Miša Anđelković, Lucian Covaci, Tatiana G. Rappoport, João M. V. P. Lopes and Aires Ferreira, R. Soc. open sci, 7:191809 (2020). DOI: 10.1098/rsos.191809
[3] D. A. Bahamon, G. Gómez-Santos, and T. Stauber, Nanoscale, 12, (2020), [15383-15392], DOI https://doi.org/10.1039/D0NR02786C.
[4] Vladimir A. Mandelshtam and Howard S. Taylor, J. Chem. Phys. 102, 7390 (1995); DOI: 10.1063/1.469051
[5] G. Bouzerar and D. Mayou, Phys. Rev. B 103, 075415 (2021), DOI: 10.1103/PhysRevB.103.075415

Figures

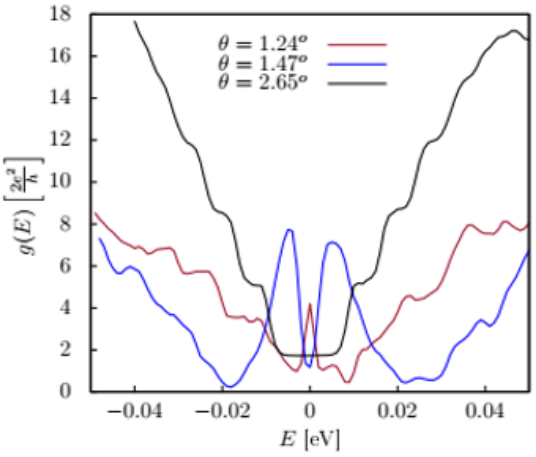


Figure 1: Conductance of the 100nm x 100nm TBG device as a function of the Fermi energy for different twist angles.

Investigation of Microstructure and Stability of Amorphous Boron Nitride upon Carbon Contamination

Onurcan Kaya[1]
Aleandro Antidormi[1]
Luigi Colombo[,2]
Stephan Roche[1,3]
[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), Bellaterra 08193, Barcelona, Spain*
[2] *Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, TX, 75080, United States*[3]*ICREA-Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain*
onurcan.kaya@icn2.cat

Abstract

The development of barrier materials with low dielectric constant, good thermal and mechanical properties is the key to progress in further miniaturisation of interconnects and downscaling microelectronics. A recent study [1] shows that amorphous boron nitride (aBN) possesses very low dielectric constant and low metal diffusivity and high mechanical robustness. Moreover, since it can be grown at much lower temperatures than its hexagonal counterpart (hBN), its integration in silicon-based devices is much easier. Even though the excellent properties of atomically thin aBN shows that it has great potential for barrier applications, we need a deeper understanding of its microscopic structure and its relationship with device performance. In this study, the effect of varying level of carbon (C) contamination on structural, thermal, and mechanical properties of aBN are investigated using classical molecular dynamics, given that C is one of the typical contaminants in dielectrics grown at lower temperature. To ensure the reliability of calculations and describe the atomic interactions more accurately, a Gaussian Approximated Potentials (GAP) is trained on a large dataset of atomic structures which obtained via ab-initio calculations [2]. We report that C contamination of aBN samples causes a significant change in thermal stability and mechanical properties.

References

[1] Hong, S., Lee, CS., Lee, MH. et al. Nature 582 (2020) 511–514.
[2] Bartók, A. P., Payne, M.C., Kondor, R, Csányi, G. Physical Review Letters, 104 (2010) 136403. Bartók, A. P., Csányi, G. Quantum Chem. 115 (2014), 1051– 1057.
[3] A. Antidormi, O. Kaya, L. Colombo, M. Lanza and S. Roche, in preparation.

Figures

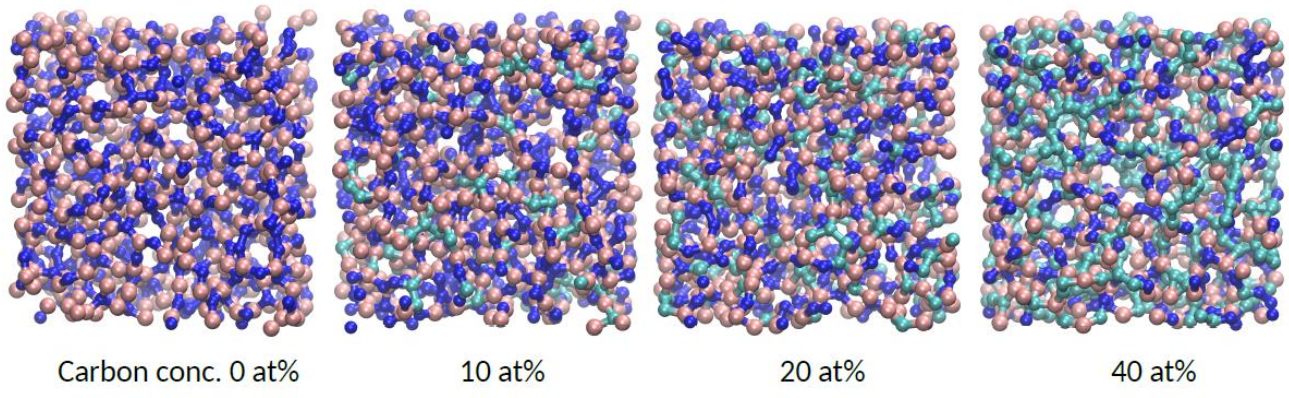


Figure 1: aBN samples with different level of C concentration.

Electronic structure of exfoliated black phosphorus and black arsenic measured by μ-ARPES

Florian Margot
Simone Lisi, Irène Cucchi, Edoardo Cappelli, Andrew Hunter, Ignacio Gutiérrez-Lezama, KeYuan Ma, Fabian von Rohr, Christophe Berthod, Marco Gibertini, Samuel Poncé, Nicola Marzari, Anna Tamai, Alberto Morpurgo and Felix Baumberger
Departement of quantum matter physics, University of Geneva, quai Ernest-Ansermet 24, CH-1211 Geneva, Switzerland
florian.margot@unige.ch

2D semiconducting materials represent an interesting opportunity to pursue the desired scaling of transistors for the electronic industry. Black phosphorus (BP) and black arsenic (BAs), direct gap semiconductor with strongly thickness dependent anisotropic properties, are two prominent candidates to replace silicon in this application. Experiments have indeed shown that in relatively thin body BP FETs (7-15 nm), mobilities of the order of 1000 cm^2/Vs can be achieved at room temperature, with appropriate on-off ratio of the order of 10^5 and near ideal subthreshold swing [1-3]. However, despite the interest in BP and a large body of transport and optical studies, little is known about its momentum-dependent electronic structure. To date, one thus commonly resorts to electronic structure calculations to interpret a range of measurements. Given the large spread of results from ab-initio electronic structures, the validity of this approach for the precise evaluation of device behaviour and performance is unclear. To remedy this situation, we performed μ-ARPES experiments on very thin encapsulated BP and BAs flakes. Our measurements unveil the layer-dependent quantum well state structure in the valence band of these two materials and allow us to characterise the anisotropy of the quasi-particle band structure near the valence band edge. We further propose an eight parameters tight-binding model that captures the dispersion of the subbands in the relevant portion of the Brillouin zone. Finally, our measurements also uncover satellite peaks, present for all measured thicknesses and for each subband. We tentatively attribute these satellites to electron-phonon coupling.

References

[1] Chen, X. et al., ACS nano, 2018, 12, 5003-5010
[2] Chen, X., Wu, Y., Wu, Z. et al., Nat. Commun 6, 2015, 7315
[3] Liu, X., Ang, KW., Yu, W. et al., Sci Rep 6, 2016, 24920

Figures

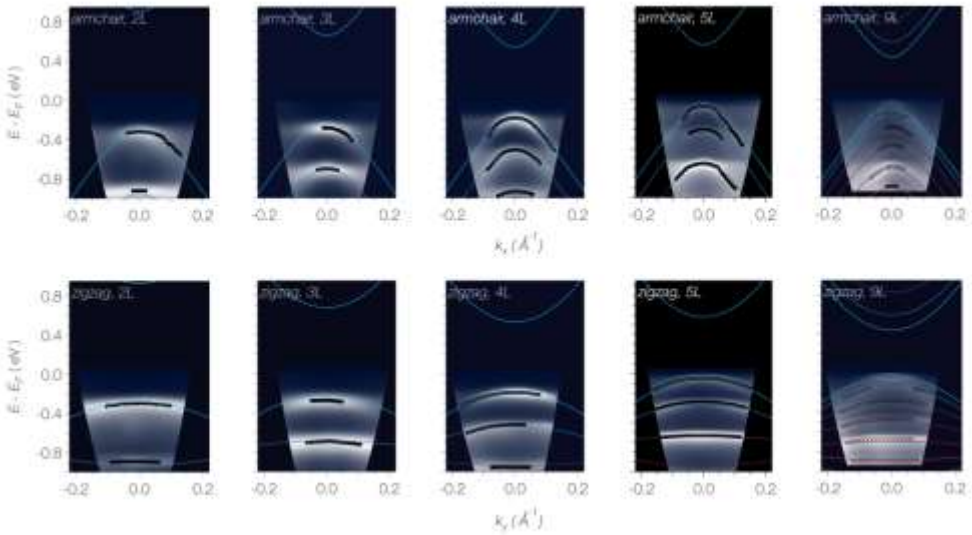


Figure 1: ARPES spectra acquired along the high symmetry directions (armchair, zigzag) of few layer encapsulated BP flakes from 2L to 5L and for a thicker 9L sample. Filled black and hollowed dots are extracted quasi-particle dispersions. The continuous coloured lines are the tight-binding bands obtained by fitting the extracted dispersions.

Rapid Analysis of 2D Material Quality Using Raman Spectroscopy

Crystal A. Nattoo*
Kirstin Schauble, Connor S. Bailey, Eric Pop
Dept. of Electrical Engineering, 420 Via Palou Mall, Stanford University, Stanford, CA, U.S.A.
*E-mail: cnattoo@stanford.edu

As silicon reaches its intrinsic scaling limits, emerging thin-film materials like transition metal dichalcogenides (TMDs) must adhere to the quality control standards set by decades of fine-tuning silicon. Unfortunately, current synthesis methods of TMDs by chemical vapor or atomic layer deposition (CVD or ALD) result in generally defective films, which hinder their electrical performance. In this work, we use Raman spectroscopy to study defects in MoS_2 and WSe_2 films prepared using multiple synthesis methods, including higher quality (exfoliated and CVD-grown) and more defective (e.g. sputtered or ALD) films. We optimized the tool parameters of our Raman system (532 nm laser) to obtain the best spectral resolution possible (0.3 cm^{-1}) and minimize peak fitting error. We then fit the Raman features of both TMDs using the phonon confinement (also known as RWL) model [1-4], which uses the phonon dispersion of the TMD to capture Raman peak broadening based on defect density ($n_D = 1/L_D^2$, where L_D is the defect spacing). Both MoS_2 and WSe_2 have phonon modes which are degenerate at the Γ point (momentum $k = 0$) but disperse away from it ($k \neq 0$), causing "shoulder" peaks to appear (Fig. 1a), whose intensities depend on the defectivity of the films. For WSe_2, we refer to the doubly degenerate peaks (E' and A_1') as E' for simplicity (Fig. 1b). Using the RWL model, we uncover three Raman-based metrics for the electrical quality (i.e. mobility) of MoS_2 and WSe_2: 1) the ratio between the shoulder and E' peak heights, 2) the E' peak width, and 3) the presence of the LA(M) peak. The first two criteria can distinguish between two (relatively) low-defect samples, whereas the third one appears only in more defective samples ($n_D > 2.5 \times 10^{13}$ cm^{-2}) [2]. By comparing this Raman analysis with measured electrical mobility, our Raman-based metrics allow us to predict the electrical quality of the TMDs without extensive device fabrication. We also uncover a clear difference in film quality after photolithography-based nanofabrication, suggesting that usual device fabrication [5] must be more carefully tuned in future work. In summary, we provide a comprehensive approach for evaluating the quality of TMD films from a variety of sources using simple Raman mapping, also correlating the Raman metrics with electrical data. This is an important advance which can be used to probe the electrical quality of TMDs using fast, nondestructive Raman characterization.

References

[1] K. Schauble, R. Grady, E. Pop, *Virtual MRS Spring/Fall Meeting*, Nov 2020
[2] S. Mignuzzi et al., *Physical Review B* 91 (2015) 195411
[3] W. Shi et al., *Chinese Physics Letters* 33 (2016) 057801
[4] W. Shi et al., *2D Materials* 3 (2016) 025016
[5] A. Daus, K. Schauble, E. Pop et al., *Nature Electronics* 4 (2021) 495

Figures

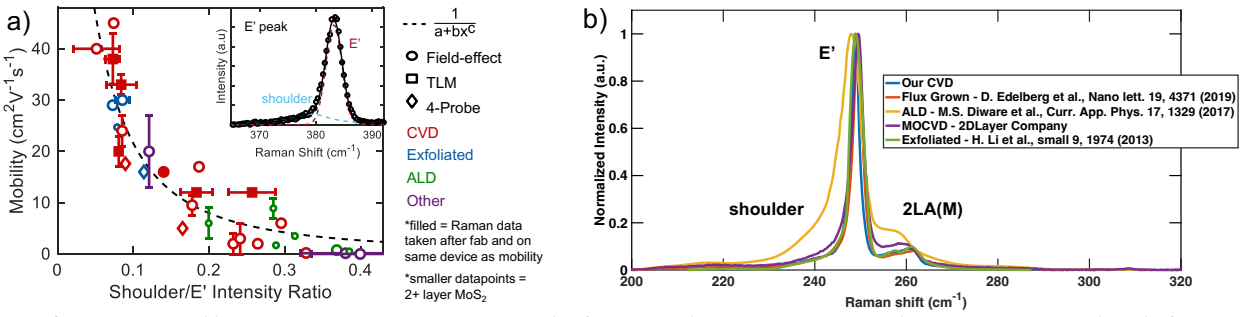


Fig. 1: a) MoS_2 mobility vs. shoulder/E' peak ratio from various sources; an inverse correlation is found. b) Raman spectra of WSe_2 obtained by various growth methods. Broader peak shoulders mark higher defect density. Our CVD sample is grown by solid-source (Se and WO_3 powder) CVD.

Transition metal dichalcogenide alloys as a new class of materials

K. Olkowska-Pucko[1],
E. Blundo[2], N. Zawadzka[1],T. Woźniak[3], S. Cianci[2], M. Felici[2], D. Vaclackova[4], P. Kapuściński[4], D. Jana[4], K. Watanabe[5], T. Taniguchi[5], C. Faugeras[4], M. Potemski[4], A. Babiński[1], A. Polimeni[2], and M. R. Molas[1]
[1]*Institute of Experimental Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland*
[2]*Physics Department, Sapienza University of Rome, Rome, Italy*
[3] *Wrocław University of Science and Technology, Wrocław, Poland*
[4]*Laboratoire National des Champs Magnétiques Intenses, CNRS, Grenoble, France*
[5]*National Institute for Materials Science, Tsukuba, Japan*
kolkowska@fuw.edu.pl

Alloys of semiconducting transition metal dichalcogenides have emerged as materials with tunable electronic structures and valley polarizations [1]. It is therefore crucial to uncover their basic optical properties. To this end we investigate the low-temperature magneto-photoluminescence (PL) of $Mo_{0.5}W_{0.5}Se_2$ monolayers (ML) embedded in hexagonal boron nitride (hBN) flakes. Measurements were done in magnetic field up to 30 T applied in two configurations: out-of-plane and in-plane. The $MoWSe_2$ ML should combine the properties of both "parents", which are members of different ML families. The WSe_2 MLs belong to the so called "darkish" MLs, in which the excitonic ground state is optically inactive (dark), while the $MoSe_2$ MLs is a representative of "bright" MLs with optically active ground state [2]. Fig. 1(a) shows the low-temperature PL spectra at selected out-of-plane magnetic field. The zero-field spectrum is composed of two well resolved emission lines, denoted as X and T, which we attribute correspondingly to the neutral and charged excitons. Upon application of the out-of-plane magnetic field, these transitions split into two circularly polarized components (σ±) due to the excitonic Zeeman effect. The extracted transition energies are presented in Fig. 1(b) along with the extracted effective Lande g-factors. It is seen that the g-factors for both transitions significantly differ. While the g-factor of the T line of about -4.7 is similar to the reported value of about -4 [3], the g-factor of the X line is much bigger and equal to -7.3. Using DFT calculations, we predict that this value can be understood in terms of particular arrangements of bands in the investigated $Mo_{0.5}W_{0.5}Se_2$ ML. Moreover, the application of the in-plane magnetic field to the ML reveals an additional line observed in magnetic fields above 25 T. This transition is apparent around 16 meV below the X line. We show how our results support the conclusion that the $Mo_{0.5}W_{0.5}Se_2$ ML is a "darkish" material with bright-dark exciton splitting very similar to that of the MoS_2 ML [4].

References

[1] Y. Meng, et al., Nano Letters, 19 1 (2019) 299-307
[2] M. R. Molas et al., 2D Materials, 4 (2017) 021003
[3] M. Koperski et al., 2D Materials, 6 (2019) 015001
[4] C. Robert et al., Nature Communication, 11 (2020) 4037

Figures

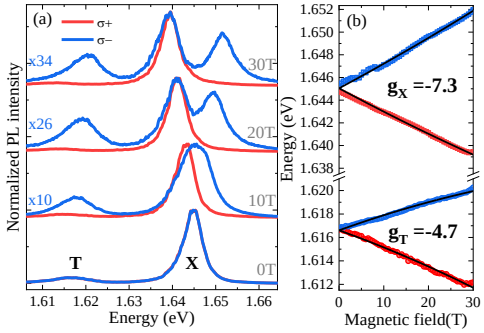


Figure 1: (a) Helicity-resolved PL spectra of $Mo_{0.5}W_{0.5}Se_2$ ML at selected out-of-plane magnetic fields. (b) Extracted transition energies of the X and T lines from panel (a).

Raman thermometry reveals efficient heat dissipation to air molecules in ultimately thin free-standing $MoSe_2$ crystals

D. Saleta Reig[1]
S. Varghese[1], R. Farris[1], A. Block[1], J. D. Mehew[1], O. Hellman[2], P. Wozniak[3], M. Sledzinska[1], A. El Sachat[1], E. Chávez-Ángel[1], S. O. Valenzuela[1,4], N. F. van Hulst[3,4], P. Ordejón[1], Z. Zanolli[5], C. M. Sotomayor Torres[1,4], M. J. Verstraete[6], and K.-J. Tielrooij[1,*]
[1]*Catalan Institute of Nanoscience and Nanotechnology (ICN2), BIST and CSIC, Campus UAB, 08193 Bellaterra (Barcelona), Spain.* [2]*Dept of Molecular Chemistry and Materials Science. Weizmann Institute of Science, Rehovoth 76100, Israel.* [3]*ICFO—Institut de Ciències Fotòniques, Mediterranean Technology Park, Castelldefels (Barcelona) 08860, Spain.* [4]*ICREA, Pg. Lluís Companys 23, 08010 Barcelona, Spain.* [5]*Chemistry Department and ETSF, Debye Institute for Nanomaterials Science, Utrecht University, the Netherlands.* [6]*Nanomat, Q-Mat, CESAM, and European Theoretical Spectroscopy Facility, Université de Liège, B-4000 Liège, Belgium.*
david.saleta@icn2.cat

The prospect of heat management via 2D-material based nanodevices is rapidly gaining attention within the scientific community. In this regard, the ability to tune thermal transport properties of layered materials is of utmost relevance [1]. Here, we study the effects of flake thickness (in the range of 0.7—50 nm) and environment (vacuum, air and N_2) on the in-plane thermal conductivity (κ) of large, free-standing $MoSe_2$ single-crystals using Raman thermometry [2,3]. In vacuum, our results suggest a weak influence of flake thickness on κ (~20—40 W m^{-1} K^{-1}) given by a unique in-plane cooling channel from the hot spot towards the heat sink. Interestingly, the results in air and N_2 environments suggest enhancement heat dissipation capabilities for the thinnest flakes. Owing to the large surface-to-volume ratio, the presence of an out-of-plane cooling channel from $MoSe_2$ to the environmental molecules results in an apparent thermal conductivity (κ_{app}) increase by an order of magnitude (~200 W m^{-1} K^{-1}) for monolayer flakes. We estimate the out-of-plane heat transfer coefficient to adjacent gas molecules as large as 60,000 W m^{-2} K^{-1}. These results are crucial for the design of (sub-)nanometer-thick TMD-based devices with engineered thermal properties that can be comparable, or even better, to those of nanometer-thick Si-based devices.

References

[1] Y. Zhao, et. al. *Advanced Functional Materials*. 30, 1903929 (2020)
[2] S. Varghese, et. al. *Journal of Physics: Materials*. 4, 046001 (2021)
[3] D. Saleta Reig, et. al. *Advanced Materials*. 2108352, (2022)

Figures

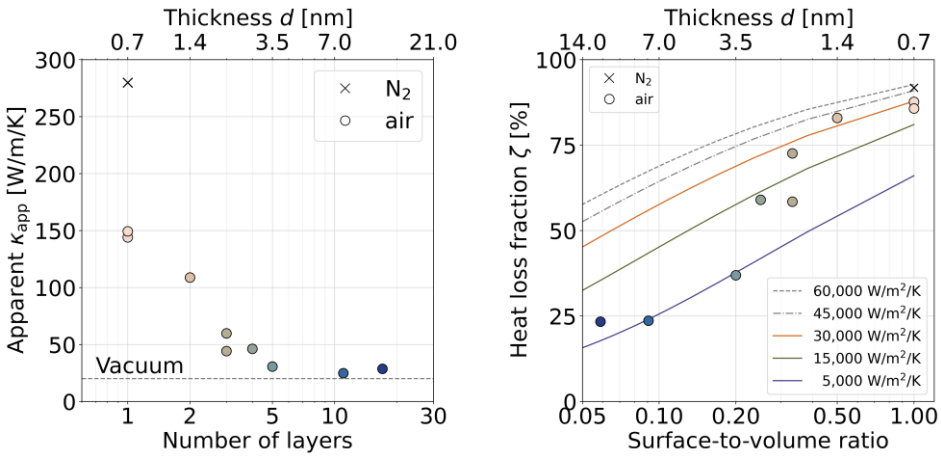


Figure 1: Apparent thermal conductivity of $MoSe_2$ in vacuum, air and N_2 environments (*left*) and heat loss fraction (in air and N_2) as a function of flake thickness (*right*).

Unbiased plasmonic-assisted graphene photodetectors in near and mid-wave infrared

Ioannis Vangelidis[1]
Sebastián Castilla[2], Tatiana Slipchenko[3], Luis Martín-Moreno[3], Frank H. L. Koppens[2], Andrea C. Ferrari[4], Nikos Pleros[5], Elefterios Lidorikis[1]
1 University of Ioannina, 45110, Ioannina, Greece
2 ICFO, 08860, Castelldefels (Barcelona), Spain
3 CSIC-Universidad de Zaragoza, 50009, Zaragoza, Spain
4 University of Cambridge, CB3 0FA, Cambridge, UK
5 Aristotle University of Thessaloniki, 57001, Thessaloniki, Greece
i.vangelidis@uoi.gr

Current photodetection technology aims for layouts with high optoelectronic bandwidth, improved efficiency, dynamic tunability, low energy operation and improved noise characteristics. Single layer graphene (SLG) can meet these requirements as it exhibits ultrafast interactions, high room temperature mobility, field-effect tunability and broadband detection. Furthermore, low noise graphene photodetectors (GPDs) can operate without bias exploiting the photo-thermoelectric (PTE) effect whereby an electronic temperature gradient gives rise to a photovoltage due to the Seebeck effect. To get a net photoresponse from such devices, the symmetry between source and drain contacts must be broken, which can be achieved by either an architecture supporting asymmetric light absorption [1] or by an asymmetric gate creating a lateral pn-junction configuration [2]. Here we present a self-consistent multi-physics modelling framework including optical, thermal, and electrostatic simulations, that can accurately predict the response of PTE driven GPDs operating in either free-space or integrated platforms and put the model to the test by direct comparison to experiments. We model two different devices. In the free-space device, we concentrate mid-infrared light onto a graphene pn junction by efficiently exciting hyperbolic phonon-polaritons (HPPs) in the hBN encapsulation through their resonant coupling with a metallic bowtie antenna and H-shape gates. This detector exhibited ultrafast response (response time < 15 ns (setup limited)) and excellent sensitivity with noise-equivalent power (NEP) down to 82 pw/√Hz at 6 μm [3]. Comparison to experiment is excellent. The integrated device, on the other hand, is a simple architecture of hBN/SLG/hBN on top of a Si waveguide with asymmetric Au contacts. Here, the optical mode excites and hybridizes with, surface plasmon polaritons (SPPs) on the Au contact edge increasing the local SLG absorption and resulting in strong temperature gradient across the SLG channel. We show that such device can reach for both transverse-electric and transverse-magnetic modes (at λ = 1550 nm) ~A/W responsivity and ~100 GHz operation speed at zero power consumption [4]. Comparison to experiments is again excellent. Our approach, fully validated by experiments, sets up a new standard for future simulation works and can be applied for modelling a range of different unbiased GPDs architectures.

References

[1] R. J. Shiue et al. Nano Letters, 15, (2015) 7288–7293
[2] S. Castilla et al., Nano Letters, 19 (5), (2019) 2765–2773
[3] S. Castilla, et al. Nature Communications, 11, (2020) 4872
[4] I. Vangelidis et al. ACS Photonics, under revision

Acknowledgement

The research leading to these results has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 881603 Graphene Flagship for Core3 and Grant Agreement No. 871391 Plasmoniac.

Quantifying Nanoscale Heat Transport in 2D Materials using Pre-Time-Zero Spatiotemporal Pump-Probe Microscopy

S. Varghese[1]
J. D. Mehew[1], A. Block[1], D. Saleta Reig[1], P. Wozniak[2], N. F. van Hulst[2,3], K. J. Tielrooij[1]

[1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, 08193 Barcelona, Spain
[2]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels, Barcelona, Spain
[3]ICREA-Institució Catalana de Recerca i Estudis Avancats, 08010 Barcelona, Spain
sebin.varghese@icn2.cat

2D materials, particularly transition metal dichalcogenides (TMDs), have attracted significant research interest over the last decade, due to their many intriguing electrical, mechanical, optical and thermal properties. In-depth knowledge and control of the heat transport properties in these materials will help heat management in optoelectronic devices and in designing novel materials for energy conversion and storage [1]. Consequently, scientists have developed several techniques [2] to determine the heat transport in 2D materials, nevertheless, these techniques usually require accurate knowledge of material parameters, such as thickness, optical absorption and heat capacity, and require relatively strong heating (ΔT ~ 100 K).

Here, we address these limitations and present a pre-time-zero spatiotemporal pump-probe microscopy technique [3] to obtain the in-plane thermal diffusivity (D) by examining the spatial profile at a small negative pump-probe delay time, i.e., when the probe pulses arrive before the pump pulses. Thus, the probe is sensitive to remnant heat created by previous pump pulses from the pulse train. We demonstrate the working principle of our method by quantifying the D of four TMD materials: $MoSe_2$ (0.18 ± 0.01 cm^2/s), WSe_2 (0.20 ± 0.03 cm^2/s), MoS_2 (0.35 ± 0.03 cm^2/s), and WS_2 (0.59 ± 0.07 cm^2/s), in excellent agreement with reported thermal properties [4, 5]. We also predict that our proposed technique will facilitate an advance in the understanding of unconventional nanoscale thermal transport phenomena, for example non-diffusive phonon transport, in low-dimensional materials.

References

[1] Zhao, Bei, et al., Adv. Funct. Mater. 31(48), 2105132 (2021).
[2] Sandell, Susanne et al., J. Appl. Phys. 128, 131101 (2020).
[3] Varghese, Sebin et al., *In preparation*.
[4] Jiang, Puqing, et al., Adv. Mater. 29 (36), 1701068 (2017).
[5] Reig, David Saleta et al., Adv. Mater. 2108352 (2022).

Figures

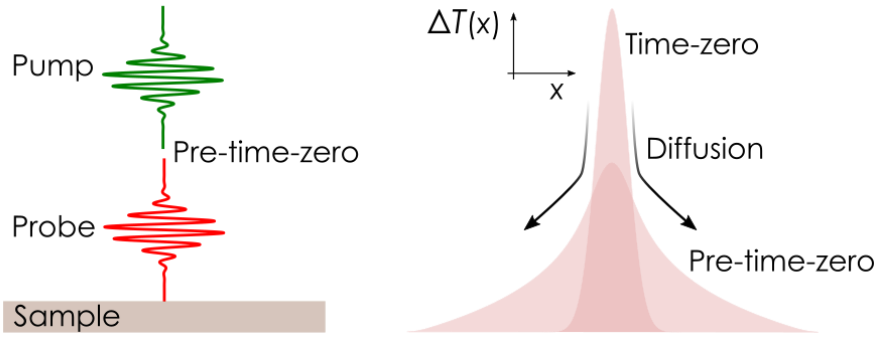


Figure 1: Schematic of the concept behind the pre-time-zero spatiotemporal microscopy technique.

Nonlocal Signals of Orbital Angular Momentum Transport in Graphene

L. M. Canonico
M. Vila, T.G. Rappoport and Stephan Roche
ICN2, Universitat Autònoma de Barcelona, Edifici ICN2 Campus de la, Av. de Serragalliners, s/n, 08193 Bellaterra, Barcelona, Spain.
luis.canonico@icn2.cat

In the last decades, the development and the successes accumulated by the field of spintronics demonstrated that harnessing the quantum degrees of freedom of the matter is the most prominent pathway for further technological development. Following the lines set by spintronics, orbitronics explore the possibility of manipulating the orbital angular momentum of the carriers to store and process information using the orbital Hall effect as its main lever. In resemblance to the spin Hall effect, the orbital Hall effect refers to the appearance of a transverse orbital angular momentum current after applying a longitudinal electrical field [1].

Contributions for the orbital Hall effect are separated as intra- and inter-atomic contributions since they refer to the localized atomic and motion orbital angular momentum, respectively [2,3]. Despite being studied for 3D systems, recent works on 2D materials demonstrated that materials with vanishing spin Hall conductivity such as mono- [4] and bilayers [5] of transition metal dichalcogenides and gaped graphene monolayers [6] exhibit finite orbital Hall conductivity, which is given by intra- and interatomic contributions, respectively. Using the Landauer-Büttiker formalism, we show that gapped graphene devices present sizable non-local resistance signals related to conduction through dispersive edge states. Investigating the effect of weak magnetic fields on these non-local signals, we find that they exhibit a chiral behaviour with the field direction. Our results suggest that the origin of the non-local resistance signals in gapped graphene devices are described more transparently in terms of orbital angular momentum currents.

References

[1] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, PRL, 95, (2005), 06660.
[2] Cysne, T. P., Bhowal, S., Vignale, G., & Rappoport, T. G. arXiv preprint arXiv:2201.03491 (2022).
[3] Pezo, A., Ovalle, D. G., & Manchon, A. arXiv preprint arXiv:2201.05807 (2022).
[4] Canonico, L. M., et al. PRB (R) 101 (2020) 161409.
[5] Cysne, T. P., Costa, M., Canonico, L. M., Nardelli, M. B., Muniz, R. B., & Rappoport, T. G. PRL, 126(5), 056601 (2021).
[6] Bhowal, S., & Vignale, G. Physical Review B, 103(19), 195309 (2021).

Figures

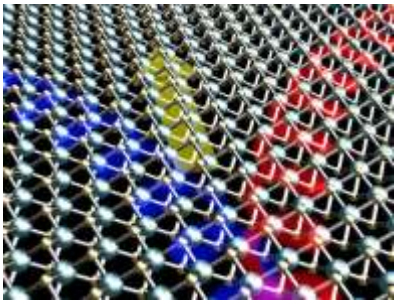


Figure 1: Schematic representation of the orbital-Hall effect.

Channel Hot Carrier degradation of back-gated GFETs exposed to air: a combined nanoscale and device level study

Sergi Claramunt[a]
Javier Arrese[b], Ana Ruiz[a], Marc Porti[a], Albert Cirera[b], Montserrat Nafria[a]
[a]*Electronic Engineering Department, Universitat Autònoma de Barcelona, Edifici Q-Carrer de les Sitges, 08193, Cerdayola del Vallés (Barcelona), Spain*
[b]*Electronics and Biomedical Engineering Department and Institute of Nanoscience and Nanotechnology, Universitat de Barcelona, Carrer Martí i Franqués 11, 08028, Barcelona, Spain*
sergi.claramunt@uab.cat

In this work we study the Channel Hot Carrier (CHC) degradation [1] of back-gated graphene field-effect transistors (GFETs) with their channel exposed to air [2]. A measurement-stress-measurement procedure has been adopted, using a Semiconductor Parameter Analyzer (SPA) to stress and measure at the device level and a Conductive Atomic Force Microscope (CAFM) to measure the graphene properties at the nanoscale. To combine measurements at the two scales, a custom-made system has been implemented, to avoid moving the sample and decrease the time between electrical stress and nanoscale measurement (Fig.1). Nanoscale measurements show a consistent decrease of conductive graphene area with longer CHC stress times(Fig.2a/b). Surprisingly, device level measurements do no show an important change in the conductivity of the GFET as one may expect from the level of damage of the graphene channel detected at the nanoscale. This could affect the performance, for example, of sensor devices that rely on the graphene channel morphology or defects to promote the detection of molecules [3].

References

[1] A.Bravaix, C.Guerin, V.Huard, D.Roy, J.-M.Roux, E.Vincent, Proc. IEEE Int. Rel. Phys. Symp. (IRPS) (2009), pp. 531-548.
[2] C.Hummel, F.Schwierz, A.Hanisch, J.Pezoldt, Journal, Physica Status Solidi B (2010), pp. 903-906
[3] X.Tang, M.Debliquy ,D.Lahem,Y.Yan, J.-P. Raskin, Sensors (2021), Art. No. 1443.

Figures

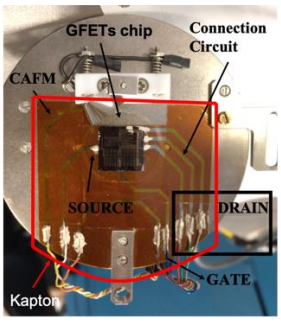


Figure 1: Detail of the custom-made measuring system of fully processed electron-devices. A switch unit (not shown) is used to alternate measurements between the SPA and CAFM. The connection of the DUT is done with an interface fabricated by means of ink-jet printing.

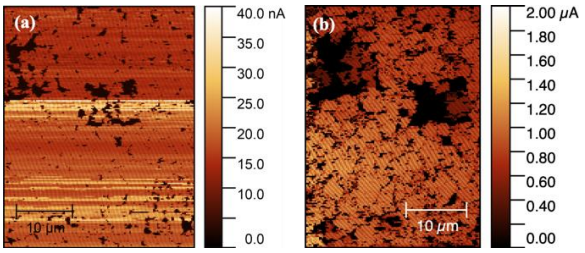


Figure 2: CAFM image of the same region of the graphene channel before (a) and after 8h of CHC stress (b). Black colour indicates zero current, that corresponds to the presence of defects in the graphene layer.

Alkali halide promoter induced synthesis of crystalline quasi-1D MoS_2 nanoribbons from PLD grown MoO_x precursor

Presenting Author Ganesh Ghimire[1]

Co-Authors

Raymond R. Unocic[2], Rajesh Ulaganathan[1], Denys I. Miakota[1], Oleksii Ilchenko[3], Henrik B. Lassen[4], Edmund Kelleher[4], Cheng Xiang[5], Tim Booth[5], and Stela Canulescu*[1]

[1]Department of Photonics Engineering, Technical University of Denmark, DK-4000 Roskilde, Denmark [2]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States, [3]Department of Health Technology Nanoprobes, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark, [4]Ultrafast Infrared and Terahertz Science Department of Photonics Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark, [5]Center for Nanostructured Graphene (CNG), Department of Physics, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

*Corresponding author: stec@fotonik.dtu.dk

Abstract

The large-scale and quality growth of semiconducting thin films form the basis of modern-day optoelectronic devices. Atomic-scale growth of traditional semiconductors is always a challenge for the growth community. To overcome this transition, metal dichalcogenides (TMDs) form a stable atomic-scale structure that provides the ideal platform. The large-scale growth of TMDs on various insulating substrates would open a promising way to explore the use of these materials. Among all the TMDs family, molybdenum disulfide (MoS_2) is a promising candidate for power electronics due to its sizeable direct bandgap and other electronic properties. Pulsed laser deposition (PLD) is one of the ways to synthesize MoS_2 monolayers, demonstrating its potential for 2D materials synthesis via both direct growth and a two-step process. In this work, we present a two-step process of synthesizing quasi-one-dimensional (1D) MoS_2 nanoribbons. In the first step, the precursor film of oxygen-deficient molybdenum oxide films is grown by PLD on sapphire, followed by sulfurization process at the desired temperature. The vapor-liquid-solid (VLS) growth of quasi-1D-MoS_2 nanoribbons gives highly anisotropic crystalline structure with a height of few nm, several microns in length, and a few hundred nm width. The VLS growth happens due to the reaction between MoOx precursors and sodium fluoride (NaF) as a promotor forming liquid droplets. An epitaxial growth of quasi-1D nanoribbons was analyzed by SEM, AFM, and Raman spectroscopy. The structural properties of the nanoribbons possess highly anisotropic crystalline structure with predominantly 3R-stacking, which was confirmed by STEM, polarization-dependent Raman spectroscopy, second harmonic generation microscopy, and terahertz spectroscopy. The electrical measurement on the nanoribbons demonstrates reasonable value of photocurrent. All the experimental results reveal the growth of high-quality quasi 1D-MoS_2 nanoribbons and their potential use in future optoelectronic applications. Details will be presented.

Figure

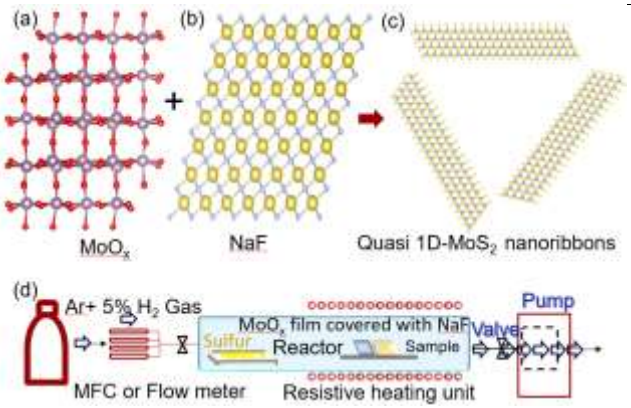


Figure 1. Schematic illustration of the sample preparation process. The schematics from a-d displayed the complete steps of fabricating the nanoribbons from oxide precursors.

The long march toward the zero friction

Mengzhou Liao
Department of Control Engineering, Faculty of Electrical Engineering, Czech Technical University in Prague, Technicka 2, 16627 Prague 6, Czech Republic
MengzhouLia@fel.cvut.cz

Abstract (Century Gothic 11)

Friction causes massive energy dissipation and mechanical abrasion between machine parts every year (costing approximately 119 EJ). Understanding the mechanism of the frictional processes and searching for an optimum material combination, ideally providing a near frictionless state, is thus essential. Recent works show that near-zero interface friction can be realized in twisted 2D materials or 2D heterostructures due to their ultra-flat interface PES. However, the origin of friction is complex. Suppressing one primary source will make friction from other mechanisms to the surface. Thus, toward the pure zero friction state will be a long march.

The speaker will report the friction phenomenon of superlubric MoS_2/graphite and MoS_2/h-BN van der Waals heterostructure interfaces in this talk. As shown in Figure 1, instead of reaching a frictionless state with a suppressed interface friction, in those interfaces, mechanisms like the edge pinning effect [1] and the variation of structure potential energy [2] start to dominate the friction processes and provide friction during the sliding and twisting. Those phenomena explain why it is hard to realize low friction on the macro scale. The speaker will further discuss the main challenges and give possible ways toward a pure zero friction state in the talk.

References

[1] Liao, M., Nicolini, P., Du, L., . . . Zhang, G. Nature Material (2022), 21(1), 47-53.
[2] Liao, M., Andrea, S., Du, L., . . . Zhang, G. The twisting dynamic of large lattice mismatch van der Waals heterostructures. Under reviewing.

Figures

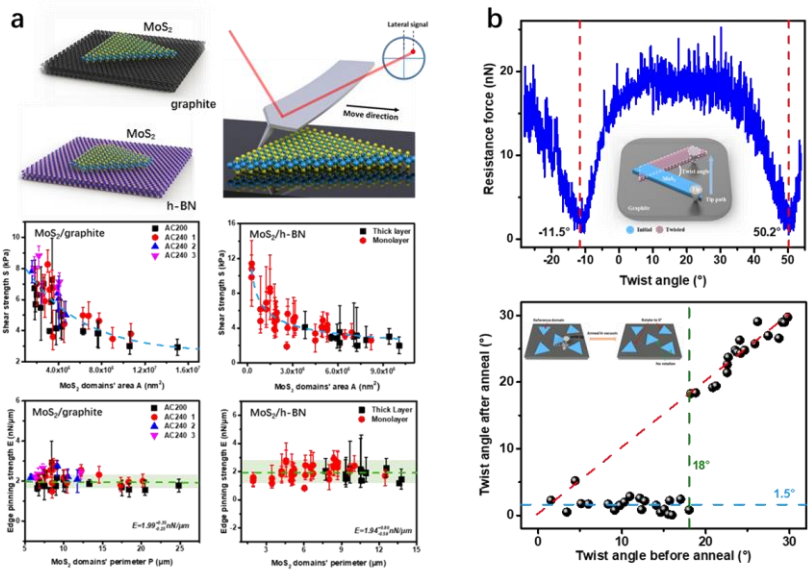


Figure 1: a and b: edge pinging effect (a) and twisting effect (b) of large lattice mismatch heterostructures at translational and rotational motions

Iron-rich phyllosilicates as 2D magnetic insulators

Aleksandar Matkovic[1],
Muhammad Zubair Khan[1], Oleg E. Peil[2], Apoorva Sharma[3], Daniel Knez[4], Lorenz Romaner[2], Dietrich R. T. Zahn[3], Ferdinand Hofer[4], Georgeta Salvan[3], Johann G. Raith[5], and Christian Teichert[1]
[1] *Institute of Physics, Montanuniversität Leoben, 8700 Leoben, Austria.*
[2] *Materials Center Leoben Forschung GmbH (MCL), 8700 Leoben, Austria.*
[3] *Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany.*
[4] *Institute of Electron Microscopy and Nanoanalysis (FELMI), 8010 Graz, Austria.*
[5] *Chair of Resource Mineralogy, Montanuniversität Leoben, 8700 Leoben, Austria.*
aleksandar.matkovic@unileoben.ac.at

Driven mainly by the potential applications in spintronics, magnetic random-access memories and sensing, magnetic van der Waals materials have attracted wide attention in the last years. While the field focuses mainly on layered iodides/tellurides and diluted layered magnetic semiconductors, the class of magnetic phyllosilicates remain almost completely unexplored. The mineral class of phyllosilicates (layered silicates) counts more than 240 members, and many of these minerals are known to incorporate local magnetic moment baring ions as Fe/Ni/Co which substitute Mg/Al sites in the central octahedral group. These naturally occurring magnetic van der Waals materials could serve as a novel and versatile platform for 2D magnetic insulators.
This talk will present our recent findings on layered magnetic minerals, mainly focusing on iron-rich talc (Fe:talc) [1] and briefly overviewing also iron-vermiculites, iron-micas, and iron end-members annite, and minnesotaite. These systems can serve as scaffolds to incorporate local magnetic moment baring ions in high concentration. Capping silicate/aluminate tetrahedral groups in their monolayers enable ambient stability, while magnetic properties could be tailored in the central octahedral site of the monolayers.

References

[1] A. Matković, *et.al.,* npj 2D Materials and Applications **5**, 2021, 94.

Figures

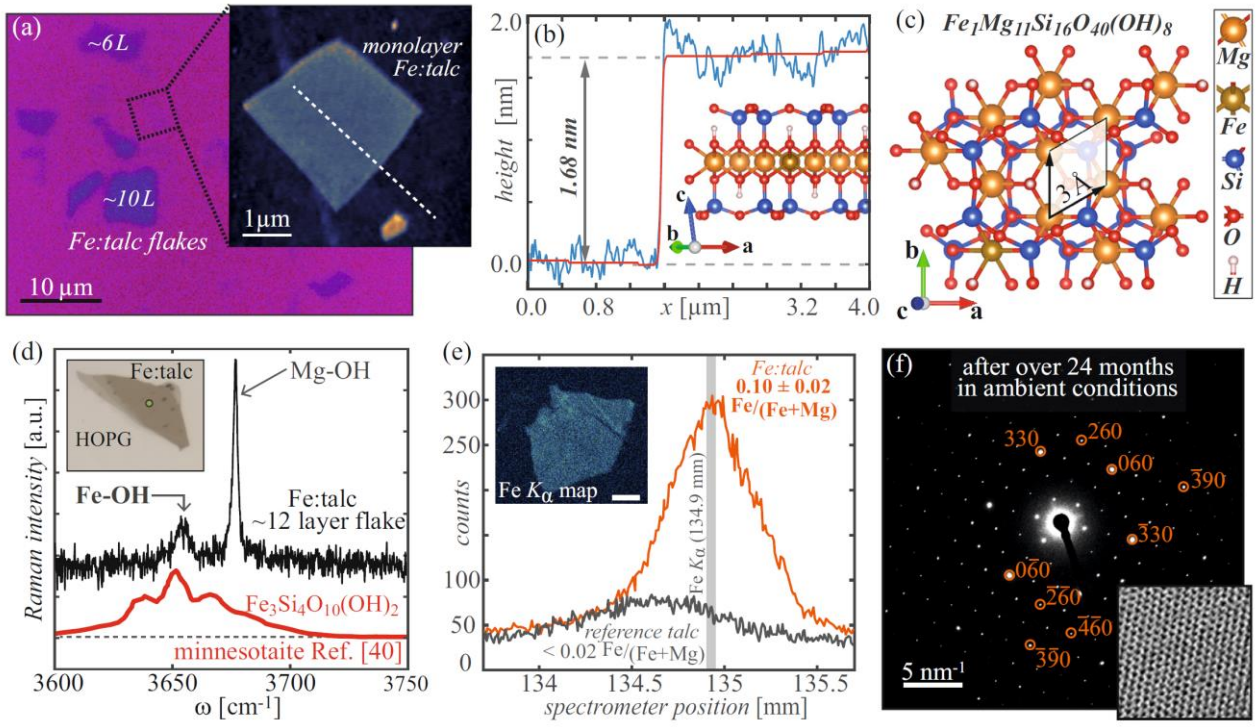


Figure 1: Iron-rich talc. (a) Fe:talc flakes exfoliated on SiO_2/Si (inset AFM topography of a monolayer). (b) step-edge cross-section with the side-view of the structural model. (c) top view of the Fe:talc-structure. (d) Raman spectra of the Mg/Fe-OH modes. (e) WDS quantitative analysis of Fe-concentration. (f) SEAD of a suspended flake after over two years of ambient storing.

Direct integration of PECVD-grown graphene electrodes into $Al_xGa_{1-x}N$-based UV-LEDs

Wolfgang Mertin
Umut Kaya, Hehe Zhang, Johanna Meier, Jan Mischke, Gerd Bacher
University of Duisburg-Essen & CENIDE, Bismarckstr. 81, 47057 Duisburg, Germany
wolfgang.mertin@uni-due.de

In anticipation of their promising applications in the deep-UV spectral range, e. g., for water disinfection or UV curing, $Al_xGa_{1-x}N$ LEDs have experienced a lot of attention over the last decade [1]. One challenge on the route to efficient devices is the poor conductivity of the p-$Al_xGa_{1-x}N$ top layer, and thus the limited lateral current spreading. While for blue GaN-based LEDs this issue is addressed by transparent conductive layers (TCL) of, e.g., ITO, this approach is not suitable for deep-UV LEDs due to the poor transparency of ITO in this spectral range.

Here, we present an attempt for using graphene as a TCL in UV $Al_xGa_{1-x}N$ LEDs, expanding our recent work on graphene TCL in blue GaN-based LEDs [2]. Hereby, graphene has been directly grown on p-doped $Al_xGa_{1-x}N$ via a PECVD process at low growth temperatures of around 670 °C to avoid surface degradation of the device. Using a N_2-flux of 200 sccm instead of the commonly used H_2, a CH_4 flux of 5 sccm and a growth time of 1 h, we routinely obtain few-layer graphene with a ratio of I_D/I_G between 1.1 and 2.7 and a ratio of I_{2D}/I_G between 0.3 and 0.95 on 2" wafers, with a maximum value of I_{2D}/I_G = 1.3 (Fig. 1). The graphene layers exhibit a transparency higher than 90 % in the UV range and a sheet resistance of less than 5 kΩ/sq. After integrating this graphene TCL directly into an $Al_xGa_{1-x}N$ LED, an I/V characteristic with a diode-like behaviour is obtained. The corresponding electroluminescence spectrum (Fig. 2) reveals a distinct UV emission with a peak wavelength at 273 nm, with some contribution in the VIS spectral range. Remarkably, UV emission starts already at about 4 V, indicating excellent current injection on both, the n- and the p-side of the device.

References

[1] M. Kneissl, Nature Photonics **13** (2019) 233
[2] J. Mischke et al., 2D Materials **7** (2020) 035019

Figures

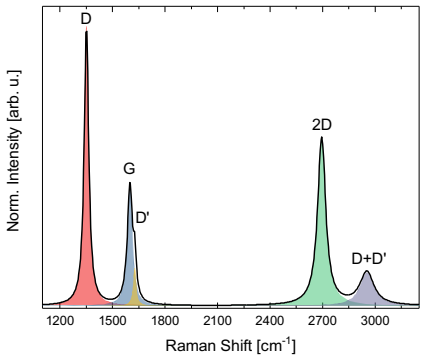


Figure 1: Raman spectrum of graphene directly grown on an $Al_xGa_{1-x}N$ LED.

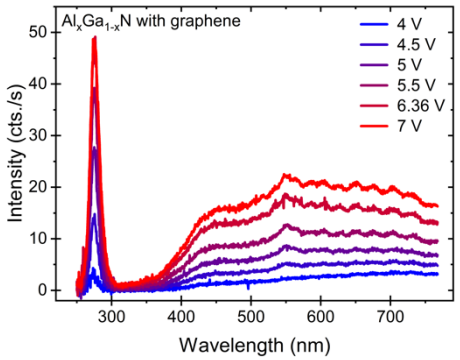


Figure 2: Electroluminescence spectra of an $Al_xGa_{1-x}N$ LED with graphene TCL for various voltages.

Acknowledgement

We thank Hans Lugauer and Adrian Avramescu from OSRAM Opto Semiconductors GmbH for their support during this work. This work is funded by the German Federal Ministry of Education and Research, funding program Photonics Research Germany, contract number 13N15461.

The use of MHz frequency surface acoustic waves for material exfoliation and manipulation

Amgad Rezk[1]
Heba Ahmed[1], Hossein Alijani[1], Ahmed El Chazaly[2], Joseph Halim[2], Per O. A. Persson[2], *Kourosh Kalantar-zadeh*[3], Johanna Rosen[2], Leslie Yeo[1]
[1]*RMIT University, 124 La Trobe street, Melbourne, Australia*
[2]*Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden*
[3]*School of Chemical Engineering, University of New South Wales (UNSW), Sydney, New South Wales 2052, Australia*
Amgad.rezk@rmit.edu.au

While the remarkable properties of 2D crystalline materials offer tremendous opportunities for their use in a variety of fields including electronics, energy systems, and catalysis, their practical implementation largely depends critically on the ability to exfoliate them from a 3D bulk state. Although much progress has been made to date to address this bottleneck, this goal nevertheless remains elusive, particularly in terms of a rapid processing method that facilitates high yield and dimension control. In this talk, I will be presenting an ultrafast exfoliation approach that utilises the use 10 MHz order nanometre surface vibrations known as surface acoustic waves (SAWs) comprised of a combination of extraordinarily large mechanical acceleration (≈10^8 ms^{-2}) and electric field (≈10^7 Vm^{-1}) [1], which in turn is shown to efficiently exfoliate a range of materials including 2D MXenes sheets[2], MXene quantum dots[3], MoS_2[4], amongst others (Fig 1). Additionally, these powerful surface acoustic waves, when used at lower powers, can be used to tailor the electrical and physical properties of many material classes including metal transition dichalcogenides (TMDs)[5] and metal organic frameworks (MOFs)[6].

References

[1] Amgad R Rezk, Heba Ahmed, Shwathy Ramesan, Leslie Y Yeo, Advanced Science, 2021, p. 2001983
[2] Hossein Alijani, Amgad R Rezk, Mohammad Mehdi Khosravi Farsani, Heba Ahmed, Joseph Halim, Philipp Reineck, Billy J Murdoch, Ahmed El-Ghazaly, Johanna Rosen, Leslie Y Yeo, ACS nano, American Chemical Society, 2021, pp. 12099--12108
[3] Ahmed El Ghazaly, Heba Ahmed, Amgad R Rezk, Joseph Halim, Per O A Persson, Leslie Y Yeo, Johanna Rosen, ACS nano, American Chemical Society, 2021, pp. 4287—4293
[4] Heba Ahmed, Amgad R Rezk, Benjamin J Carey, Yichao Wang, Md Mohiuddin, Kyle J Berean, Salvy P Russo, Kourosh Kalantar-zadeh, Leslie Y Yeo, Advanced Materials, 2018, p. 1704756
[5] Amgad R Rezk, Benjamin Carey, Adam F Chrimes, Desmond WM Lau, Brant C Gibson, Changxi Zheng, Michael S Fuhrer, Leslie Y Yeo, Kourosh Kalantar-Zadeh Nano letters, American Chemical Society, 2016, pp. 849--855
[6] Heba Ahmed, Amgad R Rezk, Joseph J Richardson, Lauren K Macreadie, Ravichandar Babarao, Edwin LH Mayes, Lillian Lee, Leslie Y Yeo, Nature communications, Nature Publishing Group, 2019, pp. 1--9

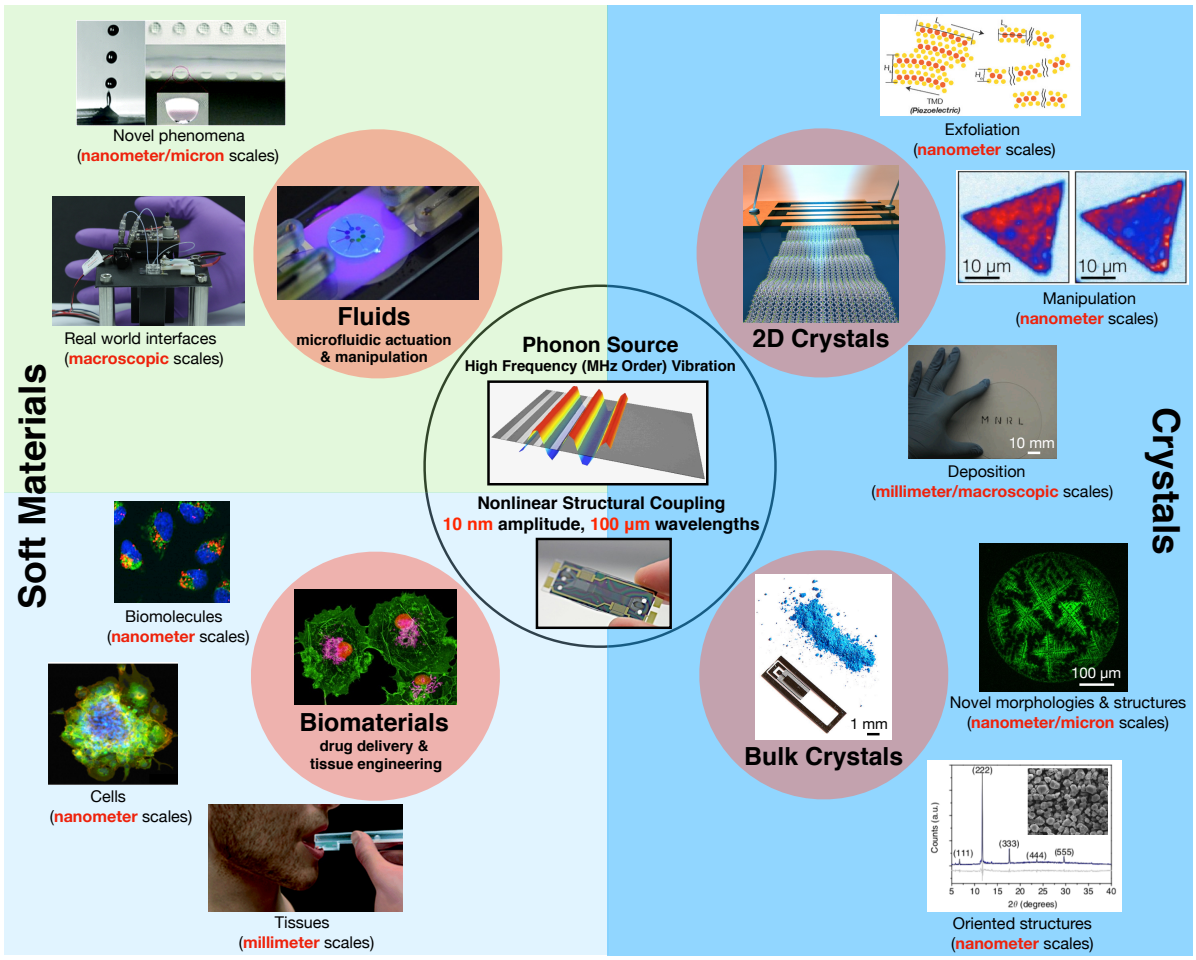


Figure 1: Examples demonstrating the use of 10 MHz order surface acoustic waves for crystals manipulation, including 3D, 2D, 1D and OD. From reference [1]

Electron-Spin-Resonance in a proximity-coupled MoS_2/Graphene van-der-Waals heterostructure

Chithra H. Sharma
Pai Zhao, Lars Tiemann, Marta Prada and Robert H. Blick
Center for Hybrid Nanostructures (CHyN), Universität Hamburg
Chithra.Sharma@physik.uni-hamburg.de

Abstract

The extended family of van der Waals (vdW) materials offers a comprehensive resource to tailor hybrid systems of semiconducting, metallic, superconducting, and insulating layers that exhibit novel properties. [1,2] MoS_2 and Graphene are two among the most widely studied vdW-systems. MoS_2 is a semiconductor transition metal dichalcogenide (TMDC) with high spin-orbit coupling (SOC) where carrier density and thus conductivity can be tuned easily by application of gate voltages. The mobility and conductivity of MoS_2 is limited predominantly due to the Schottky contact that it forms with most metals. On the other hand, graphene is a semimetal with Dirac electrons (holes) and high conductivity and carrier mobilities. The lack of a sufficiently large band gap and the relatively small intrinsic SOC of the order of 20-40 μeV [3], however, prohibits certain device applications. Proximity induced SOC is predicted in graphene on MoS_2 and has been signaled in the observation of weak-anti-localization [4] and spin Hall effects [5]. Modification in SOC will also be reflected in the deviation of *g*-factor from the free electron value of 2.0023.

Here, we report low-temperature measurements on a MoS_2/Graphene heterostructure shown in Figure 1 (a). The device is laterally separated into a pure layer of graphene (left) and an MoS_2/Graphene stack (right) that allows us to study and compare the interaction-induced changes in the graphene layer using magneto-transport. Resistively-detected electron-spin-resonance measurements (Figure 1 (b)) reveal that the *g*-factor in the hybrid system is ~1.91 further deviating from the previously measured *g*-factor of 1.952 ±0.002 for pure graphene. [3,6] Understanding the nature of the interlayer coupling will facilitate observation of topological phases and designing spin-transfer devices.

References

[1] K. S. Novoselov et al. , Science **353**, aac9439 (2016).
[2] C. H. Sharma et al. , Commun. Phys. **1**, 90 (2018).
[3] J. Sichau et al. and R. H. Blick, Phys. Rev. Lett. **112**, 046403 (2019).
[4] J. I. J. Wang et al. , Nano Lett. **15**, 1898 (2015).
[5] A. Avsar et al. , Nat. Commun. **5**, 4875 (2014).
[6] R. G. Mani et al. , Nat. Commun. **3**, 996 (2012).

Figures

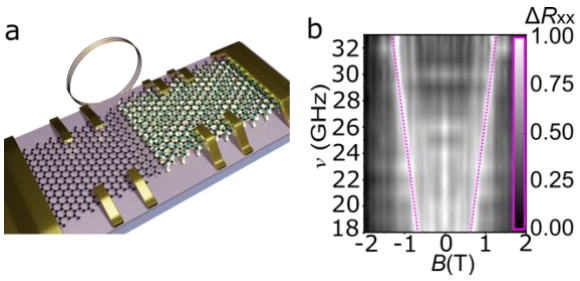


Figure 1: Schematic of the device (left). ESR measurement showing the resonance at different frequencies shown with red line as a guide to the eye (right). Measurements done at 1.5 K

Enhancement of Atomic Oxygen durability of 3D-Graphene infused Polyimide for long-term space application

Ranjana Shivakumar
Asaf Bolker, Siu Hon Tsang, Nurit Atar, Ronen Verker, Irina Gouzman, Mor Hala, Nehora Moshe, Alexandra Jones, Eitan Grossman, Timothy K. Minton, and Edwin Hang Tong Teo
Temasek Laboratories @ NTU, 50 Nanyang Drive, Research Techno Plaza, BorderX Block, 9th Storey, Singapore 637553
ranjana.s@ntu.edu.sg

In this work, Polyhedral Oligomeric Silsesquioxane (POSS) nanoparticles are used to enhance the Atomic Oxygen (AO) durability of 3D-graphene infused Polyimide (3D-C/PI) composite films in low earth orbit (LEO). Recently, 3D-C was identified as an effective filler to protect the polyimide films from electrostatic discharge when used as thermal blankets for satellites.[1-3] However, the carbon-based composite film is susceptible to erosion due to long term AO exposure at LEO altitudes. [4, 5] Here, POSS is added to the composite film in three ways, and the resulting samples (3D-C-POSS/PI, 3D-C/PI-POSS and 3D-C-POSS/PI-POSS) are studied and compared to 3D-C/PI. These samples are subjected to ground-based AO exposure. Their electrical and mechanical properties are also investigated. It is seen that adding POSS to PI results in lower AO erosion yield since most of the film mass, including the top surface, is PI. The 3D-C/PI-POSS film has the lowest erosion yield of 4.67 X 10^{-25} cm^3/AO when subjected to AO fluence equivalent to 5 months at an altitude of 500 km. By adding POSS in PI, the durability of 3D-C/PI composite film has been extended beyond ten years, making it an ideal material for long term missions in LEO.

References

[1] Zhang, L.; Liu, M.; Bi, S.; Yang, L.; Roy, S.; Tang, X.-Z.; Mu, C.; Hu, X., Journal of Colloid and Interface Science, 493 (2017), 327-333.
[2] Wu, Y.; Wang, Z.; Liu, X.; Shen, X.; Zheng, Q.; Xue, Q.; Kim, J.-K., ACS Applied Materials & Interfaces,10 (2017), 9059-9069.
[3] Loeblein, M.; Bolker, A.; Tsang, S. H.; Atar, N.; Uzan-Saguy, C.; Verker, R.; Gouzman, I.; Grossman, E.; Teo, E. H. T., Small, 48 (2015), 6425-6434.
[4] Reddy, M. R., Journal of Materials Science, 2 (1995), 281-307.
[5] Iskanderova, Z. A.; Kleiman, J. I.; Gudimenko, Y.; Tennyson, R. C., Proceedings of ICPMSE-4, 4(2001); 33-50.

Figures

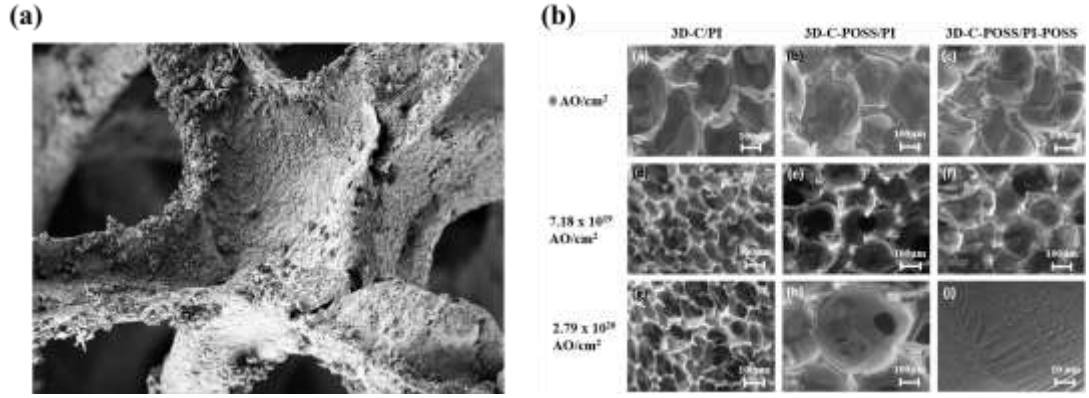


Figure 1: SEM images showing a) 3D-C with POSS nanoparticles on the foam surface; b) Composite film surface before and after AO exposure showing the effect of AO exposure.

Self-Healable and Self-Powered Graphene-based Polymer Composites for Strain Sensors

Barış Şimşek
Jasper Ruhkoph, Ulrich Plachetka, Max Christian Lemme
Çankırı Karatekin University, Department of Chemical Engineering, 18100, Çankırı, Turkey
RWTH Aachen University, Chair of Electronic Devices, Otto-Blumenthal-Strasse 2, Aachen, Germany
baris.simsek@eld.rwth-aachen.de

Abstract

Smart electronic devices have become very attractive in recent years with the rapid development of science and technology and graphene-polymer-based strain sensors come to the forefront due to their significant advantages over semiconductors and metals such as high flexibility, low-cost fabrication [1]. In addition, graphene-polymer-based strain sensors are preferred regarding to their self-healing, self-powered capabilities [2]. Noncovalent interactions such as hydrogen bonding, electrostatic, hydrophobic and host-guest interaction plays a key role in imparting these properties to strain sensors [3]. In this study, the effect of intermolecular interactions on self-healing properties was evaluated.

References

[1] Xiao-Lu Xu, Shun-Xin Li, Ying Yang, Xiang-Chao Sun, Hong Xia, High-performance strain sensor for detection of human motion and subtle strain by facile fabrication, Measurement, 189 (2022)110658.
[2] Yang Lu, Manik Chandra Biswas, Zhanhu Guo, Ju-Won Jeon, Evan K. Wujcik, Recent developments in bio-monitoring via advanced polymer nanocomposite-based wearable strain sensors, Biosensors and Bioelectronics, 123 (2019) 167-177.
[3] Lei Zhai, Ameya Narkar, Kollbe Ahn, Self-healing polymers with nanomaterials and nanostructures, Nano Today 30 (2020) 100826.

Figures

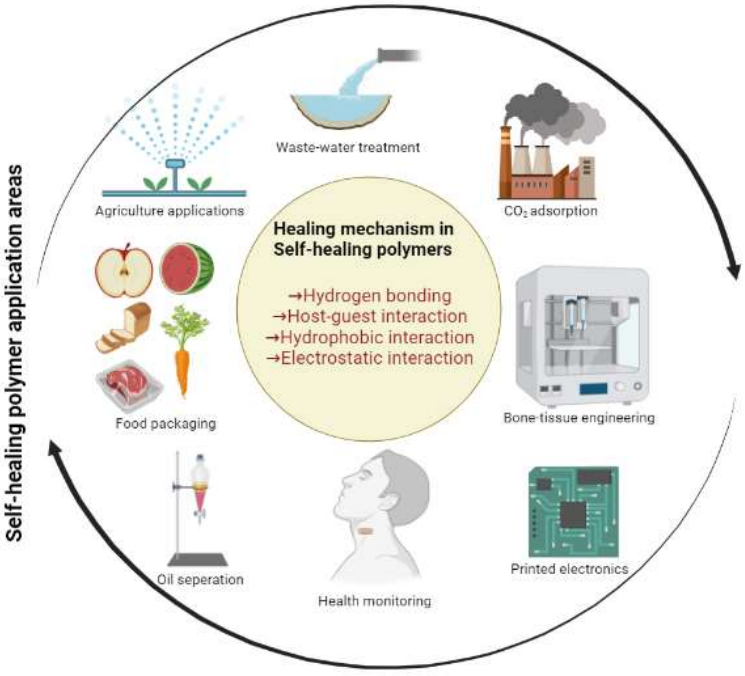


Figure 1: Noncovalent interaction in self-healing polymers and their application areas

Atomic layer deposition of MoS_2 and the influence of subsequent annealing on the optical and structural properties

Christian Tessarek
Tim Grieb, Andreas Rosenauer, Martin Eickhoff
Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany
tessarek@ifp.uni-bremen.de

MoS_2 belongs to the 2D transition metal dichalcogenide material family. It is an indirect band gap semiconductor for bulk to bilayer thickness, while monolayers are characterised by a direct band gap having an energy of ~ 1.9 eV. The 'Scotch-tape-method' is a simple but a not well controllable exfoliation technique to produce small flakes of different layer thickness. Homogeneous wafer scale deposition is possible using chemical vapor deposition (CVD). Atomic layer deposition (ALD) is a CVD based process usually using pulsed precursor supply at low pressure and low temperature.

In this study, growth of MoS_2 layers on SiO_2/Si substrates is performed by ALD. Raman spectroscopy is used to determine the number of layers by analyzing the frequency difference of the E^1_{2g} and A_{1g} modes. It will be shown that the number of layers can be controlled by the number of ALD cycles (Fig. 1a). The influence of ALD growth parameters on the structural properties will be discussed.

As-grown MoS_2 layers by ALD suffer from poor photoluminescence (PL) properties [1]. To obtain typical PL activity with A and B excitonic emission (Fig. 1b), a subsequent annealing step at higher temperature is required. The influence of different annealing temperatures and atmospheres on the structural, optical and morphological properties is investigated and compared to exfoliated MoS_2. MoS_2 grown directly on free-standing graphene layers dispersed on transmission electron microscopy (TEM) grids enables plan view high resolution TEM measurements for insights in the crystalline quality and the grain size.

References

[1] L. K. Tan, B. Liu, J. H. Teng, S. Guo, H. Y. Low and K. P. Loh, Nanoscale **6** (2014), 10584

Figures

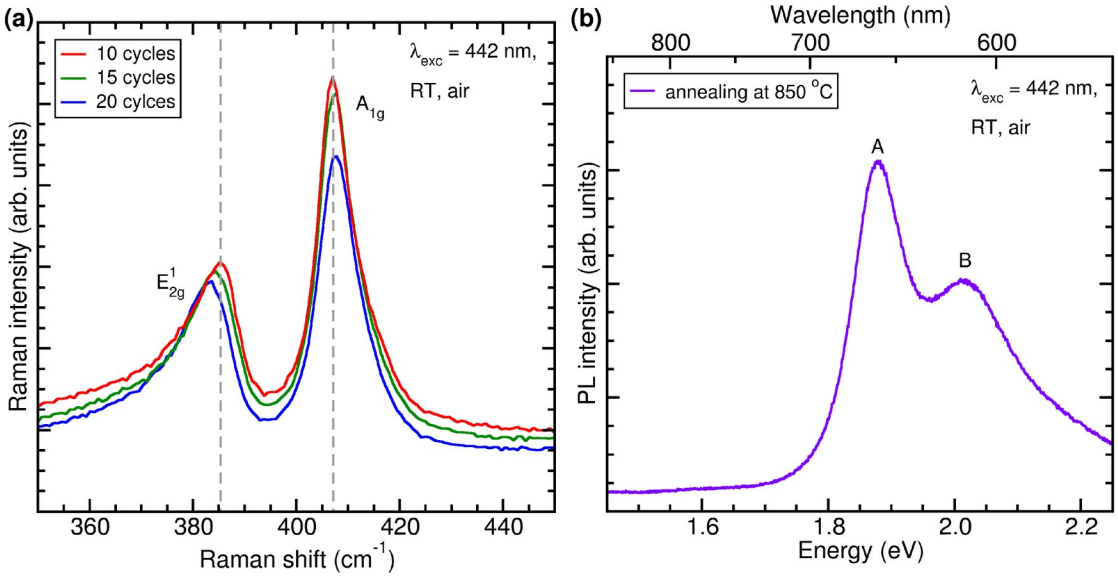


Figure 1: a) Raman spectra of MoS_2 layers: reduction of number of ALD cylces leads to a decrease of the frequency difference of E^1_{2g} and A_{1g} modes. b) PL spectrum of MoS_2 monolayer after annealing showing typical A (1.88 eV) and B (2.01 eV) exciton related emission.

On-Water Surface Synthesis of Charged Two-Dimensional Polymers Enabling Effective Ion Transport

Zhiyong Wang[1,2]
Renhao Dong[2], Xinliang Feng[1,2]
[1]*Max Planck Institute for Microstructure Physics, D-06120 Halle (Saale), Germany*
[2]*Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany*
wang.zhiyong@tu-dresden.de

Synthetic two-dimensional polymers (2DPs) are an emerging class of structurally-defined crystalline materials that comprise covalent networks with topologically planar repeat units. Yet, synthesizing 2DP single crystals via irreversible reactions remains challenging. Herein, utilizing the surfactant-monolayer-assisted interfacial synthesis (SMAIS) method, few-layer, large-area, skeleton-charged 2DP (C2DP) single crystals were successfully synthesized through irreversible Katritzky reaction, under pH control. The resultant periodically ordered 2DPs comprise aromatic pyridinium cations and counter BF_4^- anions. The representative C2DP-Por crystals display a tunable thickness of 2-30 nm and a lateral size up to 120 μm^2. Using imaging and diffraction methods, a highly uniform square-patterned structure with the in-plane lattice of a = b = 30.5 Å was resolved with near-atomic precision. Significantly, the C2DP-Por crystals with cationic polymer skeleton and columnar-like pore arrays offer a high chloride ion selectivity with a coefficient up to 0.9, thus ensuring the integration as the anion-selective membrane for the osmotic energy generation. Our studies reveal a route to synthesize 2DP single crystals using a kinetically controlled irreversible reaction and will propel the development of membrane-based energy-conversion technologies.

References

[1] Z. Wang, Z. Zhang, H. Qi, A. Guerrero, L. Wang, K. Xu, M. Wang, S. Park, F. Hennersdorf, A. Dianat, A. Croy, H. Komber, G. Cuniberti, J. J. Weigand, U. Kaiser, R. Dong, and X. Feng, Nat. Synth. 1 (2022), 69–76.
[2] Z. Wang, X. Jia, P. Zhang, Y. Liu, H. Qi, P. Zhang, U. Kaiser, S. Reineke, R. Dong, and X. Feng, 34 (2022), 2106073

Figures

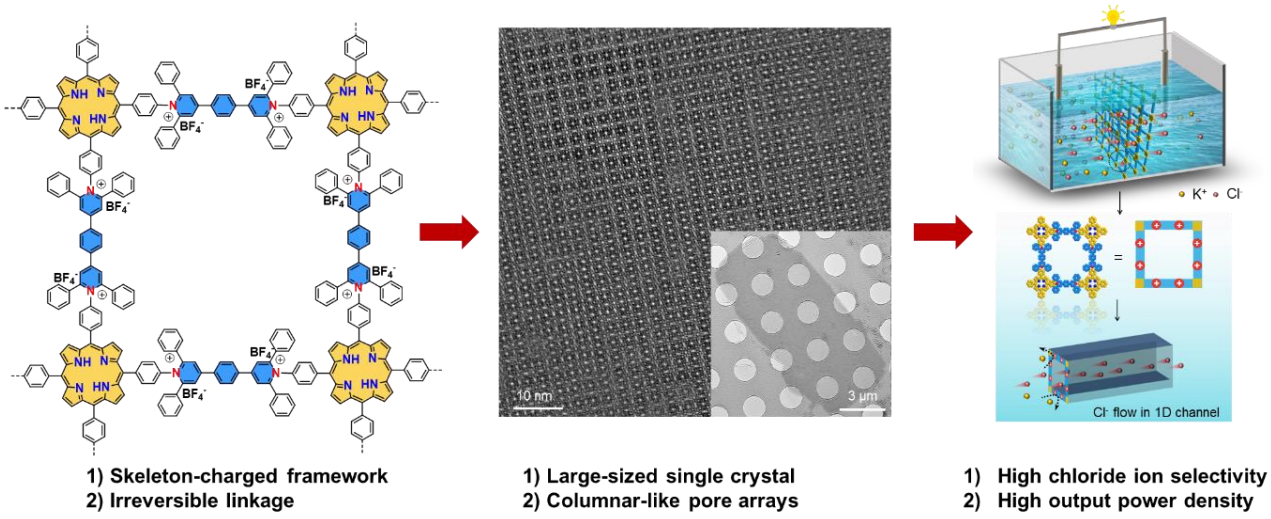


Figure 1: On-water surface synthesis of charged 2DP single crystal via irreversible reactions towards osmotic energy generation.

Tuning the Many-body Interactions in a Helical Luttinger Liquid

Bent Weber
School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371
b.weber@ntu.edu.sg

Abstract

The interplay of topology, superconductivity, and many-body correlations has become a subject of intense research in condensed matter physics for the pursuit of non-trivial forms of superconducting pairing. Atomically thin topological materials – amongst them the quantum spin Hall (QSH) insulator [1] – provide a fertile ground to engineer electronic states and phases in van-der-Waals heterostructures. The topological edge states of such systems – strictly 1D electronic structures with linear (Dirac) dispersion and spin-momentum locking – have recently been shown to harbour a strongly correlated 1D low temperature ground state – the helical Tomonaga-Luttinger Liquid (TLL) [2]. The strength of its many-body correlations can be quantified by a single dimensionless parameter, the Luttinger parameter *K*, characterising the competition between the electrons' kinetic and electrostatic energies.

Here we show [3] that the many-body Coulomb interactions in such helical Luttinger Liquid – realized in epitaxial QSH heterostructures of monolayer 1T'-WTe_2 – can be effectively screened by the edge state's dielectric environment. This is inferred from temperature-dependent scanning tunnelling spectroscopy down to 4.2K, confirming universal scaling of the tunnelling density of states in bias voltage and temperature. We demonstrate tunability of the Luttinger parameter *K*, distinct on the different edges of the crystal, and extracted to high accuracy from a statistical analysis of tens of tunnelling spectra. We expect that our results will stimulate experimental and theoretical investigation into the interplay of topology and strong electronic interactions in 1D, also in the superconducting state, in which non-Abelian parafermions have been predicted.

References

[1] Lodge et al., *Atomically Thin Quantum Spin Hall Insulators.* Advanced Materials **33,** 2008029 (2021).
[2] Stuehler et al. *Tomonaga–Luttinger liquid in the edge channels of a quantum spin Hall insulator*. Nat. Phys. **16,** 47 (2020).
[3] Jia et al. *under review*

Alternative strategy to grow large surface hBN on Ge films by Molecular Beam epitaxy

Walter Batista Pessoa[1]
Max Franck[2], Jaroslaw Dabrowski[2], Xavier Wallart[1], Nicolas Nuns[3], Mindaugas Lukosius[2], Dominique Vignaud[1]
[1]*Univ. Lille, CNRS, Centrale Lille, JUNIA ISEN, Univ. Polytechnique Hauts de France, UMR 8520- IEMN Institut d'Electronique, de Microélectronique et de Nanotechnologie F59000 Lille France*
[2] *IHP - Leibniz-Institut fuŕ innovative Mikroelektronik, Frankfurt (Oder) 15236, Germany*
[3] *Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. d'Artois, IMEC-Institut Michel-Eugène Chevreul, 59000 Lille, France*
walter.batista-pessoa@iemn.fr

Hexagonal Boron Nitride is a two-dimensional insulator with a wide bandgap (~6 eV), chemically and thermally stable. Its 2D nature makes it exceptionally interesting as an ultrathin barrier, tunneling or passivation layer for integrated electronics and photonics, noticeably for the encapsulation of graphene or other 2D materials for next generation electronics [1]. In the case of germanium, Ge oxides are unstable and might induce thermal pits, limiting its applications [2]. Hence, hBN could be a good candidate not only for Ge passivation but also for ultra-capacitors (e.g., metal/hBN/Ge) and for graphene devices on Ge (e.g. graphene/hBN heterostructures)[1,3].
In this work, we study the growth of large surface atomically thin hBN on Ge (001) films by molecular beam epitaxy using boron effusion cell and a remote nitrogen plasma cell. Firstly, we discuss how the B/N precursor ratio influences the BN composition from B-rich to stoichiometric films (figure 1). Then, we consider the challenges related to the limitation of growth temperature due to Ge thermal pits formation. A BN buffer layer strategy was developed which significantly allows to increase the growth temperature without thermal pits formation, so that better quality BN can be grown.

References

[1] Lopes, J.M.J., Vignaud, D., "Molecular Beam Epitaxy of Graphene and Hexagonal Boron Nitride." in *Molecular Beam Epitaxy*, Ed. M. Henini, Elsevier (2018), 487-513
[2] Diallo, T.M., et al. , 'CVD Growth of High-Quality Graphene over Ge (100) by Annihilation of Thermal Pits', Carbon 174 (2021), 214–26
[3] Jang, S.K., et al., 'Synthesis and Characterization of Hexagonal Boron Nitride as a Gate Dielectric', Sci. Reports 6 (2016), 30449

Figures

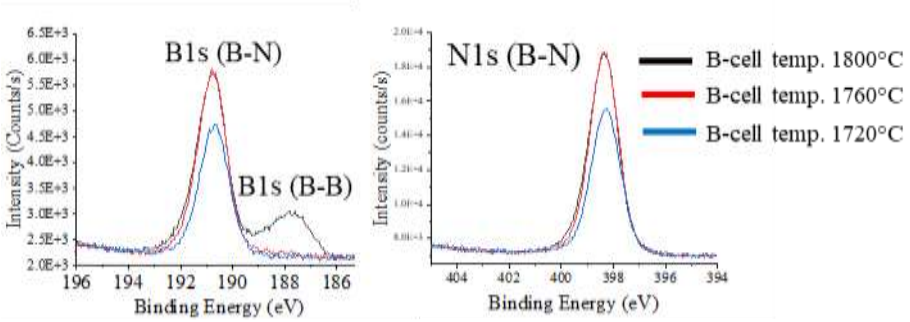


Figure 1: XPS measurements of BN grown as a function of the B-cell temperature (i.e., B flux), B1s (left) and N1s (right) components. BN films are B-rich above 1760°C, and stoichiometric below 1760°C.

Single Atom Fe-N-C Electrocatalysts for Oxygen Reduction Reaction

Guangbo Chen
Xinliang Feng
Center for Advancing Electronics Dresden (cfaed) and Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Mommsenstasse 4, 01069 Dresden, Germany.
guangbo.chen@tu-dresden.de

Electrocatalytic oxygen reduction reaction (ORR) is the vital process in the cathode of next-generation electrochemical storage and conversion technologies, such as, metal-air batteries and fuel cells. Single-atom Fe-N-C carbonous electrocatalysts have emerged as attractive alternatives to noble-metal platinum to catalyze the kinetically sluggish ORR due to the high electrical conductivity, large surface area, structural tunability at the atomic/morphological levels. However, the ORR activity of current Fe-N-C is seriously limited by the low density, inferior exposure of active Fe-N_x species and low intrinsic activity of the Fe-N_x sites.[1] Here, a novel zinc-mediated template synthesis strategy is demonstrated for constructing densely exposed Fe-N_x moieties on hierarchically porous carbon (SA-Fe-NHPC). As a result, the SA-Fe-NHPC electrocatalysts exhibit an unprecedentedly high ORR activity in a 0.1 M KOH aqueous solution, which outperforms those for Pt/C catalyst and state-of-the-art noble metal-free electrocatalysts.[2] Furthermore, we discovered an edge tensile strain effect strategy to efficiently weaken the interaction between the single Fe site and the O* intermediate through atomic engineering of FeN_4 active sites at the armchair-edge of nitrogen-doped hierarchically porous carbon (e-FeN_4(A)-NHPC), thereby boosting its intrinsic ORR activity in acidic solution.[3] Increasing the site density and enhancing the intrinsic activity of the Fe-N_x site pave a new avenue toward high-performance ORR electrocatalysts.

References

[1] G. Chen, H. Zhong, X. Feng. Chem. Sci., 12 (2021) 15802–15820.
[2] G. Chen, X. Feng et al, Adv. Mater., 32 (2020) 1907399.
[3] G. Chen, X. Feng et al, Under Revision in Energy & Environ. Sci.

Figures

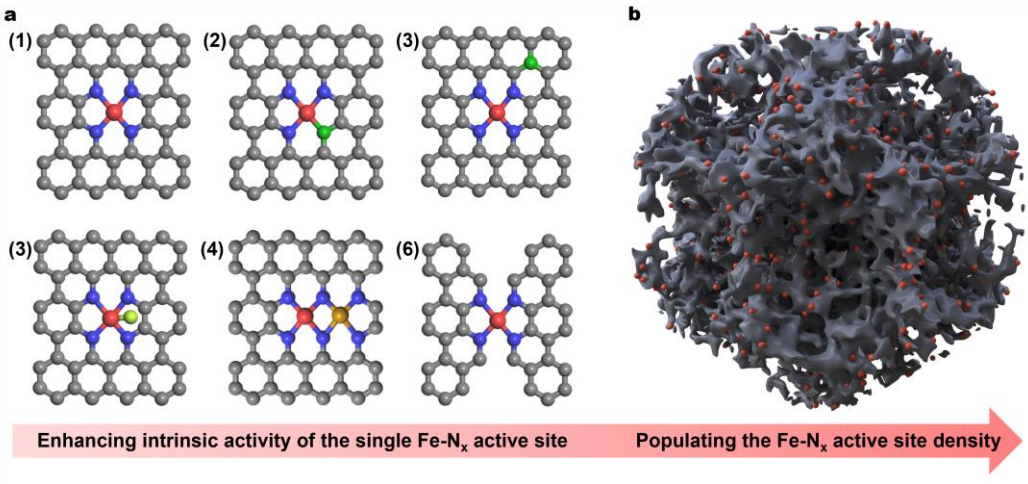


Figure 1: Promoting the ORR activity of Fe-N-C materials via (a) enhancing the intrinsic activity of single Fe-N_x site and (b) populating the Fe-N_x site density.

Fermi level depinning in two-dimensional materials using flourinated bilayer graphene

Manh-Ha Doan[1,2]
Cunzhi Sun[1,2,3], Cheng Xiang[1,2], Rongdun Hong[3], Feng Zhang[3], Timothy J. Booth[1,2], Peter Bøggild[1,2]
[1]*Department of Physics, Technical University of Denmark*
[2]*Centre for Nanostructured Graphene (CNG), Technical University of Denmark, Kgs. Lyngby 2800, Denmark*
[3]*Department of Physics, Xiamen University, Xiamen, 361005, P. R. China*
mando@dtu.dk

Two-dimensional (2D) materials, such as graphene and transition-metal dichalcogenides (TMDs), have drawn tremendous attention recently due to their promising advantages including atomic thickness and smooth channel-to-dielectric interface without dangling bonds [1]. However, while the absence of bandgap in graphene results in a high off-current of the field effect transistor, the large contact resistance of metal/TMD junctions makes it difficult to inject charge carriers to the channel [2, 3].

In this report, we first demonstrate the energy gap opening in bilayer graphene (BLG) *via* a mild fluorination using SF_6 gas. Raman scattering and X-ray photoelectron spectroscopy measurements indicate that only the top layer of BLG is fluorinated with the covalent C-F bonding at the surface, while the bottom layer remains intrinsic. The current-voltage characteristics of the fluorinated bilayer graphene (FBLG) transistor show a nonlinear behaviour. The fluorination induces an asymmetry between the top and bottom graphene layers due to differences in carrier concentrations and/or disordered lattice structure, leading to an opening of a gap between valence and conduction bands of BLG [4]. The calculated energy gap is from 70 to 100 meV, which is in a similar range of molecular doped BLG [5].

As a proof of concept, we fabricate and investigate transport properties of the metal/FBLG/MoS_2 transistors using contact metals with different work functions. The extracted Schottky barrier heights (SBH) at the metal/MoS2 junctions are almost similar for all metals, manifesting the strong Fermi level pinning. By insertion of FBLG, the SBH dramatically reduces for the low-work function metals, resulting in higher on-current of the transistor. In addition, it alleviates the line-up effect of the work function of the metal at the interface, leading to a better pinning factor.

Our results define a straightforward method to generate thin dielectrics for de-pinning the Fermi level at the interface of metal/TMD and as well as for various applications in advanced electronics and optoelectronics.

References

[1] Y. Liu, X. Duan, H.-J. Shin, S. Park, Y. Huang, X. Duan, Nature 591 (2021) 43-53.
[2] A. Allain, J. Kang, K. Banerjee, A. Kis, Nat. Mater. 14 (2015) 1195-1205.
[3] R.-S. Chen, G. Ding, Y. Zhou, S.-T. Han, J. Mater. Chem. C 9 (2021)11407-11427.
[4] T. Ohta, A. Bostwick, T. Seyller, K. Horn, E. Rotenberg, Science 313 (2006) 951-954.
[5] J. Park, S. B. Jo, Y.-J. Yu, Y. Kim, J. W. Yang, W. H. Lee, H. H. Kim, B. H. Hong, P. Kim, K. Cho, K. S. Kim, Adv. Mater. 24 (2012)407–411.

Simulation of graphene based macromaterials: the influence of flake properties and atomic intercalation

Florian Fuchs[1,2]
Tom Rothe[1,2], Leo Rizzi[3], Jörg Schuster[1,2]
[1]*Fraunhofer Institute for Electronic Nano Systems (ENAS), 09126 Chemnitz, Germany*
[2]*Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, 09107 Chemnitz, Germany*
[3]*Robert Bosch GmbH, Robert-Bosch-Campus 1, 71272 Renningen, Germany*
florian.fuchs@enas.fraunhofer.de

The excellent properties of graphene can be utilized in macroscopic conductor materials if the individual flakes are decoupled from each other, for example by misalignment of the lattices or by intercalation.

We show the results of a network model [1] to assess the properties of the macromaterial (Fig. 1 left) as a function of relevant parameters such flake size, packing density, the graphene flake conductivity, and the interlayer conductance. The model allows us to evaluate the anisotropy of the current flow in the in-plane and the out-of-plane directions of the graphene-based macromaterial [2].

Intercalation of the graphene-based macromaterial with additional atoms or molecules can also be used to enhance the material properties [3]. We show density functional theory calculations of graphite intercalated with AlF_3 and discuss the decoupling as well as the modulation of the electronic properties of the graphene flakes. Fig. 1 right shows the band structure before and after the intercalation with AlF_3.

References

[1] L. Rizzi, A. Zienert, J. Schuster, M. Köhne, S.E. Schulz, Computational Materials Science 161 (2019), 264
[2] D. Slawig, L. Rizzi, T. Rothe, J. Schuster, C. Tegenkamp, Journal of Materials Science 56 (2021), 14624
[3] A.E. Candia, S.J. Rodríguez, E.A. Albanesi, G. Bernardi, D.Fregenal, G.E. Zampieri, M.C.G. Passeggi Jr., G. Ruano, Carbon 186 (2022), 724

Figures

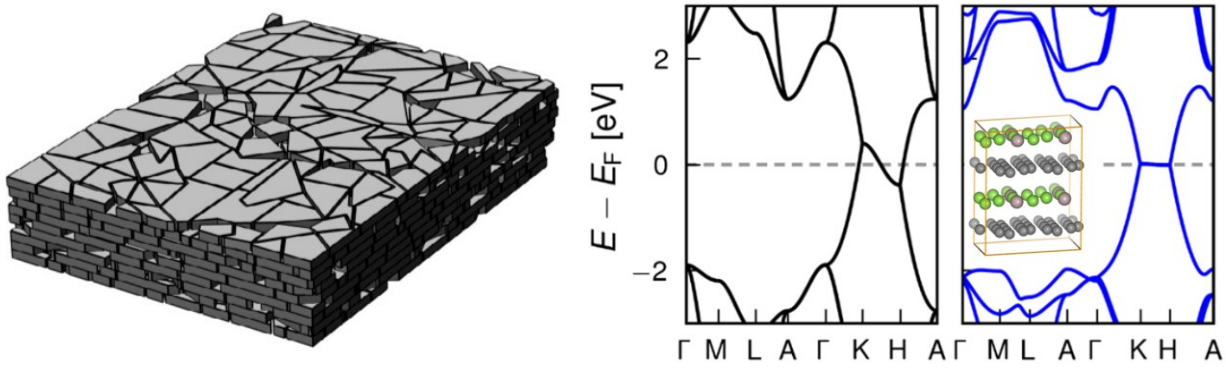


Figure 1: Left: Model system of a graphene based macromaterial. Right: Band structure of AA-stacked graphite without and with AlF_3. A 2×2×2 repetition of the model system is given in the inset.

Nonlinear analysis of the rectifying performance of zero-bias MoS_2-FETs for energy harvesting

A. Godoy[1,*], A. Medina-Rull[1], F. Pasadas[1], E. Reato[2], P. Palacios[3], M.C. Pardo[1], F. Ruiz[1], E.G. Marín[1], M. Saeed[3], Z. Wang[2], D. Neumaier[2], R. Negra[3] and M.C. Lemme[2]

[1]*Departamento de Electrónica y Tecnología de Computadores, PEARL Laboratory, Facultad de Ciencias, Universidad de Granada, 18071, Granada, Spain.*

[2]*AMO GmbH, Otto-Blumenthal-Strasse 25, 52074 Aachen, Germany.*

[3]*Chair of High Frequency Electronics, RWTH University, Kopernikusstraße 16, 52074 Aachen, Germany.*

*agodoy@ugr.es

The main purpose of wireless energy harvesting is converting the far-field radiofrequency (RF) energy into direct current (DC) energy, able to power electronic devices, by using a rectenna. The central element that enables this conversion is the rectifier and the choice of such nonlinear device is critical as it is the central component that limits the overall efficiency and operation frequency [1]. In this work, we analyse the rectifying performance of zero-bias MoS_2 field-effect transistors (FETs) as power detectors. In doing so, we have fabricated MoS_2-FETs on wafer-scale flexible substrates (Figure 1) [2] and calibrated our physics-based large-signal model of 2D-semiconductor FETs [3] with DC (Figure 1b) and RF (Figure 1c) measurements. We have incorporated our technology computer-aided design (TCAD) tool in a commercial circuit simulator to explore and optimize the rectifying performance in terms of maximum current responsivity and cut-off frequency. In order to assess the feasibility of our MoS_2-FETs as rectifiers for future flexible rectennas targeting energy harvesting purposes, different practical ambient/dedicated RF sources have been considered and the results have been put into context against the state of the art.

References

[1] X. Gu, S. Hemour, and K. Wu, "Far-Field Wireless Power Harvesting: Nonlinear Modeling, Rectenna Design, and Emerging Applications," *Proc. IEEE*, vol. 110(1), pp. 56–73, 2022.

[2] E. Reato, P. Palacios, B. Uzlu, M. Saeed, A. Grundmann, Z. Wang, D. S. Schneider, Z. Wang, M. Heuken, H. Kalisch, A. Vescan, A. Radenovic, A. Kis, D. Neumaier, R. Negra, and M. C. Lemme, "Zero Bias Power Detector Circuits based on MoS_2 Field Effect Transistors on Wafer-Scale Flexible Substrates," *Adv. Mater.*, p. 2108469, Jan. 2022.

[3] F. Pasadas, E. G. Marin, A. Toral-Lopez, F. G. Ruiz, A. Godoy, S. Park, D. Akinwande, and D. Jiménez, "Large-signal model of 2DFETs: Compact modeling of terminal charges and intrinsic capacitances," *npj 2D Mater. Appl.*, vol. 3, no. 47, pp. 1–7, 2019.

Figures

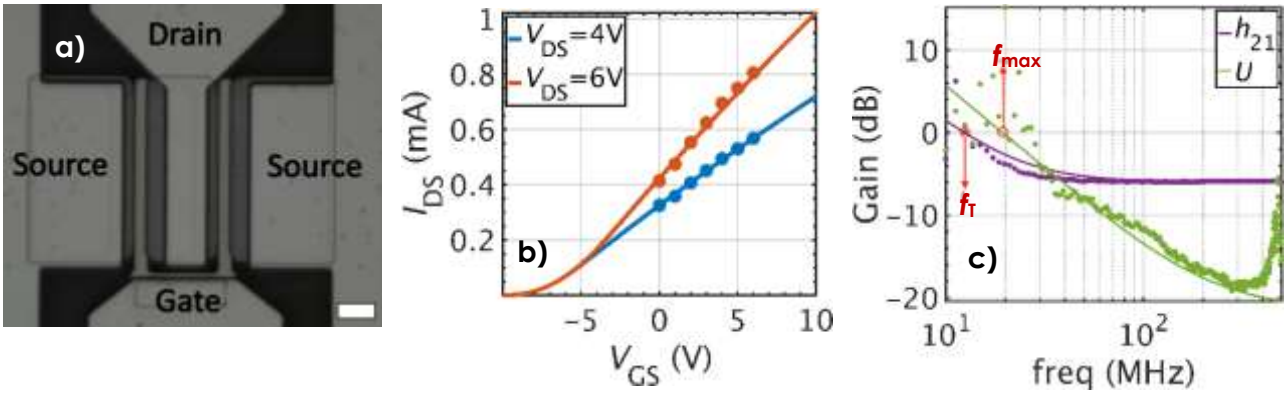


Figure 1: a) Optical micrograph of the fabricated MoS_2-FET. The MoS_2 channel is 6 µm long and 60 µm width and the scale bar is 16 µm long. Measurements (symbols) and simulations (solid lines) of **b)** the transfer characteristics and **c)** the RF performance at a bias point V_{GS} = 4V; V_{DS} = 6V. The cut-off (f_T) and the maximum oscillation (f_{max}) frequencies are highlighted in red.

Machine Learning-Enabled Smart Gas Sensing Platform for Identification of Industrious Gases

Shirong Huang[1]
Alexander Croy[2], Bergoi Ibarlucea[1], Gianaurelio Cuniberti[1,3,4]
1 Institute for Materials Science and Max Bergmann Center for Biomaterials, TU Dresden, 01062 Dresden, Germany
2 Institute for Physical Chemistry, Friedrich Schiller University Jena, Helmholtzweg 4, 07743, Jena, Germany
3 Center for Advancing Electronics Dresden (cfAED), TU Dresden, 01062 Dresden, Germany
4 Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany
Shirong.huang@tu-dresden.de

Abstract

Both ammonia and phosphine are widely used in industrial processes, and yet they are noxious and exhibit detrimental effects on human health.[1] A variety of gas sensors have been developed to detect and monitor them in an industrial environment.[2,3] Despite the remarkable progress on sensors development, there are still some limitations, for instance, the requirement of high operating temperatures, and that most sensors are solely dedicated to individual gas monitoring.[4] Here, we demonstrate an ultrasensitive, highly discriminative platform for the detection and identification of ammonia and phosphine at room temperature using graphene nanosensor. Graphene is exfoliated and successfully functionalized by copper phthalocyanine derivate. In combination with highly efficient machine learning techniques, the developed graphene nanosensor demonstrates an excellent gas identification performance even at ultralow concentrations, 100 ppb NH_3 (accuracy-100.0%, sensitivity-100.0%, specificity-100.0%), 100 ppb PH_3 (accuracy-77.8%, sensitivity-75.0%, and specificity-78.6%). Molecular dynamics simulation results reveal that the copper phthalocyanine derivate molecules attached on the graphene surface facilitate the adsorption of ammonia molecules owing to hydrogen bonding interactions. The developed smart gas sensing platform paves a path to design a highly selective, highly sensitive, miniaturized, low-power consumption, non-dedicated, smart gas sensing system towards a wide spectrum of gases.

References

[1]. Wu Z, et al. Sensors and Actuators B: Chemical 178, 485-493 (2013).
[2]. Wu H, Ma Z, Lin Z, Song H, Yan S, Shi Y. Nanomaterials (Basel) 9, (2019).
[3]. Huang S, et al. Carbon 173, 262-270 (2021).
[4]. Panes-Ruiz LA, et al. ACS Sens 3, 79-86 (2018).

Figures

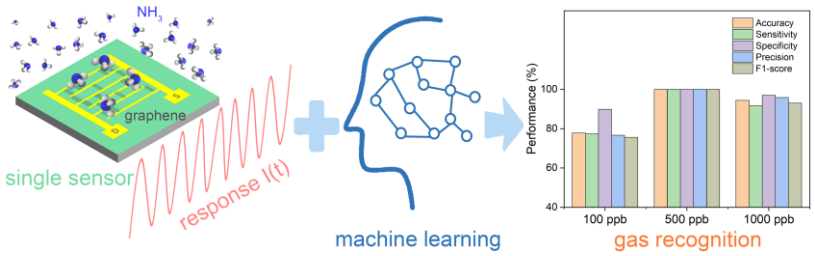


Figure 1: Schematic illustrations of the smart graphene nanosensor platform.

Towards Sustainable Fabrication of hybrid Graphene-QD Photodetectors by Laser Transfer Techniques

Doron Naveh[1]

Michal Poplinger[1], Adamantia Logotheti[2], Yehiel Nagar[1], Pilkhaz Nanikashvili[1], Adi Levi[1], Rajesh Kumar Yadav[1], Amaia Pesquera[3], Amaia Zurutuza[3], Ioanna Zergioti[2]

[1]*Faculty of Engineering and Nanotechnology Institute, Bar-Ilan University, Ramat-Gan, Israel*
[2]*School of Applied Mathematical and Physical Sciences, National Technical University of Athens, Athens, Greece*
[3]*Graphenea Headquarters, San Sebastian, Spain*

Doron.naveh@biu.ac.il

Abstract

Nanoelectronic device processing holds great promise for a continual technological progress and prosper economic development. Complementary to that, a positive impact of the field may be achieved by the adoption of sustainable nanomaterials processing methods that would not compromise device performance or the environment. To that end, hybrid graphene-quantum dots (QDs) photodetectors are known for their enhanced responsivity over the QDs absorption spectral range. However, typically this advantage comes at the cost of long response time, leading to one of the main challenges of graphene photodetectors.
Here we report on a hybrid graphene-$Bi_2Se_{(3-x)}S_x$ QDs photodetector fabricated by a laser transfer technique, necessitating the use of commonly involved chemicals and solvents in standard processing techniques. The laser-processed devices present an improved response time in the range of μ-sec and a high responsivity in the visible to near infrared spectral range, attributed to the cleanliness and quality of the interface of graphene with the QDs.

Figures

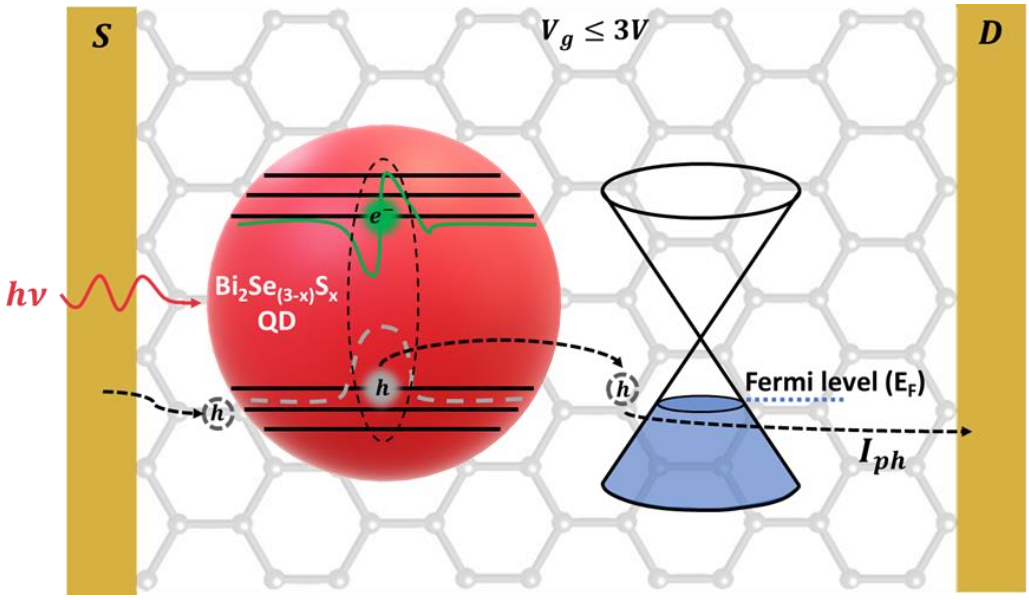


Figure 1: Schematic illustration of the photodetector gain mechanism.

Impact of heavy ions on large-area monolayer WS_2

Fahrettin Sarcan[1, 2, *]
Nicola J. Fairbairn[3], Panaiot Zotev[4], AXITRON[5], Ayse Erol[2], Alexander Tartakovskii[4], Thomas F. Krauss[1], Gordon J. Hedley[3], Yue Wang[1,**]

[1]*Department of Physics, School of Physics, Engineering and Technology, University of York, York, YO10 5DD, United Kingdom*
[2]*Department of Physics, Faculty of Science, Istanbul University, Vezneciler, Istanbul, 34134, Turkey*
[3]*School of Chemistry, University of Glasgow, Glasgow, G12 8QQ, United Kingdom*
[4] *Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, United Kingdom*
5AXITRON

*fahrettin.sarcan@istanbul.edu.tr
**yue.wang@york.ac.uk

Abstract

Focused ion beam has been employed as an effective tool for precise nanoscale fabrication, as well as tailored defect engineering in functional materials such as two-dimensional transition metal dichalcogenides (TMDCs). It has led to new functionality in 2D materials, providing desirable and customisable properties in TMDC-based optoelectronic devices. In this work, we investigate lateral damage caused by gallium focused ion beam (Ga^+ FIB) milling in large-area monolayer WS_2. Three distinct zones away from the milling location are identified and explained via steady-state photoluminescence (PL) and Raman spectroscopy. With high special resolution time-resolved PL spectroscopy, a bright ring-shaped emission around the milled location has been revealed for the first time. This ring emission originated from enhanced trion emission at the edge of the milled monolayer. Our study also provide evidence that while some localised damages are inevitable, the distant damaging can be eliminated by reducing the ion beam current used during the milling process. The correlation between lateral ion beam effects and optical properties of 2D TMDCs is important in fabrication of high-performance optoelectronic nanodevices.

Air-Stable Polymer-Capped Graphene Hall-Sensor

Ayush Tyagi[1,2]
Leonardo Martini[2] Zewdu M. Gebeyehu[2,3], Vaidotas Mišeikis[2,3], Camilla Coletti[2,3]
1. NEST, Scuola Normale Superiore, Piazza San Silvestro 12, I-56127 Pisa, Italy.
2. Center for Nanotechnology Innovation @NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, I-56127 Pisa, Italy.
3. Graphene Labs, Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy
ayush.tyagi@sns.it

Protecting CVD graphene from ambient exposure, provides an excellent platform for high quality graphene-based air stable electrical devices for different technological applications[1]. Polymethyl methacrylate (PMMA) is a commonly used capping layer for protecting graphene-based devices from environmental exposure[2,3]. Here, we show PMMA-capped, air-stable, and highly sensitive CVD graphene-based Hall-sensors. Detailed characterizations, including electrical and magnetic transport measurements at room temperature (RT), are performed to assess the quality of the PMMA/graphene Hall sensors. We find that as-fabricated back-gated PMMA/graphene Hall-sensors maintain, after 15 days in air, a current related RT sensitivity (S_I) up to ~ 2422 $VA^{-1}T^{-1}$, with low residual carrier density of (n^*) ~ 2.11×10^{11} cm^{-2}, and hole and electron mobility (μ) of ~ 7554 $cm^2V^{-1}s^{-1}$ and ~ 6600 $cm^2V^{-1}s^{-1}$, respectively. Furthermore, the minimum magnetic field (B_{min}) of the PMMA/graphene Hall-sensor was observed to be around ~ 2.0×10^{-3} $T/Hz^{0.5}$ after 15 days of ambient exposure. The overall performance of PMMA/graphene Hall-sensors shows minimal degradation (i.e., <7%) after 15 days of air exposure. This study contributes to the achievement of air-stable and highly-sensitive CVD graphene Hall sensors on wafer scale[4].

References

[1] H. He et al. Nat. Commun. 9, 2018, 3956.
[2] P. H. Ho, et al., Chen, Energy Environ. Sci., 8, 2015, 2085–2092.
[3] A. Sundararajan et al., Appl. Phys. Lett.,103, 2013, 253505.
[4] A. Tygai et al., in preparation.

Figures

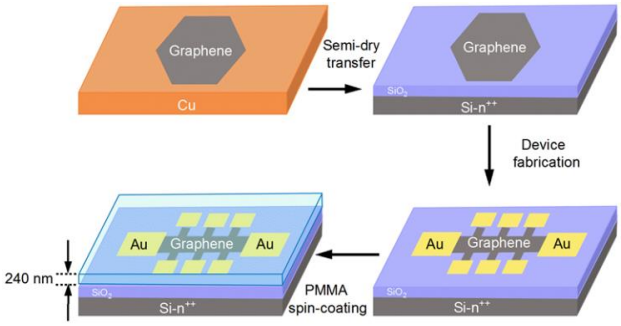


Figure 1: Schematics of graphene transfer and PMMA/graphene Hall-sensor fabrication process.

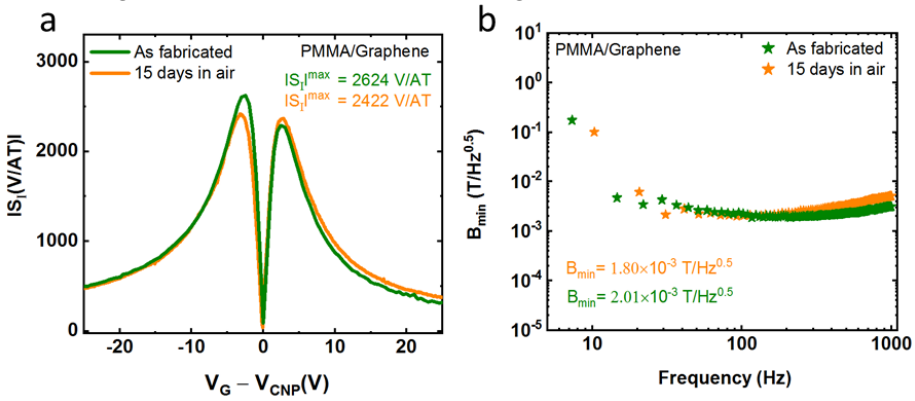


Figure 2: (a) Current related sensitivity $|S_I|$ vs gate voltage and (b) minimum magnetic field (B_{min}) vs frequency of as fabricated PMMA/graphene Hall-sensor and after 15 days of air exposure.

"This work has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement 881603"

Band transport by large Fröhlich polarons in MXenes

Hai Wang[1]
Wenhao Zheng[1], Boya Sun[2], Dongqi Li[2], Sai Manoj Gali[3], Heng Zhang[1], Shuai Fu[1], Lucia Di Virgilio[1], Zichao Li[4], Sheng Yang, [2] Shengqiang Zhou[4], David Beljonne[3], Minghao Yu[2], Xinliang Feng[2], Mischa Bonn[1]
[1] *Max Planck Institute for Polymer Research, Mainz, Germany;*
[2] Technische Universität Dresden, Dresden, Germany
[3] Université de Mons, Mons, Belgium
[4] Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany
wanghai@mpip-mainz.mpg.de

Abstract
MXenes are newly emerging layered two-dimensional materials with great promise for electrochemical energy storage and (opto)electronic applications.[1] A fundamental understanding of charge transport in MXenes is essential for such applications, but has remained under debate. While theoretical studies pointed to efficient band transport[2], device measurements have revealed thermally activated, hopping-type transport[3].
Here we present a unifying charge transport picture in two model MXenes by combining ultrafast terahertz and static electrical transport measurements to distinguish the short- and long-range transport characteristics.[4] We find that band-like transport dominates short-range, intra-flake charge conduction in MXenes, whereas long-range, inter-flake transport occurs through thermally activated hopping. Our analysis of the intra-flake, i.e., inherent charge transport, shows that carrier scattering is dominated by scattering from longitudinal optical phonons with relatively weak electron-phonon coupling (coupling constant $\alpha \approx 1$) in MXenes. The weak electron-phonon coupling gives rise to the formation of large polarons in MXenes: electrons and holes locally deform the lattice, and are dressed by a lattice distortion extending over several lattice units. Our work provides insight into the polaronic nature of free charges in MXenes, and unveils intra- and inter-flake transport mechanisms in the MXene materials, relevant for both fundamental studies and applications.

Reference
[1] A. VahidMohammadi et *al.* ***Science*** 65, 372, eabf1581 (2021);
[2] Z. Jing et *al.* ***J. Phys. D: Appl. Phys.*** 54, 015301(2021);
[3] J. Halim, et *al.*, ***Phys. Rev. B*** 98 104202, (2018);
[4] W. Zheng et *al.* ***Nat. Phys.***, in press (2022), https://doi.org/10.1038/s41567-022-01541-y.

Figures

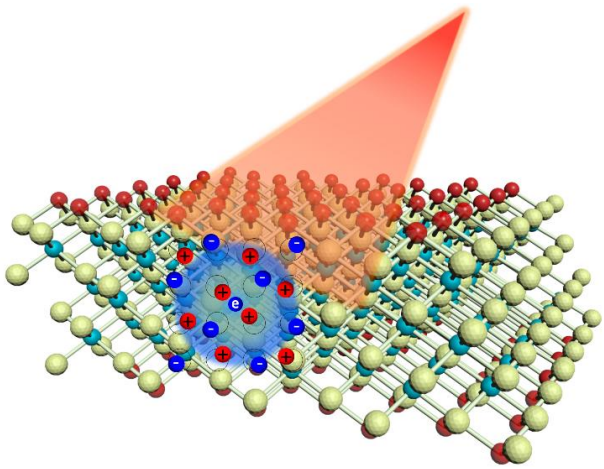


Figure 1: Schematic of large polaron formation in MXenes following optical excitations.

2-dimensional perovskite nanosheet-based synaptic devices for mimicking heterosynaptic plasticity

Haena Yim[1]
Chansoo Yoon[2], So Yeon Yoo[1], Bae Ho Park[2], and Ji-Won Choi[1,*]
[1]*Korea Institute of Science and Technology, Seongbuk-gu, Seoul, Republic of Korea*
2 Konkuk University, Gwangjin-gu, Seoul, Republic of Korea
jwchoi@kist.re.kr

Abstract

Electrical synaptic devices are the basic components for neuromorphic computational systems, which are expected to break the bottleneck of current von Neumann architecture. Especially, the development of artificial synapses having tunable multiple synaptic response can be an essential step forward for the advancement of novel neuromorphic computing [1]. Three-terminal based transistors, which modulate the channel conductance through a floating gate and/or charge trapping layer use gate pulses, have been reported to realize multiple synaptic response. However, the vertical 2-terminal device, which provides more energy-efficient system, with heterosynaptic behavior have not been reported so far. Herein, high-performance and low-power consumption Pt/bi-layer A-site modified $Sr_2Nb_3O_{10}$ (3 nm)/Nb:$SrTiO_3$ memristors are demonstrate. We successfully controlled oxygen vacancies as trap site in 2-dimensional $Sr_2Nb_3O_{10}$ nanosheet through the A-site modification, and the tunneling current of Pt/Nb:$SrTiO_3$ interface is modulated by controlled electron trap/detrap amounts in $Sr_2Nb_3O_{10}$ nanosheet layer. The A-site modified perovskite nanosheets were synthesized by 2-step cation exchange method and deposited Langmuir-Blodgett method via solution-based process. The synaptic devices exhibit good biological synaptic functions of excellent stability, high endurance, long-term potentiation/depression, and paired-pulse facilitation.

References

[1] Shilei Dai,Yiwei Zhao,Yan Wang,Junyao Zhang,Lu Fang,Shu Jin,Yinlin Shao,Jia Huang, Advanced Functional Materials, Volume29, Issue42 (2019) 1903700.

Figures

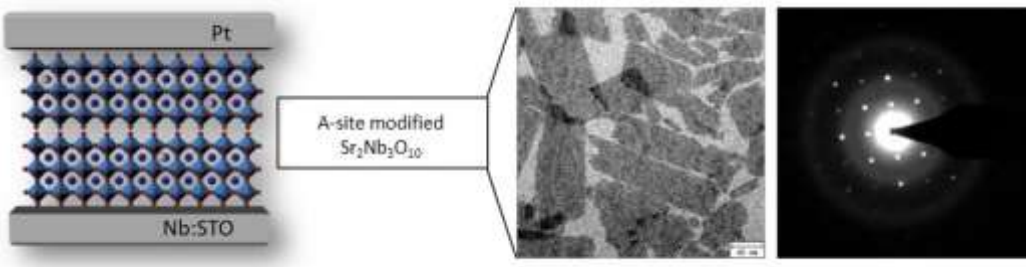


Figure 1: Schematic diagram of Pt/bi-layer $Sr_2Nb_3O_{10}$ (3 nm)/Nb:$SrTiO_3$ memristors and TEM image of nanosheets.

Theoretical Study of Viscosity in Monolayer and Bilayer Graphene

Indra Yudhistira
Ramal Afrose, Aydin Cem Keser, Oleg. P. Sushkov, Shaffique Adam
National University of Singapore, 6 Science Drive 2, Singapore 117546
yudhist87@gmail.com

Abstract:

The advancements in technology in recent years have allowed for the experimental realisation of ultraclean monolayer and bilayer graphene samples where impurity or phonon scattering are no longer the dominant scattering mechanism. The strong electron-electron interaction in these ultraclean samples results in the emergence of hydrodynamic electron behaviour where electron transport is governed by an electronic Navier- Stokes equation analogous to classical fluids. In this theoretical study, we carry out a theoretical calculation of dynamic viscosity in monolayer and bilayer graphene from a microscopic theory. We find a non-monotonic temperature dependence of the dynamic viscosity in both monolayer and bilayer graphene that approaches a universal limit at high temperature and strong electron-electron interaction. We show that our results agrees very well with available experimental data.

Figures

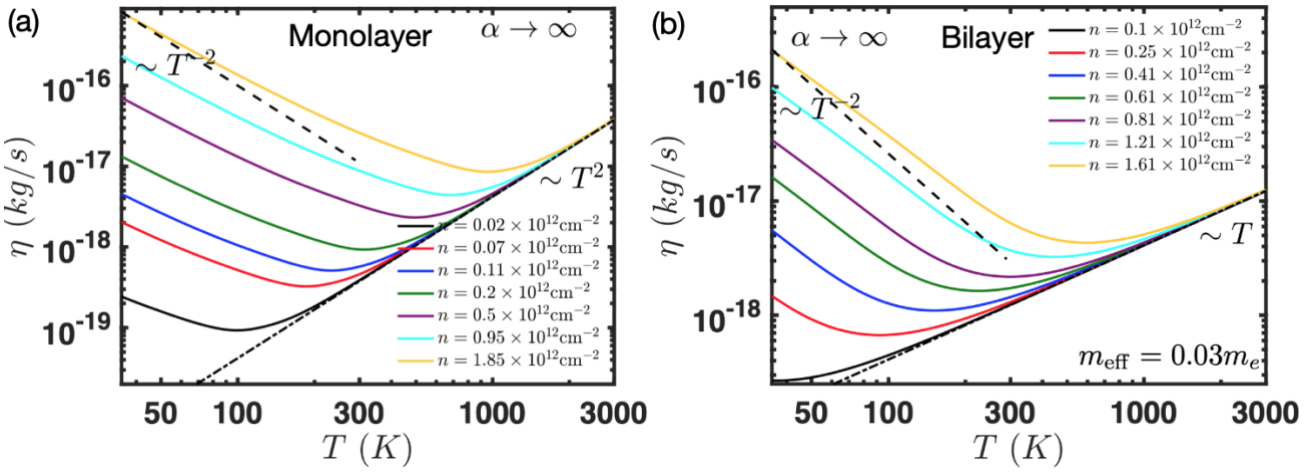


Figure 1: Dynamic viscosity as a function of temperature and Coulomb interaction strength. For both monolayer (a) and bilayer graphene (b), the viscosity is non-monotonic with temperature. At low temperature, the degenerate regime for unipolar hydrodynamics gives a density-dependent viscosity that increases at low temperature in contrast to high-temperature, where the ambipolar transport becomes density independent.

Extreme Extraordinary Magnetoresistance in Encapsulated Monolayer Graphene Devices

Bowen Zhou
Technical University of Denmark, Fysikvej, building 309, 2800 Kgs. Lyngby, Denmark
bowez@dtu.dk

Abstract
We report a proof-of-concept study of extraordinary magnetoresistance (EMR) in devices of monolayer graphene encapsulated in hexagonal boron nitride having a central metal shunt [1]. Extremely large EMR values, $MR=(R(B)-R_0)/R_0 \sim 10^7\%$ are achieved, exceeding that achieved in state-of-the-art semiconductor devices by one order of magnitude [2]. The zero-field resistance R_0 approaches or crosses zero as a function of the gate voltage due to ballistic transport. We highlight the sensitivity, dR/dB~30KΩ/T, which in two-terminal measurements is the highest reported for EMR devices and exceeds previous results in graphene-based devices by a factor of 20 [3]. An asymmetry in the zero-field transport is traced to the presence of pn-junctions at the graphene-metal shunt interface. We are improving EMR effect to make better magnetic field sensors.

References

[1] Bowen Zhou, K. Watanabe, T. Taniguchi, and E. A. Henriksen, Appl. Phys. Lett. 116, 053102 (2020)
[2] S. A. Solin, T. Thio, D. R. Hines, and J. J. Heremans, Science 289, 1530–1532 (2000)
[3] J. Lu, H. Zhang, W. Shi, Z. Wang, Y. Zheng, T. Zhang, N. Wang, Z. Tang, and P. Sheng, Nano Lett. 11, 2973–2977 (2011)

Figures

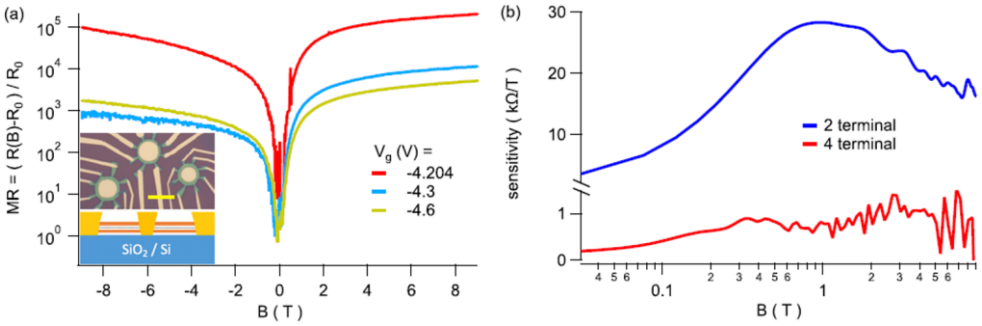


Figure 1: The highest observed magnetoresistance (a) and sensitivity dR/dB (b) for the device at room temperature. The inset shows the microscopic image and schematic side view of the devices; the yellow scale bar is 10 μm long.

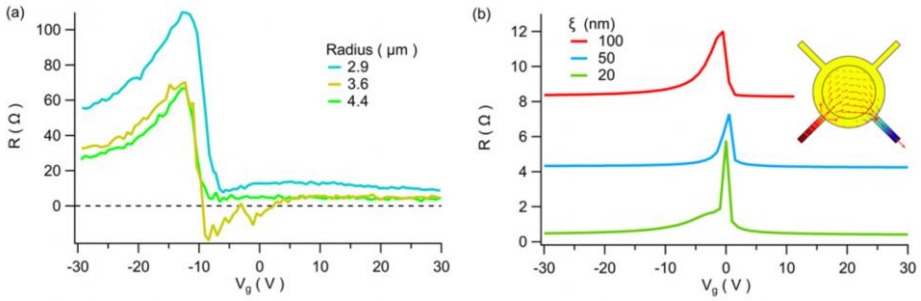


Figure 2: Experimental data (a) and model prediction (b) for asymmetry in the gate-voltage-dependent resistance near the metal-graphene interface at B = 0 T and room temperature. The traces in (b) are offset for clarity. Inset: geometry of the EMR device used in finite element simulation.

Industrial Graphene Growth and Transfer – Challenges and capabilities

Mira Baraket
General Graphene Corporation, 10239 Cogdill Road, Knoxville, TN, USA
Mira@generalgraphenecorp.com

Graphene is a monolayer of sp^2-bonded carbon atoms assembled in a honeycomb lattice structure that has attracted incredible attention for its many promising properties. It has been said that Graphene can do anything you need - except get out of the laboratory. The CVD-grown large area graphene has yet to become useful outside the laboratory due to its cost which is usually well over $10,000 dollars per square meter. Consequently, graphene's accessibility has been severely restrained with virtually no chance to integrate into industrial applications requiring high product volumes. To address this, General Graphene has scaled-up the graphene growth using an atmospheric pressure CVD process to produce cost effectively truly large-scale mono and multilayers graphene. This led us to produce different graphene types from polycrystalline graphene grown on polycrystalline copper to single oriented grown on single oriented copper to various forms of multilayer. All this can be produced with a single machine with production rates exceeding >30,000 m^2/year. Now that costs and production are in line with industrial applications – the final step is to integrate graphene into targeted applications where its unique properties and abilities provide significant competitive advantages. On the other hand, there is not a single transfer method that works for all applications. This leads to a variety of transfer methods, each with their strengths and weaknesses.
In this talk a brief history of graphene will be presented with emphasis on the challenges faced in growth and transfer along with current state-of-the-art applications with real-world performance and cost data.

Transfer and interface characterization of 2D materials for microelectronic devices

Brunet Paul[1], Sharma Kshipra[2], David-Vifflantzeff Julien[1], Ligaud Clotilde[1], Okuno Hanako[2], Krothus Simonas[3] , Pasko Sergej[3], Wang Xiaochen[4], Conran Ben[4], Le Van-Jodin Lucie[1]
[1] CEA, LETI, MINATEC Campus, F-38054 Grenoble, France and Univ. Grenoble Alpes, F-38000 Grenoble, France
[2] CEA, IRIG, MINATEC Campus, F-38054 Grenoble, France and Univ. Grenoble Alpes, F-38000 Grenoble, France
[3] Aixtron SE, Dornkaulstr. 2, 52134 Herzogenrath, Germany
[4] Aixtron LTD, Anderson Road Buckingway Business Park Swavesey Great Britain, Aixtron Ltd, UK
paul.brunet@cea.fr

Abstract: 2D materials have attracted a lot of attention since the last decade due to their unique properties especially in the microelectronics field [1]. However thermal budgets engaged for the synthesis of high quality 2D materials are, most of the time, not compatible for the direct growth into device structures. Therefore, transferring synthesized layers from the growth substrate to a desired one is required for functional device fabrication [2]. However, the transfer process could modify or degrade the material properties, and the quality of interface between the transferred materials and the targeted substrates should be carefully controled to achieve the expected properties. [3]

Our work focuses on the development of a clean room compatible large-scale transfer process based on spalling method for its integration into microelectronic devices such as photonics, RF switches or memories.

We report here a physico-chemical characterization of 2D layers before and after transfer using microscope SEM and TEM, AFM, XPS and Raman spectroscopy to study the impact of our transfer process. The electrical properties are also studied using four probes and Van Der Pauw measurement after transfer to verify the electrical interface while optimizing the process to get a good copy of the as grown materials by keeping the growth interface safe from solvent or other impurities.

References

[1] Wu, M, Xiao, Y, Zeng, Y, et al. *InfoMat*. 2021; 3: 362– 396
[2] Shim et al., Science 362, (2018) 665–670
[3] Yuan Liu, Xidong Duan, Hyeon-Jin Shin, Seongjun Park, Yu Huang & Xiangfeng Duan, Nature | Vol 591 | 4 March 2021

Figures

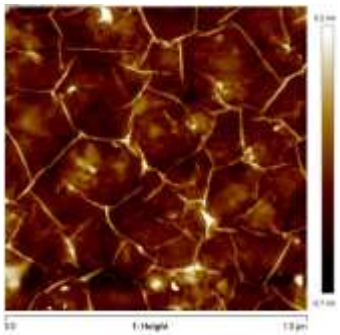


Figure 1: Atomic force microscopy of h-BN from Aixtron

Fabrication of transparent all-solid-state thin film lithium ion battery

Ji-Won Choi
Yaelim Hwang, Haena Yim
Korea Institute of Science and Technology (KIST), 5, Hwarang-ro 14 gil, Seongbuk-gu, Seoul 02792, Republic of Korea
jwchoi@kist.re.kr

Abstract

In recent years, as the development of smart paper, smart windows, medical diagnostic smart lenses, and transparent displays is accelerated, the development of next-generation energy sources with flexibility or transparency is required. However, the production of transparent batteries is difficult to fabricate since the materials acceptable in Lithium Ion Batteries are not transparent except electrolyte. All of the transparent battery research reported so far has a structure using a fine line width, and this method is a battery made to appear opaque but transparent by creating a micro-pattern below the human eye resolution. This method has limitations such as complicated process, low energy density, and packaging system occupying a large volume. [1,2] Therefore, we have developed a battery in which all materials are transparent by laminating transparent battery materials.

In previous research, we have developed transparent cathode, $LiFePO_4$.[3] Its wide bandgap of 3.7 eV, high transparency (76.3%) makes it promising candidate for cathode of transparent battery. However, a full-cell has never been fabricated due to the absence of a transparent anode. Therefore, we developed a transparent anode that does not require an anode current collector for full cell production.

In this study, we developed an Zn doped SnO_2(ZTO)/$AgTi_{0.0007}Cr_{0.067}$(ATC)/Zn doped SnO_2 (ZTO) multilayer anode that exhibits high transmittance (90%), low sheet resistivity (8.8 Ω /sq), and high discharge capacity (1036.9 μAh/cm^2·μm). Due to the high electrical conductivity of the anode itself, anode current collector is not required, therefore the fabrication process can be simplified.

All-solid-state full cell was fabricated with $LiFePO_4$ cathode and ZTO/ATC/ZTO anode, LiPON with radio frequency (RF) sputter. Using glass substrate with ITO deposited as a cathode current collector, we created a cell with a total thickness of 1.5μm excluding substrate. Electrochemical analysis is done in the glove box, checking charge/discharge profiles with 100 cycles. The transparency of full cell was verified by UV Spectroscopy in 550 nm.

References

[1] Yuan Yang et al., PNAS , 108 (2011) 13013-13018
[2] Sami Oukassi et al., ACS Appl. Mater. Interfaces, 11 (2019) 683-690
[3] HyunSeok Lee et al., J. Nanosci. Nanotechnol., 15 (2015) 8627-8631

Figures

Figure 1: Photographic image of transparent thin film battery.

Raman investigation of graphene whiskers

P. Ciepielewski
J.M. Baranowski
Łukasiewicz - Institute of Microelectronics and Photonics, al. Lotników 32/46, 02-668 Warsaw, Poland
pawel.ciepielewski@imif.lukasiewicz.gov.pl

Some organic (e.g. cellulose or keratin) materials containing the carbon atoms when subjected to high temperature sintering (over 2000 Co) in Ar atmosphere. After sintering these material evolve to multilayer graphene structures often in a form three dimensional cigar-shaped object (Fig1) . They were previously observed in graphite and called whiskers [1]. The Raman experiment on the whiskers was realized in back-scattering configuration with laser beam (532nm) parallel to the whiskers axis. The Raman spectrum close to the axis is presented in Fig.2. It shows extremely narrow and symmetric 2D Raman mode with FWHM as low as 14 cm -1. The FWHM parameter is usually consider as a measure of graphene quality and low FWHM indicates high mobility. In whiskers the graphene stripes are arranged in a conical and helical structure where consecutive layers are twisted of about 27o . This is the most likely one of the reason why we observed single and symmetric 2D Raman mode. The correlation of 2D and G Raman modes is presented in Fig.3. The almost constant 2D mode energy with simultaneous spread in G mode energy indicates both the ideal homogeneity of the whisker from the point of view of strain (tensile strain) and suggests the n - type of the carriers. This ideal strain homogeneity is the most likely responsible for the extremely low FWHM.

Figures

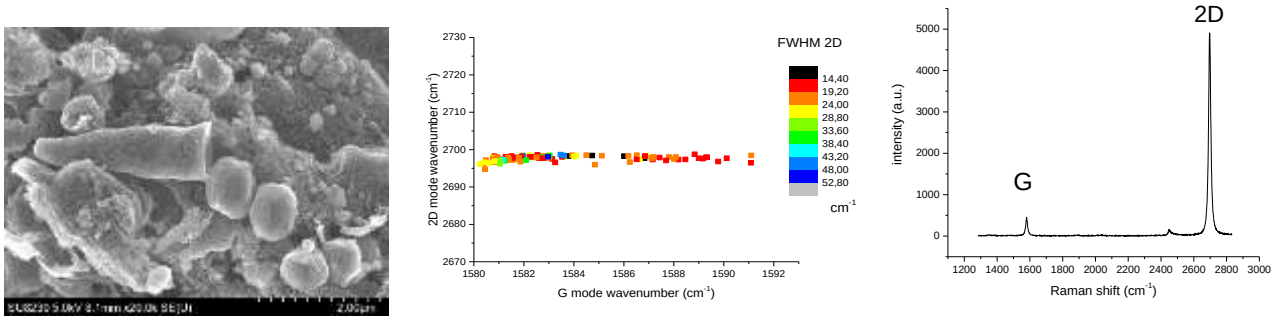


Figure 1: PingHeng Tan et all., PHYSICAL REVIEW B, 64, 214301 (2001)

Active thermography for the analysis of graphene

Christoph Geers[1]
Giulia Mirabello[2], Mathias Bonmarin[3], Marco Lattuada[2]
1 *NanoLockin GmbH, Route de la Fonderie 2,1700 Fribourg, Switzerland*
2 *University of Fribourg – Department of Chemistry, Fribourg, Switzerland*
3 *Zürich University of Applied Sciences – Institute of Computational Physics, Winterthur, Switzerland*
christoph.geers@nanolockin.com

A large variety of methods exists to analyze mostly inorganic engineered nanoparticles (NPs) in dispersions, as thin films or embedded (e.g. in nanocomposites). However, many standard analyses (e.g. chemical analysis) fail when it comes to carbon-based nanomaterials and the analysis often requires complicated sample preparation (e.g. microtome cutting) or labelling.
Methods used to detect and quantify carbon-based nanomaterials or analyze their size, size distribution, and colloidal state in analytically complex environments (e.g. cell culture media, serum) like dark-field hyperspectral imaging, electron microscopy or dynamic light scattering require complex and time-consuming sample preparation, are lacking spatial information and only analyze a small portion of the sample. Additionally, the quantification of carbon nanomaterials is even more challenging and methods for their quantification are simply missing.
Carbon nanomaterials have the ability to produce heat upon external stimulation by absorbing and scattering light [1], [2].
In this talk I will present a new technique based on lock-in-thermography (LIT) to measure and quantify the heat produced by carbon nanomaterials upon light stimulation. This heat can be recorded with an infrared camera and is processed by a specially developed LIT algorithm to yield 2D-images for analyzing carbon nanomaterials. The advantage of this set-up is the fast and accurate analysis of carbon nanomaterials in a variety of matrices, without requiring complicated sample preparation. Additionally, the method can be used for semi-quantitative analysis [3], [4].

References

[1] K Jiang, DA Smith, A Pinchuk, J. Phys. Chem. C, 55 (2013) 27073–27080
[2] D Jaque, L Martínez Maestro et. al, Nanoscale, 6 (2016) 9494-9530
[3] L Steinmetz, J Bourquin, et. al, Nanoscale, 12 (2020) 17362
[4] L Steinmetz, C Geers et. al, J. Phys. Chem. C, 10 (2021) 5890-5896

Figures

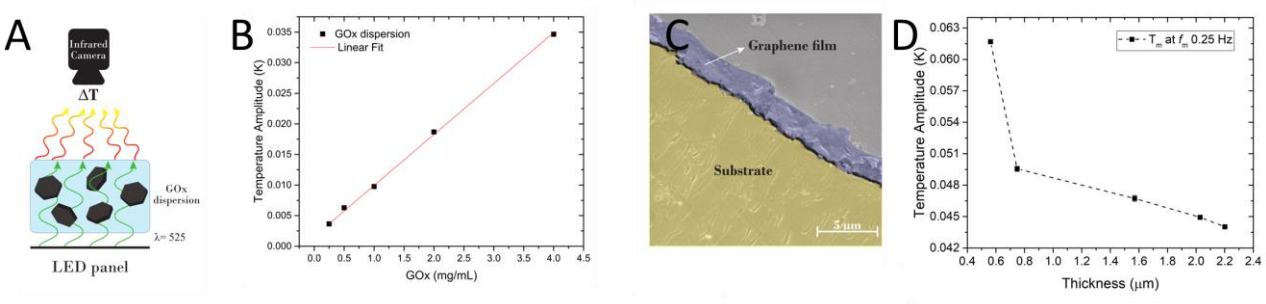


Figure 1: A: Measurement principle; B: Measurement of the average heating signal versus graphene oxide concentration; C: Graphene film on polymer substrate; D: Film thickness versus average heating signal

Top Gate Length Dependence of Hysteresis in 300mm FAB MoS_2 FETs

Yu.Yu. Illarionov[1,2], T. Knobloch[1], M. Waltl[1], Q. Smets[3], L. Panarella[3,4], B. Kaczer[3], T. Schram[3], S. Brems[3], D. Cott[3], I. Asselberghs[3], T. Grasser[1]

[1]*Institute for Microelectronics (TU Wien), Gusshausstrasse 27-29/E360, 1040 Vienna, Austria*

[2]*Ioffe Institute, Polytechnicheskaya 26, 194021 St-Petersburg, Russia*

[3]*imec, Kapeldreef 75, B-3001 Leuven, Belgium* [4]*KU Leuven, 3000 Leuven, Belgium*

illarionov@iue.tuwien.ac.at

The use of MoS_2 as a channel in FETs can potentially enable outstanding scaling opportunities which are not accessible with Si [1]. Recently, imec has demonstrated the FAB line processing of top-gated WS_2 FETs on 300mm substrates [2]. We now present the integration of MoS_2 grown on sapphire and transferred to 300mm wafers (Figure 1a,b). These devices can exhibit promising performance with an on/off current ratio up to 10^4 when operated via the top gate (Figure 1c). However, their stability has not been studied so far. Here we have performed a detailed analysis of the hysteresis in these devices and found that it is typically more pronounced in FETs with larger top gate lengths L_{TG} (Figure 2a), as confirmed by the obtained statistics of the hysteresis width vs. reciprocal sweep time t_{sw} traces measured on multiple devices with L_{TG} between 70nm and 10µm (Figure 2b). However, our subsequent measurements at higher temperatures up to 175°C have revealed that for the shortest devices with L_{TG} = 70nm the hysteresis not just becomes smaller but also becomes counterclockwise at slow sweeps (Figures 2c,d). This suggests the involvement of thermally activated oxide traps situated close to the top gate electrode, which partially compensates standard charge trapping by border oxide traps situated close to the channel. Thus, we conclude that scaling of FAB MoS_2 FETs would require an in-depth study of charge trapping at both sides of the top gate insulator.

References

[1] S. Das et al., Nature Electronics, 4 (2021), 786.
[2] T. Schram et al., IEEE Symposium on VLSI Technology, pp. 1-2 (2021).

Figures

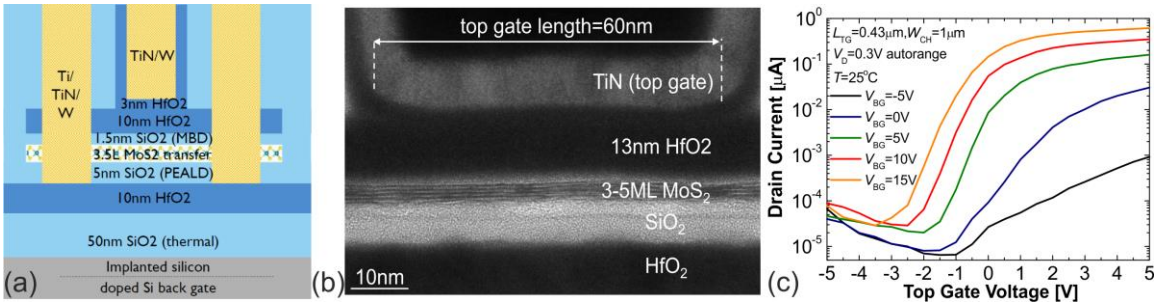


Figure 1: (a) Schematic layout of our FAB MoS_2 FETs. (b) TEM image of a device with L_{TG}=60nm. (c) I_D-V_{TG} curves of these devices vs. varied V_{BG}.

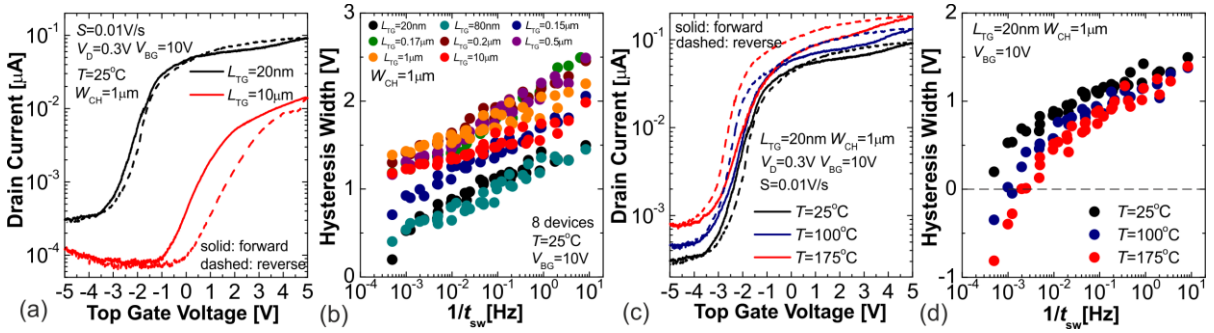


Figure 2: (a) Comparison of slow sweep I_D-V_{TG} curves for MoS_2 FETs with L_{TG} = 20nm and 10µm. (b) $\Delta V_H(1/t_{sw})$ traces for 8 devices with L_{TG} between 20nm and 10µm. (c) Slow sweep I_D-V_{TG} curves for the device with L_{TG} = 20nm measured at different temperatures. (d) The $\Delta V_H(1/t_{sw})$ traces show switching of the hysteresis towards the counterclockwise direction for slow sweeps and high temperatures.

Exploring the Interplay of Layered Materials: Atomic Force Microscopy as a Path to Morphology and Functional Properties of Heterostructures

Presenting Author: Alexander Klasen[1]
Co-Authors: James Kerfoot[1], Andrea Cerreta[1]
[1]*Park Systems Europe GmbH, Schildkrötstraße 15, Mannheim, Germany*
klasen@parksystems.com

Heterostructures of 2D materials often are more than the mere sum of their parts. Novel mechanical, electronic and optical properties can arise from the interplay of stacked 2D structures. This becomes particularly evident when orientation mismatch or strain between subsequent layers significantly modifies the properties of the involved materials with respect to bulk. Such complex phenomena require equally versatile means of characterization that allow studying such features on a local scale, be it functional parameters like the morphology, conductance, surface potential, piezoelectricity, or local mechanic features like stiffness and adhesion. Atomic force microscopy (AFM) has been established as a most versatile tool since it allows to quantitatively measure a holistic pool of parameters non-destructively with sub-nanometer resolution.
In this talk, we provide several state-of-the-art examples for the fundamental characterization of layered 2D heterostructures using AFM. As introduced in several recent accounts, stacks of graphene and hexagonal boron nitride (hBN) can be deposited on Si/SiO_2 with a controlled twist angle to give rise to different properties ranging from moiré pattern in the local conductance [1,2] to ferroelectric superlattices [3-5]. We describe the characterization of ferroelectric domains in such parallel stacked hBN by both electrostatic force microscopy (EFM) and Kelvin probe force microscopy (KPFM) in addition to manipulation of these domains by applying a bias to the sample via the AFM probe. These highly resolved electrical measurements can be further correlated with local mapping of the nanomechanical response of the sample, providing a complete set of information about the properties of hBN and similar 2D materials and allowing their optimization for applied research.

References

[1] C. R. Woods et al., Nature Phys, 10 (2014) 451-456
[2] R. Ribeiro-Palau et al., Science, 361, 6403 (2018) 690-693
[3] C. R. Woods et al., Nat Commun., 12 (2021) 347
[4] K. Yasuda et al., Science, 372, 6549 (2021) 1458-1462
[5] M. Vizner Stern et al., Science 372, 6549 (2021) 1462-1466

Figures

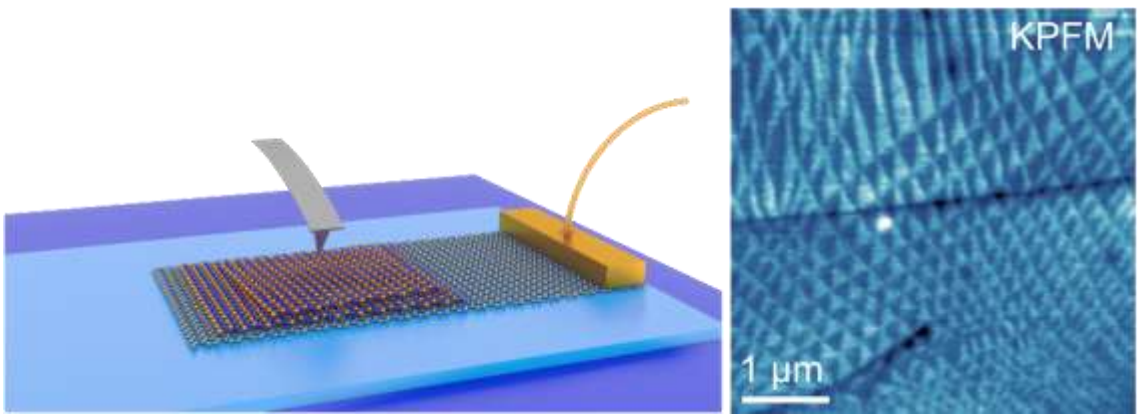


Figure 1: Example of the electrostatic characterization of layered heterostructures using AFM: Mapping of interfacial ferroelectricity in parallel stacked hBN using KPFM.

Industrial graphene coating of low-voltage copper wires for power distribution

Neeraj Mishra[1,2,],Ylea Vlamidis[1,2], Leonardo Martini[1,2], Arianna Lanza[1], Alex Jouvray[3], Marco La Sala[4], Mauro Gemmi[1], Vaidotas Mišeikis[1,2], Stiven Forti[1], Kenneth B.K. Teo[3], Camilla Coletti[1,2]

[1]Center for Nanotechnology Innovation@NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro, 12−56126 Pisa, Italy,[2]Graphene Labs, Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy,[3]AIXTRON LTD, Anderson Road, Swavesey, Cambridge CB24 4FQ, United Kingdom,[4]Baldassari Cavi, Viale Europa 118/120, 55013 Capannori (Lucca), Italy.

contact@neeraj.mishra.iit.it

Abstract

Copper (Cu) is the electrical conductor of choice in many categories of electrical wiring, with household and building installations being the major market of this metal [1-2]. In this work, we demonstrate that Cu wires with diameters relevant for low voltage (LV) applications, can be coated with graphene via chemical vapor deposition (CVD). The CVD process is rapid, safe, scalable and industrially-compatible. Graphene-coated Cu wires display oxidation resistance and increased electrical conductivity (up to 1% immediately after coating and up to 3% after 24 months), allowing for wire diameter reduction and thus significant savings in wire production costs. Combined spectroscopic and diffraction analysis indicate that the conductivity increase is due to a change in Cu crystallinity, induced by the coating process conditions, while electrical testing of aged wires elucidates that graphene plays a major role in maintaining improved electrical performances over time. Finally, we demonstrate graphene coating of Cu wires using an open-end roll-to-roll (R2R) CVD reactor, which will enable the in-line production of graphene-coated metallic wires in industrial settings.

References

[1] Zhong, Z.; Lee, H.; Kang, D.; Kwon, S.; Choi, Y. M.; Kim, I.; Kim, K. Y.; Lee, Y.; Woo, K.; Moon, J.; *ACS Nano, 10* (8) (2016) 7847–7854.
[2] Kashani, H.; Kim, C.; Rudolf, C.; Perkins, F. K.; Cleveland, E. R.; Kang, W.; *Adv. Mater. 33* (51)(2021)1–14.
[3] Mishra et al,; Industrial graphene coating of low-voltage copper wires for power distribution manuscript under preparation

Figures

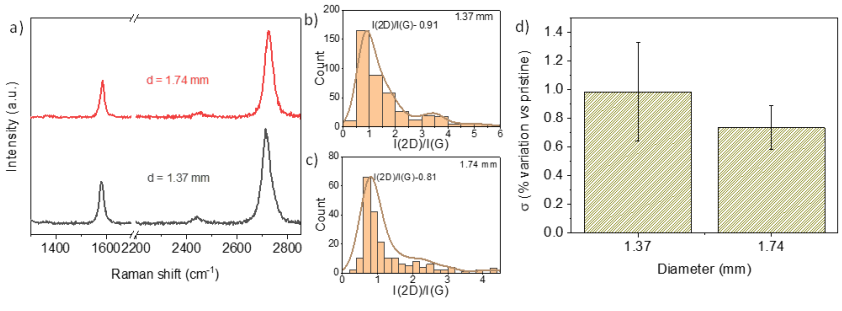


Figure 1: Spectroscopic and electrical properties of Gr-coated Cu wires. Representative Raman spectra (a) and mapping intensity ratio of 2D/G bands (b and c). Electrical conductivity improvement of Gr-coated wires with respect to pristine ones (d). Error bars represent the SDM.

Acknowledgement: This work has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement 881603"

Vertical and Lateral Electrodeposition of 2D Material Heterostructures

Yasir J Noori[1]
Shibin Thomas[1], Nema Abdelazim[1], Sami Ramadan[2], Victoria Greenacre[1], Yisong Han[3], Richard Beanland[3], Norbert Klein[3], Gill Reid[1], Philip N Bartlett[1], Kees de Groot[1]
[1]*University of Southampton, Southampton, UK*
[2]*Imperial College, London, UK*
[3]*University of Warwick, Coventry, UK*
y.j.noori@southampton.ac.uk

Abstract

Developing scalable techniques for growing 2D materials and their heterostructures is a major challenge that needs to be overcome before these materials can make an impact in industries. Electroplating (electrodeposition) is an industrially acceptable deposition technique that offers unique advantages. This work is divided into two main parts. First, we demonstrate controlled electrodeposition of uniform and continuous MoS_2 and WS_2 layers over a large-area and micropatterned graphene electrodes. Second, we present a novel electrode design that enables MoS_2 to be grown laterally over insulating substrates, demonstrating lateral photodetector devices based on TiN/MoS_2/TiN structure. Our goal is to show that electrodeposition can produce competitive quality of 2D materials which can potentially be scaled to wafer sizes in fabrication industries for device applications.

References

[1] Y. J. Noori, S. Thomas, S. Ramadan, et al., IOP 2D Mater., 9 (2022) 15025
[2] Y. J. Noori, S. Thomas, S. Ramadan, et al., ACS Appl. Mater. Interface, 12 (2020) 49786.
[3] N. Abdelazim, Y. J. Noori, S. Thomas, et al., Wiley Adv. Electron. Mater., (2021) 2100419.
[4] S. Thomas, DE Smith, V. Greenacre, et al., J. Electrochem. Soc., 167 (2020) 106511.

Figures

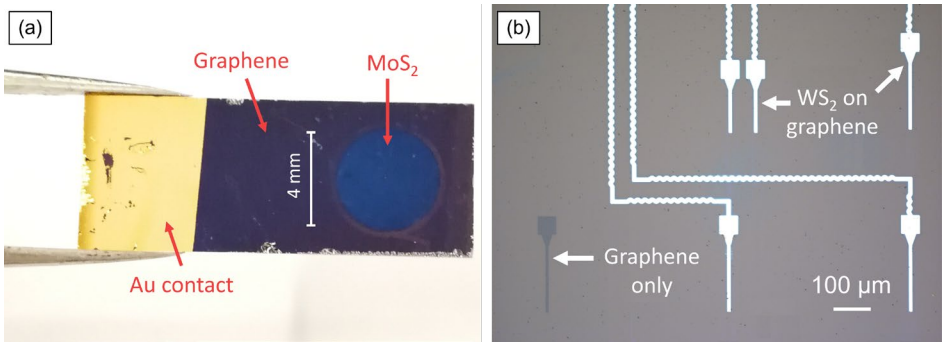


Figure 1: (a) Image of a large area MoS_2 that is electrodeposited over graphene (b) Optical microscope image of micropatterned WS_2/graphene heterostructures and a graphene only film.

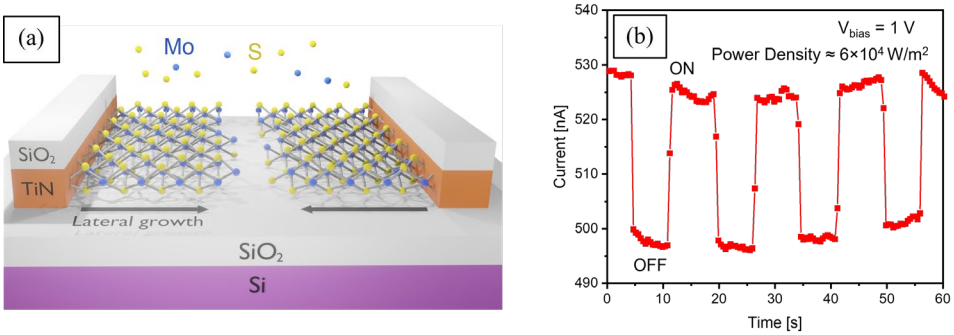


Figure 2: (a) Schematic of MoS_2 that is laterally electrodeposited over an insulator from TiN electrodes. (b) Illumination response of a photodetector device based on laterally grown MoS_2.

Investigation and Characterization of 2D Materials using Transmission Electron Microscopy – recent advances

Dr. Philipp Wachsmuth
Dr. Dietmar Weber
JEOL (Germany) GmbH, Gute Änger 30, 85356 Freising, Germany
wachsmuth@jeol.de

Abstract

The detailed characterization of materials at the nanoscale down to the atomic level is highly important to better understand many different material properties. Transmission electron microscopy (TEM) and scanning TEM (STEM) are essential tools as they offer a variety of different characterization methods ranging from imaging at the atomic level to the analysis of the chemical composition and the detailed investigation of the electric structure. In addition, these methods can readily be combined with a wide range of in-situ techniques like heating, electrical biasing or laser excitation, to name a few.
The characterization of graphene and many other 3D materials can be a very challenging topic in S/TEM especially if the goal is the direct observation of the atomic structure. In particular, electron beam induced modifications and damage during image tuning can make visualizing the sample at atomic resolution an extremely difficult task.
Here we will give an overview of recent advances in instrumentation and methods highlighting new low-dose imaging techniques [1] as well as application examples detailing the various characterization possibilities of modern TEMs. We also discuss the possibilities combining S/TEM techniques with ultra-fast electron shutters and continuous wave laser systems [2,3].

References

[1] Kousuke Ooe et al., Ultramicroscopy 220, 2021, 113133
[2] A B. W. Reed, A. A. Moghadam, R. S. Bloom, S. T. Park, A. M. Monterrosa, P. M. Price, C. M. Barr, S. A. Briggs, K. Hattar, J. McKeown, and D. J. Masiel, Struct. Dyn. 6, 054303 (2019)
[3] B. W. Reed, S. T. Park, R. S. Bloom, and D. J. Masiel, Microsc. Microanal. 23 (Suppl 1), 84 (2017)

Application of Graphene-based 2D materials in composites for aerospace applications

Muhammad Zahid[1,*], Nicola Gallo[2], Ignazio Scavo[2] and Stefano G. Corvaglia[2]

[1]*Leonardo Labs, Aerostructure division-Leonardo SpA, str. prin. Grottaglie-Monteiasi, 83/84, Monteiasi (TA), Italy*
[2]*Product Engineering and IP Management, Aerostructure division-Leonardo SpA, str. prin. Grottaglie-Monteiasi, 83/84, Monteiasi (TA), Italy*
*muhammad.zahid.ext@leonardocompany.com

Abstract

Carbon fibre reinforced composites (CFRPs) show excellent features like high strength to weight ratio, zero corrosion, ease of manufacturing and high resistance to fatigue [1]. These features translate into enhanced fuel efficiency, low maintenance costs, improved life span as well as reduced carbon foot prints of transportation sectors such as aviation and automotive [2]. Therefore, the CFRPs are being employed increasingly to replace current metallic structures in those sectors. However, the CFRPs lack several functionalities that would be a pre-requisite for the future zero-emission mobility. For instance, the CFRPs do not exhibit high electrical conductivity, thermal management, gas barrier and moisture barrier properties. The epoxy resin that constitutes 40% by volume of an aerospace composite is vulnerable to impacts, resulting in crack formation and their subsequent propagation. To overcome these shortcomings, external devices or coatings are employed that not only increase fabrication and maintenance costs as well as add significant weight to the structures. For instance, hydrogen (H2), as a green fuel, has tremendous potential to solve future energy and pollution crisis. Automotive and aerospace vehicles will be major beneficiaries of this technology and are developing CFRP-based storage cylinders. To stop the vapour escape, a metallic barrier layer is used in those composite-based cylinders. Similarly, lightning strike protection and anti-icing/de-icing require additional devices to keep the aircraft operational in extreme weather conditions. Carbon-based nanomaterials, specifically graphene, have exceptional electrical, mechanical, and thermal properties in addition to its lightweight [3]. Graphene with broad set of properties is fully capable to modify surface properties of the conventional CFRPs. The graphene-based films or coatings exhibit the enhanced electrical, thermal and gas barrier properties that can be exploited to protect the aerospace structures against high atmospheric temperatures, icing, static charges, lightning strikes, corrosion, humidity and gases. Whereas, their incorporation to the epoxy matrix can modify resin properties significantly. For example, the graphene enhanced epoxy resin display improved tensile and compression strength, better fracture toughness and fatigue resistance, as compared to the baseline CFRPs (without graphene). The epoxy polymers filled with graphene-based 2D materials can also be co-cured in a single cycle with CFRPs to reduce process time, cost and complexity. Therefore, the graphene-based 2D materials have huge potential to enhance capabilities of the current CFRPs rendering them multifunctional smart composites.

References

[1] Roeseler W. G. at el., 16th International Conference on Composite Materials, (2007). Authors, Journal, Issue (Year) page (Century Gothic 11) Indicate references with sequential numbers within [square brackets].
[2] Traveller, viewed 13 May 2022, https://www.traveller.com.au/airline-weight-reduction-to-save-fuel-the-crazy-ways-airlines-save-weight-on-planes-h14vlh
[3] K. S. Novoselov, et al., Nature, 490 (2021) 192- 200.