

Name

XXXVth
International Winterschool
on Electronic Properties
of Novel Materials

Molecular Nanostructures

Program



Hotel Sonnalp
Kirchberg/Tirol
Austria

18 - 24 March, 2023

IWEPNM 2023

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Verein zur Durchführung der International Winterschool on Electronic Properties of Novel Materials

Verein zur Förderung der Internationalen Winterschulen in Kirchberg Austria

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This year's Logo of the IWEPM shows a schematic image of two irregular arching graphene monolayer sheets.

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Financial assistance from the sponsors and supporters is greatly acknowledged.

Dear Friend:

Welcome to the 35th International Winterschool on:

Electronic Properties of Novel Materials!

This Winterschool is a sequel of thirty-four previous meetings held in Kirchberg in the last decades on problems related to the electronic structure of novel materials. The idea of the meeting is to bring together experienced scientists from universities and industry with advanced students working in the selected field and thus create a fruitful and prosperous community for the exchange of scientific information and personal experience. It is a tradition of the Winterschools in Kirchberg that this exchange is not restricted to the lectures and poster sessions but occurs throughout the whole week.

The Winterschool is dedicated to molecular nanostructures as a new class of materials. Like the previous Winterschools it runs on an informal level.

If you have any questions concerning the organization and the program, come and see one of us or one of the colleagues involved in the preparation of the meeting. These persons are:

Program	Janina Maultzsch
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Finances	Antonio Setaro
Accommodation Finances	Kati G.-Hubmann
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Abstract Booklet & Giveaways	Sabrina Juergensen
Conference Publications	Antonio Setaro
Announcements	Stefan Wolff
Technique	Patryk Kusch & Oisín Garrity

We want to thank our colleagues who helped in organizing this winterschool: Charlotte Berrezueta, Alphonse Fiebor, Gabriela Luna Amador, Aditiya Singh, Angelin See, Gudrun May-Nesseri

Also the manager of the hotel, Karin Brudermann, and their staff promised to help us wherever they can. We want to acknowledge their help.

We wish you an interesting, successful, and pleasant week in Kirchberg. We are very much looking forward to your contributions at the event.

Sincerely yours,
Janina, Stephanie, Andreas, and Christoph

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J. Maultzsch (Erlangen)

S. Reich (Berlin)

A. Hirsch (Erlangen)

C. Stampfer (Aachen)

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Scope

This winterschool will provide a platform for reviewing and discussing new developments in the field of electronic properties of molecular nanostructures and their applications. The scope of the winterschool covers experimental and theoretical work in the following fields:

- Materials science of graphene, nanographene, and carbon nanotubes
- Novel two-dimensional materials
- Optics, electronics, growth, and selection of carbon nanotubes and graphene
- Theory of novel materials
- Applications of novel materials
- Nanostructure spintronics
- Topological materials
- Plasmonic nanostructures
- Single-molecule experiments

INFORMATION FOR PARTICIPANTS

Time and location

The IWEPNM 2023 starts on Saturday, 18 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Friday, 24 March, breakfast. There will be a reception party on Saturday, 18 March, after dinner, and a farewell party including dinner on Thursday, 23 March.

Transport

The hotel Sonnalp can be reached by private car from downtown Kirchberg by driving about one kilometer towards Aschau. Participants arriving at the railway station in Kirchberg or Kitzbühel should hire a taxi to get to the hotel.

Addresses

The address of the Winterschool is:

IWEPNM 2023 Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria

e-mail: info@hotelsonnalp.info, web: www.hotelsonnalp.info

All questions concerning the IWEPNM 2023 should be directed to:

Prof. Dr. Janina Maultzsch,

Department für Physik, FAU Erlangen, Staudtstr. 7, 91058 Erlangen, Germany

or

Prof. Dr. Stephanie Reich,

Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

email: iwepnm@posteo.de, web: www.iwepnm.org

Participation

Participation at the IWEPNM 2020 is possible for students and scientists working in the field covered by the scope of the meeting. Because of the limited space the participation requires prearranged acceptance by the organizers.

Contributions

All oral contributions will be presented in the big seminar room of the Hotel Sonnalp. All participants are invited to contribute comments to research and tutorial lectures, where 10 minutes for discussion are reserved within each lecture. Video projection will be available for presentations. Invited speakers please test the video projection with the technical staff at the latest a few minutes before your session begins. Posters will be presented in the hall of the seminar room.

We kindly ask you NOT to take any pictures or videos of the presentations.

Childcare

Childcare is provided by Theresa Leitgeb (theresa.leitgeb@gmx.at). If you need childcare during the winterschool, please contact us at the registration desk.

Ski pass and internet connection

If you wish to buy a ticket for the ski lifts, please ask at the hotel reception. Internet connection through WLAN is available for all participants, even if they are not accommodated at the Hotel Sonnalp. Please check at the front desk.

Poster awards

There will be a poster award for the best poster presentation in each poster session on Monday, Tuesday, and Wednesday. Poster awards are kindly provided by Wiley VCH.

Conference Publication

Invited and contributed presentations from IWEPNM 2023 are scheduled for publication as a special issue in physica status solidi (pss) (b). **Manuscript submission is due on April 28th.** In selected cases articles are highlighted in pss (RRL) (Reviews@RRL, Rapid Research Letters) or Advanced Electronic Materials. Accepted manuscripts will become directly their DOI right after acceptance and will be fully citable.

Accepted manuscripts will fulfill the standards and requirements of the journal and are peer-reviewed in the same way as regular submissions. Acceptance of a contribution for presentation at the winterschool does not automatically include acceptance for publication in the special issue. Detailed information will be provided at the winterschool.

Manuscript preparation and submission

Preparation instructions and templates are available at <http://www.pss-b.com> → **Author guidelines.** Original Papers in pss (b) have typically 6 to 10 pages, Letters in pss (RRL) have 4 pages.

Please **submit one complete PDF- or Word-file for review** (Word or Latex source files are required after acceptance for production). The submission system can be found here: <http://www.editorialmanager.com/pssb-journal>

Please select article type "Original Paper" of the journal of your choice and subsequently the section "IWEPNM: Electronic Properties of Novel Materials. If you intend to submit a "Rapid Research Letter", a "Feature Article" or a manuscript to Advanced Electronic Materials, please consult with the editors at iwepnm-publication@physik.fu-berlin.de.

IWEPNM 2023
CHAIRPERSONS FOR THE ORAL SESSIONS

The following participants are asked to support the program of the Winterschool by serving as chairperson:

Sunday, 19.03.	morning	Janina Maultszch
	morning, after coffee break	Otakar Frank
	evening	Claudia Draxl
Monday, 20.03.	morning	Viera Skakalova
	morning, after coffee break	Francesco Mauri
	evening	Ralph Krupke
Tuesday, 21.03.	morning	Andreas Hüttel
	morning, after coffee break	Carola Meyer
	evening	Stephanie Reich
Wednesday, 22.03.	morning	Shigeo Maruyama
	morning, after coffee break	Tobias Korn
	evening	Hans Kuzmany
Thursday, 23.03.	morning	Andreas Hirsch
	morning, after coffee break	Ardemis Boghossian
	evening	Sebastian Heeg

Chairpersons are asked to start the sessions in time and **to terminate the lectures according to schedule**. The discussions may be extended up to 5 minutes beyond the schedule.

Chairpersons please remember:

You have to ask for questions from the sideroom (bar)!

For questions from the main room please ask the speaker to repeat the question. The chairperson's microphone should only be passed on to questions from the first row.

If there are any objections to the suggested list of chairpersons, please let us know at the beginning of the Winterschool.

We acknowledge your support.

The Organizers

PROGRAM

AND

ABSTRACTS

Final program

	Sunday, March 19	Monday, March 20	Tuesday, March 21	Wednesday, March 22	Thursday, March 23
Topics	vdW Semiconductors, Strain, Moiré Effects	Microscopy, hBN, Quantum Properties	Graphene, SWNT Defects, Synthesis & Applications	Twisted Graphene, Interfaces in 2D, CNT & BNNT	Novel 2D Crystals, Graphene Structures & Hybrids
08:30	TUTORIAL Magneto-Spectroscopy of Interlayer Excitons in TMD Heterostructures KORN	TUTORIAL Discovering Atomic Behaviour with Scanning Transmission Electron Microscopy and 2D Material Heterostructures HAIGH	Quantum Phases in Natural Bilayer Graphene Accessed by Control of Bandstructure and Screening WEITZ	TUTORIAL Non-Identical Moiré Twins in Bilayer Graphene RIBERIO	Hexagonal Hybrid Bismuthene by Molecular Interface engineering ABELLÁN
09:00			Microscopic Modelling of Electrostatically Induced Quantum Nanostructures in Gapped Bilayer Graphene KNOTHE		Advances in Organic 2D Crystals - From On-Water Surface Chemistry to Functional Applications FENG
09:30	Tailoring Optical Properties of 2D Semiconductors in van der Waals Heterostructures WALDECKER	Visualizing Magnetic Phase Transitions in 2D van der Waals Materials TSCHUDIN	Large Graphene Quantum Dots for THz Technology MANGENEY	Homojunctions, Topological Points, Strain Solitons and Kohn Anomaly in Graphene Systems JORIO	Optical Signatures of the 3D Anisotropy in Black Phosphorus SCHUE
10:00	Coffee Break				
10:30	Probing and Controlling Excitons in 2D Semiconductors and Heterostructures HEINZ	The Quantum Twisting Microscope ILANI	Exploring Electronic Spins in Chemically Modified Carbon Nanotubes MA	Generating and Exploring the Effects of Ultrastrong Electric Field in 2D Materials via Molecular Gating BOLOTIN	On the Interaction Between Single-Walled Carbon Nanotubes and Encapsulated Nanostructures AYALA
11:00	Electrical Control of Excitons in Two-Dimensional Semiconductors LEISGANG	CVD Synthesis of sp ² -Hybridized Multilayer Boron Nitride Films TAILPIED	Electroluminescence from Single-Walled Carbon Nanotubes with Quantum Defects KRUPKE	Nonlinear and Noisy Dynamics of 2D Materials ALIJANI	Spatially Resolved Molecular Engineering of Graphene WEI
11:30	Excitons and Polaritons in van der Waals Semiconductors DENG	Efficient Light-Matter Interaction in Hexagonal Boron Nitride CASSABOIS	Inorganic Liquid Crystals Based On 2D Materials CHENG	Level Alignment and Excitations at Heterointerfaces DRAXL	2D Materials for 3D Smart Soft Structures VÁZQUEZ

12:00 - 17:00	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops
17:00 - 18:30	Dinner				17:00 Automated Assembly of Synthetic van der Waals Solids MANNIX
18:30	Controlling Defect Hybridization with Strain in 2D Semiconductors LIBISCH	Novel Non-Equilibrium Phenomena in Two-Dimensional Heterostructures RUBIO	Exploring Electronic Spins in Chemically Modified Carbon Nanotubes MA	1D Heterostructures : Periodically Encoded Dipolar Chains based on BNNT Template GAUFRÈS	17:30 Search for the Fractional Josephson Effect in Topological and Nontopological Materials SCHÖNENBERGER
19:00	Vibrational Moiré Coupling and Dielectric Effects in One-Dimensional Heterostructures GORDEEV	Nanochemistry on 2D Materials: Principles and Applications VOIRY	Simple Chemical Approach to Two-Dimensional Metal Iodides/Graphene heterostructures SKAKALOVA	The Alignment of Single Wall Carbon Nanotubes by Filtration FLAVEL	18:00 Summary
19:30	Electronic Excitations of Suspended Neutral Graphene and LO-TO Phonon Splitting in h-BN Monolayer by EELS MAURI	Quantum Materials for Thermoelectricity NIELSCH	A NanoBioengineering Frontier for Next-Generation Optical Devices BOGHOSSIAN	Super-Resolution Microscopy of Excitonic Photoluminescence in SWIR Emitting Single Wall Carbon Nanotubes COGNET	
20:00	Mattermorphosis HEINE	Poster I Monday	Poster II Tuesday	Poster III Tuesday	Bauernbuffet Farewell Dinner
20:30					
Topics	vdW Semiconductors, Strain, Moiré Effects	Microscopy, hBN, Quantum Properties	Graphene, SWNT Defects, Synthesis & Applications	Twisted Graphene, Interfaces in 2D, CNT & BNNT	Novel 2D Crystals, Graphene Structures & Hybrids
Sunday, March 19		Monday, March 20	Tuesday, March 21	Wednesday, March 22	Thursday, March 23

- 08:30 – 09:30 TUTORIAL: T. Korn, Rostock
Magneto-Spectroscopy of Interlayer Excitons in TMD Heterostructures
- 09:30 – 10:00 L. Waldecker, Aachen
Tailoring Optical Properties of 2D Semiconductors in van der Waals Heterostructures
- 10:00 – 10:30 Coffee Break
- 10:30 – 11:00 T. Heinz, Stanford
Probing and Controlling Excitons in 2D Semiconductors and Heterostructures
- 11:00 – 11:30 N. Leisgang, Cambridge
Electrical Control of Excitons in Two-Dimensional Semiconductors
- 11:30 – 12:00 H. Deng, Ann Arbor
Excitons and Polaritons in van der Waals Semiconductors
- 12:00 – 17:00 Mini Workshops
- 17:00 – 18:30 Dinner
- 18:30 – 19:00 F. Libisch, Vienna
Controlling Defect Hybridization with Strain in 2D Semiconductors
- 19:00 – 19:30 G. Gordeev, Belvaux
Vibrational Moiré Coupling and Dielectric Effects in One-Dimensional Heterostructures
- 19:30 – 20:00 F. Mauri, Roma
Electronic Excitations of Suspended Neutral Graphene and LO-TO Phonon Splitting in h-BN Monolayer by EELS
- 20:00 – 20:30 T. Heine, Dresden
Mattermorphosis

08:30**Magneto-Spectroscopy of Interlayer Excitons in TMD Heterostructures**

J. Holler¹, M. Selig², D. S. Smirnov³, M. Kempf⁴, J. Zipfel⁵, P. Nagler¹, M. Katzer², F. Katsch², M. V. Ballottin⁶, A. A. Mitiglu⁶, A. Chernikov^{1,7}, P. C. M. Christianen⁶, C. Schüller¹, A. Knorr², Tobias Korn⁴

¹Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Regensburg, Germany

²Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

³Ioffe Institute, St. Petersburg, Russia

⁴Institut für Physik, Universität Rostock, Rostock, Germany

⁵Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California, USA

⁶High Field Magnet Laboratory (HFML - EMFL), Radboud University, ED Nijmegen, The Netherlands

⁷Institute of Applied Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Dresden, Germany

Transition-metal dichalcogenide (TMD) monolayers are direct-gap semiconductors with peculiar spin-valley coupling. Combining two different TMDs can lead to formation of interlayer excitons (ILE), and their basic properties will be discussed in the introduction. In MoSe₂-WSe₂ heterobilayers, optically bright ILE are only observable if the interlayer twist is close to 0 (aligned) or 60 (anti-aligned) degrees.

Depending on interlayer twist, ILE transitions are either valley-conserving or occur between different valleys. This allows us to engineer the ILE g factor, changing its magnitude and even its sign. Additionally, applied magnetic fields induce a valley polarization of the ILE, and its buildup can directly be observed in helicity- and time-resolved photoluminescence (PL), with peculiar features due to the dependence of ILE optical selection rules on interlayer registry. For both, aligned and anti-aligned ILEs, we find that at 24 Tesla, the valley polarization is resonantly enhanced, even though their g factors are markedly different. This observation hints at a scattering process involving single carriers within the ILE and zone-boundary acoustic phonons.

09:30**Tailoring optical properties of 2D semiconductors in van der Waals heterostructures**Lutz Waldecker¹¹RWTH Aachen University

The opto-electronic properties of the transition metal dichalcogenides (TMDs) can be modified in different ways by embedding them into van der Waals heterostructures. For example, the presence of graphene in the vicinity of the TMDs modifies their exciton binding energy and the magnitude of the bandgap via external dielectric screening. At the same time, charge- and energy transfer determine the doping level of the TMD and the lifetime of excitations.

Here, we will describe our advances in understanding the dielectric screening as well as the energy transfer in TMD – graphene heterostructures. We will discuss how the screening modifies the dispersion of the electronic bands as well as the exciton binding energy. Furthermore, we will discuss how hBN spacer layers and the charge carrier density in graphene can be used to tune the screening and the energy-transfer times.

10:30**Probing and Controlling Excitons in 2D Semiconductors and Heterostructures**Tony F Heinz^{1,2}¹Dept. of Applied Physics, Stanford University, Stanford, CA, USA²SLAC National Accelerator Laboratory, Menlo Park, CA, USA

please use One of the key features of the optical response of 2D semiconductors is the dominant role of excitonic interactions. The strong influence of these many-body effects reflects the reduced dimensionality combined with the reduced dielectric screening of atomically thin crystals. In our talk, we will review progress in understanding the nature of optically excited states in 2D monolayers and heterostructures. We will describe how excitonic states can be tuned and probed by altering the Coulomb interaction within the layer by various approaches, including through changes in the external dielectric environment. We will particularly emphasize recent advances in applying time-resolved ARPES (angularly resolved photoemission spectroscopy) to examine the momentum-space character and dynamics of excitons in transition metal dichalcogenide semiconductors. In these studies, carried out in collaboration with the group of Keshav Dani, we have been able not only to determine the valley characteristics of both bright and dark excitons, but also to image the wavefunction of excitonic states in momentum space. TEX format or plain text

11:00**Electrical control of excitons in two-dimensional semiconductors**Nadine Leisgang¹¹Department of Physics, Harvard University, Cambridge, MA, USA

The pursuit of scalable quantum technologies has led to an increasing demand for better control of quantum properties of materials. An exciton, a bound electron-hole pair, constitutes an atomic-like solid-state system which is optically accessible. In two-dimensional (2D) semiconducting transition metal dichalcogenides (TMDs), electron-hole pairs have particularly large binding energies, such that the excitons are stable even at room temperature. However, as the excitons are charge neutral, traditional depletion traps as employed for 2D electron gases will only provide weak confinement.

Here, we focus on TMD bilayer systems. We realize optical and electrical generation of interlayer excitons, where the bound electrons and holes reside in different layers. As a result of this separation the interlayer excitons are long-lived and have a large permanent dipole moment. Modulating the out-of-plane dipole by adjusting the distance of the electrons and holes and by an applied electric field, the interlayer excitons can be controlled on a quantum level. The deterministic creation and control over interlayer exciton systems will open up new avenues for quantum optoelectronic applications.

11:30

Excitons and polaritons in van der Waals semiconductors

Hui Deng¹

¹Physics Department, University of Michigan, Ann Arbor

Van der Waals semiconductors provide a new platform for robust excitons and polaritons with novel electronic and optical properties. We will discuss a few different ways to modify the excitonic and polaritonic properties in this platform, the resulting new types of excitons and polaritons, and potential device concepts based on their novel properties.

18:30**Controlling defect hybridization with strain in 2D semiconductors**

Christoph Schattauer¹, Pablo Hernández López², Sebastian Heeg², Lukas Linhart¹, Sviatoslav Kovalchuk³, Abhijeet Kumar³, Douglas J. Bock³, Jan N. Kirchhof³, Bianca Höfer³, Kyrylo Greben³, Denis Yagodkin³, Kirill I. Bolotin³, Florian Libisch¹

¹Institute for Theoretical Physics, Vienna University of Technology, Vienna

²Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

³Freie Universität Berlin, Department of Physics, Berlin, Germany

Mechanical strain is a powerful tuning knob for excitons. We present a multiscale tight-binding simulation for the optical spectra of WSe₂ under nonuniform strain in the presence of point defects [1]. Under the application of strain, conduction-band states are brought into energetic resonance with localized defect orbitals, forming a new hybrid state that inherits the properties of the constituent species. We compare our model to photoluminescence measurements of these fragile many-body states on pristine suspended WSe₂ kept at cryogenic temperatures [2]. The characteristics of the hybridized state, including an order-of-magnitude enhanced light/matter coupling, avoided-crossing energy shifts, and strain tunability of many-body interactions, all fit to our simulation. Our results suggest such hybridized excitons may play a critical role in the operation of single quantum emitters based on WSe₂. Furthermore, the techniques we developed may be used to fingerprint unidentified excitonic states.

[1] L. Linhart et al., Phys. Rev. Lett. **123**, 146401 (2019)

[2] H. Hern

19:00**Vibrational moiré coupling and dielectric effects in one-dimensional hetero-structures**Georgy Gordeev¹¹Department of Physics and Materials Science, University of Luxembourg, Belvaux

Double-walled carbon nanotube is a fascinating system hosting one-dimensional moiré and Coulomb correlated physics. The moiré potential interconnects the electronic states between the inner and outer walls. Such coupling has chiral and radial components, the chiral component is predefined by the DWCNT chirality while radial component by the wall separation distance. During the oscillation of the radial breathing modes the atoms undergo a change in the moiré potential and their frequency shifts. We provide a tight-binding based model linearly relating the RBM frequency shifts with the energy shifts of the electronic transitions. This model is verified experimentally using resonance Raman spectroscopy of RBM modes with a system containing semiconducting inner and outer walls. The optical properties of the inner walls are dictated by the excitonic effects, provided by strong electron-hole correlation. This correlation can be altered by changing dielectric properties of the outer wall. The metallic walls provide substantially higher coupling compared to semiconducting ones and screen the inner walls exciton by reducing it to single particle.

19:30**Electronic excitations of suspended neutral graphene and LO-TO phonon splitting in h-BN monolayer by EELS**Francesco Mauri¹¹Physics, Università di Roma - La Sapienza, Roma

Electron energy loss spectroscopy (EELS) in the transmission electron microscope (TEM) makes finally possible to measure the dispersion of charge excitations of monolayers suspended in vacuum [1]. EELS of freestanding neutral graphene demonstrates the importance of many-body effects (e-e repulsion and excitonic attraction) in the description of the prominent electronic excitations, the onset and of the π -plasmon [2]. EELS of freestanding monolayer h-BN demonstrates the peculiar LO-TO phonon splitting, linear in the phonon momentum, predicted to occur in 2D membranes [3]. In both cases, the absence of the substrate dielectric-screening enhances the visibility of the interaction effects.

I acknowledge support from the MORE-TEM ERC-SYN project, grant agreement No 951215.

[1] R Senga, K Suenaga, P Barone, S Morishita, F Mauri, T Pichler, Nature 573, 247 (2019)

[2] A Guandalini, R Senga, YC Lin, K Suenaga, A Ferretti, D Varsano, A Recchia, P Barone, F Mauri, T Pichler, C Kramberger, arXiv:2302.06367 (2023)

[3] T Sohler, M Gibertini, M Calandra, F Mauri, N Marzari, Nano Letters 17, 3758 (2017)

20:00

Mattermorphosis

Thomas Heine¹

¹Theoretical Chemistry, TU Dresden, Dresden

Subtle changes in the structure of host materials can control the overall properties of the material. In the first part, I will discuss how the edge structure of graphene nanoribbons controls their properties and propose a simple scheme to cover the entire chemical space of cove- and gulf-edged zigzag graphene nanoribbons, predicting their band gap and topological character. In the second part, I will discuss governance of the superlattice emerging from relaxed MoS₂ twisted bilayers on the electronic structure of the top of the valence band, with the focus of very small twist angles. First results on twisted heterobilayers of transition metal dichalcogenides will also be discussed.

08:30 – 09:30	TUTORIAL: S. Haigh, Manchester <i>Discovering Atomic Behaviour with Scanning Transmission Electron Microscopy and 2D Material Heterostructures</i>
09:30 – 10:00	M. Tschudin, Basel <i>Visualizing Magnetic Phase Transitions in 2D van der Waals Materials</i>
10:00 – 10:30	Coffee Break
10:30 – 11:00	S. Ilani, Rehovot <i>The Quantum Twisting Microscope</i>
11:00 – 11:30	L. Tailpied, Châtillon <i>CVD Synthesis of sp^2-Hybridized Multilayer Boron Nitride Films</i>
11:30 – 12:00	G. Cassabois, Montpellier <i>Efficient Light-Matter Interaction in Hexagonal Boron Nitride</i>
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	A. Rubio, Hamburg <i>Novel Non-Equilibrium Phenomena in Two-Dimensional Heterostructures</i>
19:00 – 19:30	D. Voiry, Montpellier <i>Nanochemistry on 2D Materials: Principles and Applications</i>
19:30 – 20:00	K. Nielsch, Dresden <i>Quantum Materials for Thermoelectricity</i>
20:00	Poster Session I

08:30**Discovering Atomic Behaviour with Scanning Transmission Electron Microscopy and 2D material heterostructures**Sarah Jane Haigh¹, Nick Clark¹, Daniel Kelly¹, Yichao Zou¹, Roman Gorbachev¹¹National Graphene Institute, University of Manchester, Manchester, UK

Transmission electron microscopy (TEM) is a powerful technique to image atomic structure and behavior, generating new understanding that drives forward nanomaterials development. This tutorial will cover some of the strengths and weaknesses of the approach. For example, TEM data usually consists of two dimensional images but can be expanded to three dimensions using tomographic data sets [1] or phase retrieval methods [2]. In addition, most TEM is performed with the sample exposed to high vacuum, an environment that is not representative of most chemical and physical processes and can result in artefacts especially when studying dynamic processes. Commercial environmental cell TEM holders overcome this but compromise spatial resolution imaging and chemical analysis. Our 2D material heterostructure stacks provide an alternative route to in-situ imaging that preserves atomic resolution and analytical capabilities and can study the earliest stage of chemical synthesis and adatom motion at the atomic scale [3,4].

[1]Wang et al Nano Lett.(2019), [2]Latychevskaya et al. Proc Natl Acad Sci.(2018), [3]Kelly et al. Advanced Materials (2021), [4]Clark et al. Nature (2022)

09:30**Visualizing Magnetic Phase Transitions in 2D van der Waals Materials**Märta A. Tschudin¹, David A. Broadway¹, Patrick Reiser¹, Carolin Schrader¹, Patrick Maletinsky¹¹University of Basel, Switzerland

The recent discovery of two-dimensional (2D) magnetic materials has sparked wide interest in the scientific community due to their potential for a novel atomic-scale platform hosting exotic spin-textures and exhibiting different magnetic phases. Future advances of these materials and their applications, however, rely on quantitative understanding of their magnetic properties at the nanoscale.

Magnetic imaging using a single spin in diamond has proven to be an excellent tool for probing magnetism in van der Waals (vdW) materials with nanoscale resolution. We employ a scanning technique with single Nitrogen-Vacancy centers embedded in an all-diamond scanning probe to image nanoscale magnetization patterns in a range of 2D materials. In our studies we focus on layered, antiferromagnetic 2D magnets at cryogenic temperatures, where we image spin textures down to the monolayer limit. With our experiments we gain insight into different magnetic phases, domain formation and magnetic anisotropies in these systems. Our results pave the way for future fundamental experiments on low dimensional magnetism including also dynamical phenomena such as spin-wave detection in vdW magnets.

10:30

The Quantum Twisting Microscope

Shahal Ilani¹

¹Weizmann Institute, Rehovot

In this talk I will present a fundamentally new type of scanning probe microscope, the Quantum Twisting Microscope (QTM), capable of performing local quantum interference measurements at a twistable interface between two quantum materials. Its working principle is based on a unique tip, made of an atomically-thin two-dimensional material. This tip allows electrons to coherently tunnel into a sample at many locations at once, with quantum interference between these tunneling events, making it a scanning electronic interferometer. With an extra twist degree of freedom, our microscope becomes a momentum-resolving local probe, providing powerful new ways to study the energy dispersions of interacting electrons. I will present various experiments performed with this microscope, demonstrating quantum interference at room temperature, probing the conductance of in-situ twisting interfaces, and imaging local energy dispersions in a variety of quantum materials.

11:00**CVD synthesis of sp²-hybridized multilayer boron nitride films**

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Due to its unique properties, sp² hybridized boron nitride (BN) has been identified as a key towards integration of 2D materials into devices. Indeed, this capability has been demonstrated using mechanically exfoliated BN from low defective and highly crystalline single crystals. Yet, this process strongly limits the size of the devices. In order to develop devices at a wafer scale, it is therefore critical to master the synthesis of BN layers at low cost, large scale and desired quality.

Our synthesis effort aims at full filling these requirements. In a first step we demonstrated that heteroepitaxial growth of a few nanometer-thick BN film of well-stacked and flat layers could be achieved by CVD on Ni (111) surface of polycrystalline substrate [1]. On this basis we have developed a process on a dedicated Rapid Thermal CVD reactor using borazine as B and N sources and wafer-scale single crystalline Ni(111) pseudo substrates. We will show that thanks to an appropriate preparation of the substrate, continuous layers with a single crystalline orientation can be grown and transferred for being integrated in appropriate devices.

[1] 10.1088/2053-1583/aba8ad.

11:30**Efficient light-matter interaction in hexagonal boron nitride**Guillaume Cassaboïs¹¹Laboratoire Charles Coulomb, CNRS, Montpellier University, 34095 Montpellier, France

Hexagonal boron nitride (hBN) is an ultrawide bandgap semiconductor with a large range of basic applications relying on its low dielectric constant, high thermal conductivity, and chemical inertness. The growth of high-quality crystals in 2004 has revealed that hBN is also a promising material for light-emitting devices in the deep ultraviolet domain [1]. With a honeycomb structure similar to graphene, bulk hBN has gained tremendous attention as an exceptional substrate for graphene with an atomically smooth surface, and more generally, as a fundamental building block of van der Waals heterostructures [2].

I will discuss here our recent measurements characterizing the light-matter interaction in hBN, with record oscillator strengths in 3D bulk hBN [3], and a giant excitonic radiative broadening in 2D monolayer hBN [4]. This work highlights the outstanding light-matter interaction in hBN.

References:

- [1] K. Watanabe et al., *Nature Mater.* **3**, 404 (2004).
- [2] A. K. Geim et al., *Nature* **499**, 419 (2013).
- [3] C. Elias et al., *Phys. Rev. Lett.* **127**, 137401 (2021).
- [4] G. Cassaboïs et al., *Phys. Rev. X* **12**, 011057 (2022).

18:30**Novel non-equilibrium phenomena in two dimensional heterostructures**Angel Rubio¹¹Theory, Max Planck Institute for the Structure and Dynamics, Hamburg

We present our recent studies on the thermodynamical stability, mechanical, electronic, structural and optoelectronic properties of 2D materials. We will discuss new states of matter that are optically induced and have no equilibrium counterparts, and we will identify the fingerprints of these novel states that will be probed with pump-probe spectroscopies. A particular appeal of light dressing is the possibility to engineer symmetry breaking which can lead to novel properties of materials, e.g. coupling to circularly polarized photons leads to local breaking of time-reversal symmetry enabling the control over a large variety of materials properties (e.g. topology). By controlling the Berry curvature in 2D layered materials (metal/insulator transition metal dichalcogenides, or TMD), a new class of quantum Hall states can be induced. In these states, the valley degree of freedom can be tuned with light.

19:00**Nanochemistry on 2D materials: Principles and applications**Damien Voiry¹¹Institut Européen des Membranes (IEM), CNRS, Montpellier

2D materials such as graphene have attracted interest as fascinating materials with an impact on broad areas of chemistry and physics. In particular, their atomic thickness induces strong quantum confinement that gives rise to new and sometimes exotic phenomena not present in the pristine bulk structure. Among the family of 2D materials, transition metal dichalcogenides (TMDs) are intensively studied for optoelectronic and electrocatalytic applications. The properties of TMDs can be widely tuned by changing the elemental composition, thickness and atomic structure. Moreover, TMDs can adopt two different coordinations for the metal atoms: a trigonal prismatic coordination or an octahedral coordination that corresponds to the 2H and 1T phases, respectively. Interestingly, several TMDs are stable in both phases, resulting in radically different electronic behaviors. This led us to develop the concept of phase engineering of TMDs in order to tune the electronic properties and chemical reactivity of nanoplatelets. In this talk, using TMDs as examples, I will present how nanochemistry can be used to tune the properties of exfoliated 2D materials.

19:30**Quantum materials for thermoelectricity**Kornelius Nielsch^{1,2,3}¹Institute for Metallic Materials, Leibniz Inst for Solid State and Materials Research, Dresden²Institute of Materials Science, TUD³Institute of Applied Physics, TUD

Research in thermoelectric (TE) quantum structures was greatly propelled by the prediction in the early 1990s of a significant boost in TE efficiency by quantum size effects. Recently, research interest has shifted from quantum size effects in conventional semiconductors toward new types of quantum materials (e.g., topological insulators [TIs], Weyl and Dirac semimetals) characterized by their nontrivial electronic topology. Bi₂Te₃, Sb₂Te₃, and Bi₂Se₃, established TE materials, are also TIs exhibiting a bulk bandgap and highly conductive and robust gapless surface states. The signature of the nontrivial electronic band structure on the TE transport properties can be best verified in transport experiments using nanowires and thin films. However, even in nanograined bulk, the typical peculiarities in the transport properties of TIs can be seen. The signature of TI surface states on the thermoelectric properties of nanowire model systems will be discussed in depth and how these states can be modified by chemical modifications and in the vicinity of magnetic insulators.

MON 1**Investigation of spatially localized defects in synthetic WS₂ monolayers**

Bárbara L. T. Rosa^{1,2}, Kazunori Fujisawa^{3,4}, Joyce C. C. Santos², Tianyi Zhang^{4,5}, Matheus J. S. Matos⁶, Frederico Sousa², Tiago C. Barbosa⁷, Lucas Lafeta², Sérgio L. L. M. Ramos⁷, Bruno R. Carvalho⁸, Helio Chacham², Bernardo R. A. Neves², Mauricio Terrones^{3,4,9}, Leandro M. Malard²

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⁹Department of Chemistry and Materials Science & Engineering, The Pennsylvania State University, University Park, USA

While the spatially nonhomogeneous light emission from synthetic WS₂ monolayers is frequently reported in the literature, the nature of this phenomenon still requires thoughtful investigation. Here, we combine several characterization techniques (optical imaging, scanning probe and electron microscopy) along with density functional theory to investigate the presence of substitutional doping localized at narrow regions along the S zigzag edge of WS₂ monolayers. We verified that photoluminescence quenching along narrow regions is not related to grain boundaries but to substitutional impurities of lighter metals at the W sites, which modify the radiative and nonradiative decay channels. We also found potential candidates for occupying the W site through ADF-STEM analysis and discussed their impact on photoluminescence quenching by performing density functional theory calculations. Our findings shed light on how atomic defects introduced during WS₂ monolayer's synthesis impact the crystalline quality and, therefore, the development of high-performance optoelectronic devices based on semiconducting 2D materials.

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MON 2**Optical Properties and Resonant Raman Spectroscopy of Ferroic Oxides**

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²Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Belvaux, Luxembourg

Ferroic oxides exhibit a vast range of properties that attract attention for their applicability. We focus here on their optical and electronic properties, and our objective is to understand their electronic transitions via resonant Raman spectroscopy, showing enhanced signal for the modes of interest. The goal is to interpret these Raman spectra for ferroic oxides and relate the Raman resonances to the optical properties of the crystals.

These crystals generally possess low symmetries and anisotropic physical properties. In a first step, we focus on measuring both the real and imaginary parts of the complex refractive index, expecting to observe optically the anisotropic effect. Characterizing fully the optical properties of these materials becomes quite complicated for low symmetry. We tackle this challenge by combining two techniques: spectroscopic ellipsometry and UV-visible spectroscopy. Pros and cons of both techniques will be discussed in view of some examples of anisotropic crystals, like hexagonal ferric oxide (Fe_2O_3) and monoclinic bismuth vanadate (BiVO_4), which band-gaps are in visible range (2.1 and 2.5 eV). Then, we will show some preliminary results for BiVO_4 .

MON 3

Static and Dynamic Disorder in Formamidinium Lead Bromide Single Crystals

Guy Reuveni¹, Yael Diskin-Posner², Christian Gehrman³, Shravan Godse³, Gianis G. Gkikas⁴, Isaac Buchine⁵, Sigalit Aharon¹, Roman Korobko¹, Constantinos C. Stoumpos⁴, David A. Egger³, Omer Yaffe¹

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We show that formamidinium lead bromide is unique among the halide perovskite crystals because its inorganic sub-lattice exhibits intrinsic local static disorder that co-exists with a well-defined average crystal structure. Our study combines THz-range Raman-scattering with single-crystal X-ray diffraction and first-principles calculations to probe the inorganic sub-lattice dynamics evolution with temperature in the range of 10-300 K. Our findings suggest that the static disorder at low temperatures is related to the bulky FA molecule and demonstrate that it augments the dynamic disorder present at higher temperatures in FAPbBr_3 . The temperature evolution of the Raman spectra shows that low-temperature, local static disorder strongly affects the crystal's structural dynamics and phase transitions at higher temperatures. Our results potentially have significant implications for the optoelectronic and thermal-stability properties of FA-based lead-halide perovskites.

MON 4**Architecting New Composite Materials From One Dimensional Van der Waals Heterostructures to Halide Perovskites with Carbon Nanotubes**

Reza Kashtiban¹, Richard Walton², Christopher Patrick³, Quentin Ramasse⁴, Maria Budanova¹, Taiki Inoue⁵, Yongjia Zheng⁵, Rong Xiang⁵, Andrij Vasylenko^{1,6}, David Quigley¹, Shigeo Maruyama⁵, James Lloyd-Hughes¹, Jeremy Sloan¹

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Halide perovskite nano-structures are revolutionising the design of optoelectronic materials. We report four isolated sub-nm, or pico-scale, halide perovskite structures formed inside SWCNTs from CsPbBr₃ and CsSnI₃. Three directly relate to the ABX₃ perovskite archetype while a fourth a perovskite-like lamellar structure with alternating Cs₄ and polyhedral Sn₄I_x layers. In ~1.4 nm SWCNTs, CsPbBr₃ forms Cs₃PbI₂Br₅ nanowires one ABX₃ unit cell in cross section with Pb²⁺ maintained by ordered Cs⁺ vacancies. Within ~1.2 nm SWCNTs, CsPbBr₃ and CsSnI₃ form inorganic polymer-like bilayer structures 1/4 an ABX₃ unit cell in cross-section with ABX₃ stoichiometry. Producing these smallest halide perovskite structures at their absolute synthetic cross-sectional limit enables quantum confinement effects with first-principles calculations demonstrating band gap widening. 1D heterostructures offer tangible benefits. Stacking 1D crystals coaxially enables build of low-power logic devices or direct-current electrical transformers. Coaxially grown 1D CNT/BN/MoS₂ heterostructures and optical properties characterised by electron microscopy, Raman Spectroscopy, optical pump-optical probe spectroscopy.

MON 5**Exciton-Phonon Coupling in MoSe₂/WSe₂ Heterobilayers Probed using Resonant Raman Spectroscopy**

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²Chair of Theoretical Chemistry, Technische Universität Dresden, Germany

³Institut für Physik, Universität Rostock, Germany

Transition Metal Dichalcogenides (TMDs) monolayers can host excitonic states with strong binding energies at room temperature (40 meV to 100 meV [1]) thanks to reduced dielectric screening in monolayer. Upon laying one monolayer on top of another, making a heterostructure, the electronic states of both can hybridise and form a composite structure.

Here we use resonant Raman spectroscopy and density functional theory (DFT) to study exciton-phonon coupling of a $\text{MoSe}_2/\text{WSe}_2$ heterobilayer. Resonant Raman spectroscopy shows an induced resonance in the MoSe_2 layer at the A excitonic resonance of WSe_2 , while showing no induced resonance in the WSe_2 layer at the A excitonic resonance of MoSe_2 . Comparing experiment with DFT we show that this induced resonance is a consequence of exciton-phonon coupling, with the induced resonance in WSe_2 being too small to detect.

These findings highlight how heterobilayers change upon interaction, and how phonons play an important role in the excitonic properties of these composite systems.

[1] Patryk Kusch et al., Phys. Rev. B 103, 235409 (2021)

MON 6

Identifying and mapping stacking faults in rhombohedral graphite by scanning tunneling microscopy and Raman spectroscopy

Konrád Kandrai¹, Mohammad Syahid Mohd Isa¹, Zoltán Tajkov¹, Krisztián Márity¹, Márton Szendrői¹, Levente Tapasztó¹, Péter Nemes-Incze¹

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Few layers of rhombohedral graphite (RG) host flat bands localized to the surface graphene layers. Its low vacancy concentration makes it one of the simplest crystals with a flat band - forming a pristine platform to study correlated electron states. Recent charge transport and STM measurements have revealed that increasing the number of graphene layers in RG increases the strength of correlations. However, this also increases the number of stacking configurations. Such stacking faults and lateral domain walls formed between hexagonal and rhombohedral phases remain the only experimentally relevant crystal defects. Identifying them is critically important for sample preparation and exploring correlations in RG.

Using scanning tunneling microscopy (STM) measurements and density functional theory calculations we show that the number of graphene layers in RG can be identified by their bulk bands. Furthermore, stacking faults in slabs of RG have a unique fingerprint in the local density of states, measurable by STM. Beyond stacking faults, we also identify by Raman spectroscopy lateral domain walls and map their electronic structure by STM.

MON 7

FT-IR spectroscopy of MoTe_2 , PtTe_2 and WTe_2 thin films

Tatiana Vojteková¹, Lenka Pribusová Slušná¹, Jana Hrdá¹, Michaela Sojková¹, Martin Hulman¹

¹ Institute of Electrical Engineering, SaS, Bratislava

Molybdenum ditelluride MoTe_2 , Platinum ditelluride PtTe_2 and Tungsten ditelluride

WTe₂ belong to the transition-metal dichalcogenides (TMDCs). PtTe₂ has been identified to possess unusual band structures and topological properties. WTe₂ is interesting due to the extraordinary magnetoresistance and thermoelectric properties. MoTe₂ can exist in several crystal polymorphs: hexagonal, monoclinic, and orthorhombic. Each of them shows unique electronic properties and, therefore, applications. While the hexagonal phase is semiconducting, the monoclinic phase behaves like a semi-metal. Monoclinic MoTe₂ can undergo a phase transition to the orthorhombic structure breaking the inversion symmetry of the crystal lattice. We study the optical properties of MoTe₂, PtTe₂ and WTe₂ thin film from terahertz to UV-VIS region with Fourier-transform infrared spectroscopy. FT-IR measurements and optical characterization in a wide spectral range are essential for future applications of MoTe₂, PtTe₂ and WTe₂ thin films in electronics, optoelectronics and photonics.

MON 8

Magic-Angle Bilayer Graphene Nanocalorimeters: Toward Broadband, Energy-Resolving Single Photon Detection

Paul Seifert^{1,2}, Xiaobo Lu^{2,8}, Petr Stepanov^{2,10}, José Ramón Durán Retamal^{2,7}, John Nick Moore^{2,9}, Kin Chung Fong^{3,4}, Alessandro Principi⁵, Dmitri K. Efetov^{2,6}

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Because of the ultralow photon energies at mid-infrared and terahertz frequencies, in these bands photodetectors are notoriously underdeveloped, and broadband single photon detectors (SPDs) are nonexistent. Advanced SPDs exploit thermal effects in nanostructured superconductors, and their performance is currently limited to the more energetic near-infrared photons due to their high electronic heat capacity. Here, we demonstrate a superconducting magic-angle bilayer graphene (MAG) device that is theoretically capable of detecting single photons of ultralow energies by utilizing its record-low heat capacity and sharp superconducting transition. We theoretically quantify its calorimetric photoresponse and estimate its detection lim-

its. This device allows the detection of ultrabroad range single photons from the visible to sub-terahertz with a response time around 4 ns and energy resolution better than 1 THz. These attributes position MAG as an exceptional material for long-wavelength single photon sensing, which could revolutionize such disparate fields as quantum information processing and radio astronomy.

MON 9

How to Measure Entropy of Exotic Particles

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In recent years many candidate setups have been proposed to support exotic quasi-particles, such as Majorana fermions (MFs), which may be relevant for quantum computing, but whether these particles have been observed experimentally is currently a topic of vivid debate. Entropy measurements can unambiguously separate these quasi-particles from other, simpler excitations. The entropy of a MF is, for example, $k_B \log 2/2$, a fractional value that cannot be attributed to a localized excitation. However, standard entropy measurements applicable to bulk systems cannot be utilized in measuring the additional entropy of a mesoscopic device, which may be due to less than a single electron in the device. In this talk, I will describe recent theoretical and experimental progress in performing such measurements. Particular examples will be single and double quantum dots in the Coulomb blockade regime. Lastly, I will show how the formalism has been generalized to deduce the entropy from conductance measurements and apply it to a setup where two and three-channel Kondo physics have been observed, yielding the fractional entropy of a single MF and a single Fibonacci anyon.

MON 10

Width-dependent intercalation of graphene nanoribbons in ultra-high-vacuum with carbenes

Dominik Lüthi¹, Lin Yang², Ji Ma², Akimitsu Narita^{3,4}, Xinliang Feng², Klaus Müllen³, Pascal Ruffieux¹, Roman Fasel¹, Gabriela Borin Barin¹

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Atomically precise graphene nanoribbons (GNRs) have been synthesized by polymerization and cyclodehydrogenation of specific precursors on catalyzing metallic substrates in ultra-high vacuum (UHV). By now, on-surface synthesis allowed access to various types of GNRs with armchair and zigzag edges and with different edge extensions to the GNR backbone. GNRs containing zigzag segments have intriguing physical properties such as spin-polarized edges with a long spin lifetime and topological quantum states, making them an interesting platform for spintronic

devices. However, the enhanced chemical reactivity of the zigzag edge states has hindered the transfer and device integration of such GNRs, preventing any investigation on their transport characteristics so far. Here, we studied the intercalation with a self-assembled monolayer of carbenes (BIM) as a promising route towards dry-transfer of GNRs in UHV. Intercalation statistics, via STM analysis, of various GNRs predict increased yield of intercalation with decreasing GNR width. We further study Raman spectroscopy fingerprint modes of different GNRs, which show a clear enhancement of the Raman signal upon intercalation.

MON 11

Graphene-electrolyte charge transfer: Role of defects

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In-situ combination of Raman spectroscopy and electrochemistry localized into a small droplet of an electrolyte is an ideal method for the measurement of charge-transfer processes in 2D materials. Our microdroplet spectroelectrochemistry (μ -SEC) setup allows us to perform these measurements on the basal plane of exfoliated graphene monolayers without the influence of any surface contamination, flake edges and/or monolayer/multilayer interfaces.

Influence of structural defects on the spectroelectrochemical and electrochemical behaviour of monolayer graphene is discussed in this work. Our μ -SEC technique highlights the importance of defects on graphene charge-transfer processes. We observed splitting of the Raman G band of graphene, which was caused by defect formation in crystal structure of graphene and thus differently doped areas with different charge-transfer kinetics. We also show the evaluation of the heterogeneous electron transfer coefficient of a redox reaction between graphene and an electrochemical outer-sphere mediator with two distinct rates for pristine and defective areas.[1]

[1] Jindra et.al., J. Phys. Chem. Lett. 2022, 13, 2, 642–648

MON 12

Single-Walled Carbon Nanotubes Charge Management by Controlled Functionalization

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Managing the density of charges in carbon nanotubes opens new ways to tune their optical response, their transport properties, and their physico-chemical features. Charge transfer from molecules adsorbed onto the sidewall or filled within the

hollow cavity of the nanotubes has already been demonstrated, yet a fine-tunable control of the surface coverage/filling fraction (and thus the amount of transferred charge) remains challenging to achieve. Alternatively, we developed an optically nonperturbing covalent functionalization technique based on the inclusion of a triazine derivative into the carbon network. The nitrogen atom sustaining the attached group becomes an integrated part of the π -conjugated network and contributes with its lone electron pair to uplifting the position of the Fermi level of the tube. Since the density of attached groups can be varied by adapting the synthetic conditions, this technique offers the advantage of controlling the amount of charge injected into the tubes. Here we focus on a novel class of charge-transfer agents that either donate or withdraw electrons depending on the arrangements of their building units and how they affect the tubes features.

MON 13

Optically selective CNT coatings for concentrating solar thermal

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The optical selectivity of the receiver in solar collectors is achieved with coatings that are highly absorbing over the solar spectrum, without disrupting the intrinsically low emittance of the metallic substrate in the infrared region. These selective coatings often comprise multiple layers with highly absorbing ones close to the substrate and protective, antireflective layers at the surface.

It has been shown that thin coatings of carbon nanotubes (CNTs) can be almost perfect absorbers over the solar spectrum, making them interesting for solar collectors with high concentrating factor, where high absorptance is promoted over low emittance. Here we show that through appropriate functionalization of multi-walled CNTs, water-based dispersions devoid of additives can be produced and used for spray coating selective CNT coatings. To ensure mechanical and thermal stability the CNT coatings are then fixated with an antireflective top layer of silica. When applied on a stainless steel substrate, the resulting surface exhibit optical selectivity and an Arrhenius energy suggesting thermal stability over a 25 year lifetime in low-to mid-temperature solar thermal applications.

MON 14

Strain control of valley physics in monolayer WS₂

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Mechanical strain controls the hierarchy of energy bands and their spin/valley texture in transition metal dichalcogenides (TMDs). Here, we apply controlled biaxial strain exceeding 1% in a suspended 1L-WSe₂ at cryogenic temperatures and unveil novel strain responses. First, the conduction bands and the in-gap localized defects hybridize under strain that breaks spin/valley locking and brightens the optically dark states. Second, we observe a near 100% loss of exciton valley coherence under 1% strain and show that defect-assisted hybridization is critical for valley manipulation. At the same time, the associated dark states gain valley polarization by up to 400%. These results suggest strong strain manipulation of exciton valley lifetime. Finally, we show ultrafast strain control of spins and charges in a suspended WSe₂ device. Our observations may play a critical role in the applications of TMDs in strain-valleytronics.

MON 15

Ultra-High Vacuum Assembly of van der Waals Heterostructures

Amy Carl^{1,2}, Wendong Wang^{1,2}, Nick Clark^{2,3}, Matthew Hamer^{1,2}, Alex Summerfield², Hugo de Latour^{2,3}, Sam Sullivan-Allsop^{2,3}, Eli Castanon^{1,2}, Francisco Selles^{1,2}, Astrid Weston^{1,2}, Sarah J. Haigh^{2,3}, Roman Gorbachev^{1,2,4}

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Stacking of layered van der Waals materials into increasingly complex heterostructures has led to new discoveries across solid state physics, materials science and chemistry. Despite this, progress is hindered due to a range of limitations with the fabrication process. The most used transfer methods use polymer carrier layers which are a source of contamination and limit the assembly temperature. Volatile species present in the environment condense onto the samples between the layers adding to the contamination and many crystals that would potentially produce interesting results are highly sensitive and degrade even in inert environments.

This work presents the development of device fabrication in an ultra-high vacuum environment using a polymer free transfer method. Transfers are performed using metal coated, flexible silicon nitride membranes that allow heterostructures to be built quickly, simply and at high temperatures. This technique dramatically decreases the amount of hydrocarbon contamination trapped within the heterostructure so larger, cleaner devices can be produced. Several devices are discussed showing their use in twistronics and electronic transport measurements.

MON 16

Evidence for Dirac flat band superconductivity enabled by quantum geometry

Marc Bockrath¹, Haidong Tian¹, Xueshi Gao¹, Yuxin Zhang¹, Shi Che¹, Tianyi Xu², Patrick Cheung², Kenji Watanabe³, Takashi Taniguchi⁴, Mohit Randeria¹, Fan Zhang², Chun Ning Lau¹

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The group velocity v_F of the electrons in a flat band superconductor is extremely slow, resulting in quenched kinetic energy. Conventional BCS theory implies a vanishing superfluid stiffness, coherence length, and critical current. Using twisted bilayer graphene (tBLG), we explore the profound effect of very small v_F in a superconducting Dirac flat band system. We measure v_F via the Schwinger effect, finding an extremely slow $v_F \sim 1000$ m/s for filling fraction ν between -1/2 and -3/4 of the moiré superlattice. This same velocity yields a new limiting mechanism for the superconducting critical current, with analogies to a relativistic superfluid. We estimate the superfluid stiffness from our data, showing that it is not dominated by the kinetic energy, but by the interaction-driven superconducting gap, consistent with recent theories on quantum geometric contributions. We study the BCS to Bose-Einstein condensation (BEC) crossover, finding an unprecedented ratio of the superconducting transition temperature to the Fermi temperature exceeding unity, illustrating how this can arise for very strong coupling superconductivity in ultra-flat Dirac bands.

MON 17

Growth Optimization of Transition Metal Dichalcogenides and their Heterostructures

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Transition metal dichalcogenides (TMDs) such as WS_2 have attracted increasing attention for new generation semiconductor applications in various fields, particularly in optoelectronics. From the main synthesis methods for two-dimensional materials, chemical vapor deposition (CVD) is the most appealing for reproducible and large-scale materials of high quality. Due to its complex nature, controllability and optimization of CVD growth and its parameters remains challenging.

Through design of experiments (DoE), multivariate analysis of growth conditions and characterisation of the resultant WS_2 , we show enhanced and repeatable growth of TMDs. By adjusting CVD growth parameters, grain size and thickness can be tuned to achieve monocrystalline monolayer flakes up to quasi continuous films.

This gives a platform for further development of novel materials, such as lateral and vertical heterostructures. In particular, we demonstrate the deposition of a noble metal dichalcogenide (NMD) $PtSe_2$, creating a vertical TMD-NMD heterostructure. Modulation of the optical properties shows evidence of charge transfer and opens the possibility for band structure engineering at large scale.

MON 18**Raman spectroscopy of patterned functionalized graphene and twisted bilayer graphene**

Tobias Dierke¹, Daniela Dasler², Tamara Nagel², Frank Hauke², Andreas Hirsch², Janina Maultzsch¹

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We present an experimental study on the degree of covalent functionalization of graphene exfoliated on top of hBN stripes on Si/SiO₂ as well as on other two-dimensional (2D) materials. The underlying substrate has a strong effect on the degree of functionalization of graphene. Our results indicate that the functionalization of graphene is less effective on hBN than on SiO₂, as shown by higher defect-induced modes in the graphene Raman spectra on SiO₂. Other underlying 2D materials like MoS₂, WS₂, and MoO₃ show less contrast in functionalization density than hBN or lead to even higher degree of functionalization than the Si/SiO₂ substrate. Our method of patterning the underlying substrate leads to a spatially defined functionalization of graphene without changing its intrinsic high-quality properties. Furthermore, we show an experimental study of twisted bilayer graphene encapsulated in hBN. We observe significant differences in the Raman spectra of twisted bilayer graphene with varying twist angles. Depending on the laser excitation energy we observe an enhancement of the Raman G peak at specific twist angles ($\Theta \approx 10^\circ, 50^\circ$) near the van Hove singularities.

MON 19**Controllable Synthesis of Borophene Aerogels by Utilizing h-BN layers for High Performance Li-S Batteries**

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Borophene is emerging as a new promising electrode material especially for Lithium sulfur (Li-S) batteries due to its anisotropic Dirac properties, high charge capacity, and low energy barrier for ion diffusion. However, the practical synthesis of active and stable borophene remains very challenging along with producing electrochemical devices. Here, we introduce an original method for borophene aerogels (BoAs) by utilizing hexagonal boron nitride aerogels. In this method, borophene grows between h-BN layers utilizing boron-boron bridges, as a nucleation site, where borophene forms monolayers mixed with sp²-sp³ hybridization. The process is highly generic for producing very stable borophene aerogels and is suitable for large-scale material processing. With these BoAs, we successfully fabricate high performance lithium sulfide (Li-S) batteries with superior capacity and fast charging capability up to 1521 mAh g⁻¹ (at 0.3C, >1000 cycles) and 901 mAh g⁻¹ (at 10C, 609 cycles).

MON 20**Biosensing of Membrane Proteins utilizing Solution Gated Graphene Field Effect Transistors**

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Membrane proteins play a crucial role in numerous fundamental biological processes. The protein's dynamics that govern the protein function are not yet understood due to the lack of methods that provide spatial and temporal resolution. Here, we present the first steps on how solution-gated graphene field effect transistors (SGFETs) can be used to tackle this question. We demonstrate reversible protein immobilization on SGFETs covered with a lipid monolayer employing tris-NTA complexes to capture histidine-tagged proteins [1]. The proteins are released again upon the addition of imidazole. Furthermore, we use SGFETs to monitor the electrochemical potential during the immobilization of HOPS membrane tethering complexes on a lipid monolayer. Noise measurements reveal the influence of the different functionalization steps on the transport properties of the device. The governing dynamics of HOPS are known from recent graphene-induced energy transfer measurements on dye-labeled complexes [2]. We discuss how our method can be employed to reveal the dynamics of label-free proteins.

[1] Jorde et al, JAP 129, 094302 (2021)

[2] Füllbrunn et al., eLife 10, e62501 (2021).

MON 21**Graphene Based Two-Dimensional Material**

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Two-dimensional materials are the subject of many investigations because of their properties. Their bottom-up synthesis is mainly achieved by the epitaxial growth from a molecular source in the gas phase. Growth of one-dimensional materials based on graphene crystal structure has been described in many papers, where different graphene nano-ribbons were grown and characterized and studied made of halogenated precursor molecules on smooth surfaces of copper single crystals or thin gold on mica substrates. Growth of graphene-based sub structure by using this approach to produce large-area layers for normal conditions (atmospheric pressure) studies is a goal that could yield in the interesting material like antidote

super-lattices. The material synthesized based on this route, and characterized by Raman and atomic scanning microscopy is shown.

MON 22

Cobalt-Iron Bi-metallic catalyst for chirality-specific growth of single wall carbon nanotube

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Based on theoretical simulations, iron (Fe) and cobalt (Co) can form a very stable cluster even at temperature as high as 2000K. Therefore, we speculate that the cluster would be a good candidate for single walled carbon nanotube (SWCNT) growth since Fe and Co are effective catalysts for SWCNT production. In this work, we mixed different mass ratio of Fe and Co with zeolite, and conducted alcohol catalytic chemical vapor deposition (ACCV) at different temperatures and pressures to investigate the contribution of Fe or Co for the overall yield of SWCNT. The as-grown SWCNT as well as the dispersed SWCNT solutions are well characterized by Raman, scanning electron microscopy (SEM), absorption, photoluminescence, and transmission electron microscopy (TEM). Our results show that at the lower temperature, such as 650°C, pure Co produces the most of SWCNTs while pure Fe the least. However, at the higher temperature, such as 800°C, pure Co is less effective and the bimetallic Co-Fe can produce more SWCNTs.

MON 23

Microwave optomechanics of the transversal carbon nanotube vibration

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Recently we have demonstrated optomechanical coupling of a carbon nanotube and a coplanar microwave resonator at millikelvin temperatures [1,2]. In the measured device, the nanotube acts both as a mechanical resonator and as a quantum dot. The nonlinear electronic response of Coulomb blockade enhances the microwave optomechanical coupling by several orders of magnitude. This novel optomechanical system presents several interesting features for optimized parameters, e.g., strong optomechanical coupling (with hybridization of vibrons and photons) and the quantum coherent limit (where manipulation is faster than thermal decoherence) is within reach.

Since the publication of [1], we have achieved significant improvements of our microwave resonators integrating the nanotube transfer areas and electrodes. Ongoing work aims at optimizing the carbon nanotube growth and the transfer of the nanotubes onto the resonator chip, as well as the cryogenic millikelvin setup for the

measurements. We present the current state of our measurements, towards quantum control of the carbon nanotube vibration.

[1] S. Blien et al., Nat. Comm. 11, 1636 (2020).

[2] N. Hüttner et al., in preparation.

MON 24

From transparent conduction to Coulomb blockade at fixed, known charge

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Transport spectroscopy of a clean single-wall carbon nanotube device in high magnetic fields is presented [1,2]. We analyze the region of few holes adjacent to the semiconducting band gap. At zero axial magnetic field, the device displays with increasingly negative gate voltage a fast transition toward high contact transparency and eventually Fabry–Pérot interference of conductance. Already the first conductance oscillation may represent a Kondo ridge.

When increasing an axial magnetic field component up to $B_{||} = 17$ T, the contact transparency and the overall conductance are reduced all the way to Coulomb blockade, clearly displaying the subsequent charging with the first ten holes. The continuous transition between the transport regimes is dominated by a rich spectrum of Kondo-like resonances, with distinct features in the stability diagrams.

[1] D. R. Schmid *et al.*, pss(b) **257**, 2000253 (2020)

[2] D. R. Schmid *et al.*, doi:10.5281/zenodo.4037354, Zenodo (2020)

MON 25

Band topology of layered transition metal dichalcogenides

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Layered transition metal dichalcogenides (TMDs) exist in many forms. Such a manifold of configurations manifests itself in diverseness of electronic properties making them extremely interesting as potential key-elements of sophisticated functional devices. Here we analyze electronic-band topology of a broad spectrum of layered TMD structures using symmetry indicators approach and theory of topological quantum chemistry, establishing symmetry relations between localized and extended electronic states in 2D crystals. The latter is based on the elementary band representations for double grey layer groups [1], which enables full-symmetry-based study of the electronic-band topology of layered crystals with spin degree of freedom, time reversal symmetry and spin-orbit interaction. In order to verify presence

of the extended electronic states in semiconducting compounds, we also calculate Wilson loop operator eigenspectra for particular sets of bands.

[1] I. Milosevic, Z. P. Popovic, B. Nikolic, M. Damjanovic, *Electronic Band Topology of Monoclinic MoS₂ Monolayer: Study Based on Elementary Band Representations for Layer Groups*, Phys. Status Solidi RRL 2020, **14**, 2000351.

MON 26

Radiative suppression of exciton-exciton annihilation in 2D semiconductors

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Atomically thin semiconductors possess strongly bounded excitons, opening novel opportunities for engineering light-matter interaction at the nanoscale. However, their in-plane confinement leads to strong non-radiative exciton-exciton annihilation (EEA) processes, even at relatively low exciton densities, setting a fundamental limit for their applications. Here, we demonstrate EEA suppression via enhancement of light-matter interaction in hybrid 2D-dielectric nanophotonic platforms. We couple excitons in a WS₂ monolayer with optical Mie resonances in dielectric nanoantennas. We observe intermediate light-matter coupling regime, as well as photoluminescence enhancement factors up to 10². Probing the ultrafast dynamic via pump-probe spectroscopy, reveals suppressed EEA processes for coupled excitons even under a high exciton density > 10¹³ cm⁻². We extract EEA coefficients of 10⁻³, compared to 10⁻² for uncoupled monolayers, as well as absorption enhancement of 5.5 and Purcell factor of 4.5. Our results highlight the advantages offered by all-dielectric nanophotonics, opening new routes to low-power integrated photonic devices based on 2D semiconductors.

MON 27

Conductive AFM characterisation of twist angle variation in van der Waals heterostructures assembled in UHV

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The fertile field of twistronics relies on the ability to create pristine heterostructures to obtain a homogeneous twist angle across the stack. Despite the successes, all

current 2D material (2DM) transfer techniques rely on the use of polymers which limits the cleanliness, ultimate electronic performance, and the potential for applications of the heterostructures.

The silicon nitride membrane method is a novel polymer-free fabrication platform for rapid and facile heterostructure assembly. Here, we demonstrate the cleanliness and the uniformity of the fabricated stacks, by using conductive AFM to reveal the moiré pattern induced by a twisted bilayer graphene. Via an image processing code, we extracted the twist angle of moiré superlattices, and calculated the twist angle variation over a large distance. We were then able to observe an order of magnitude improvement in the twist angle variation of the stacks fabricated in UHV.

MON 28

Correlation nanoscopy for characterization of functional nanostructures

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For the continuous advance in synthesis and fabrication capabilities of nanoscale material systems new technologies adapted to these length-scales are required. A novel technology suitable for nanoscale materials systems is the s-SNOM (scattering-type Scanning Near-field Optical Microscopy). s-SNOM delivers material-characteristic maps of electronic and optical properties of sample surface at the spatial resolution of an atomic force microscope (AFM). s-SNOM technology excels in characterization of two-dimensional (2D) materials and semiconductor nanostructures, novel energy materials or plasmonic and photonic nanostructures.

This poster highlights some correlation nanoscopy to characterize novel material and functional nanostructures like: 2D materials, novel energy materials and light controlling materials using the neaSCOPE. neaSCOPE is product which excels in both organic and inorganic materials analysis providing the broadest range of demonstrated applications and novel near-field methodologies such as quantitative s-SNOM or sub-surface measurements.

MON 29

Modelling electronic and optical properties of graphene and boron-nitride nanoribbons

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Graphene (Gr) and hexagonal boron nitride (hBN) have similar lattice parameters ($\approx 1.5\%$ mismatch) but different properties. While Gr is a metal known by its high conductivity, hBN is a large gap insulator (≈ 6 eV) and a strong UV emitter. Moreover growth chambers can be equipped to grow the two materials conjunctly. Due to these characteristics, they are perfect candidates to be grown side-by-side in a lateral heterostructures instead of stacked one of the top of the other as in a more

common vertical heterostructures.

The properties of a lateral heterostructure are sensitive to interface shape and domain size. For instance a heterostructure composed of Gr and hBN ribbons alternatively with armchair interface (AGBN-LHS) have a direct gap tunable with the size of Gr and hBN parts. We present a theoretical study of AGBN-LHS electronic structure as a function of Gr and hBN width carried out with ab-initio methods and a tight-binding model.

MON 30

Photons as material building blocks

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We describe materials as being made of electrons and atomic nuclei. The Coulomb interaction between these building blocks produces a rich landscape of electronic and vibrational states creating the vast diversity of materials in our world. Photons, in contrast, are seen as (external) perturbations that may be used to probe and manipulate excited states. We challenge this understanding of matter by showing that photons can be as much a part of materials as electrons and atomic nuclei. Using a semi-empirical model Hamiltonian we examine various material classes (semiconductors, metals, ferroelectrics, organic crystals) and demonstrate that their ground state properties are determined by the contribution of photons. Examples include the stable phase of crystals, their mechanical response, and quasiparticle spectra. Considering photons as materials building blocks opens enticing horizons for engineering materials to reach macroscopically polarized phases, realize complex photon-coupled excited states and photon-induced mechanical response.

MON 31

Revealing the composition and structure of the universal molecular contamination layer on the surface of van der Waals materials

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We identified the molecular building blocks of the contamination layer on the surface of van der Waals (vdW) materials exposed to ambient air. The airborne molecules appear as parallel stripes on distinct vdW material surfaces (graphite, hBN, MoS₂). We revealed by STM measurements (9K) that the airborne monolayer self-organizes

into a rectangular centered monolayer consisting of alkyl-backboned, linear molecules of 20-26 carbon atoms on graphite. Additional XPS and IR spectroscopy measurements allow us to conclude that the molecular layer consists of normal alkanes. We show a direct causal link between the self-organized stripe structure of the airborne alkane monolayer and the often observed, yet unexplained friction anisotropy domains observed on vdW materials. Furthermore, we show details of the growth dynamics, manipulation of the layer by AFM and the controlled desorption through annealing. Understanding the structure and composition of the universal contaminant layer, is important for both basic science and applications of vdW materials, because the alkane layer dominates their interaction with the environment.

Nat. Commun. 13, 6770 (2022).

MON 32

Manipulation of spin-states in all-organic di-radicals molecular junctions

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We report on manipulation of spin-spin interactions for PAH di-radical molecules [1] in a mechanically controlled break junction and in a 3-terminal device (electromigration break junction EMBJ) at low temperature. Magnetic fingerprints of the molecules manifest themselves by zero-bias peaks in the differential conductance spectra attributed to a Kondo resonance arising from hybridization of one of the radical electrons with the metallic electrodes and spin-flip inelastic electron tunnelling spectroscopy (IETS) steps originating from the singlet-triplet gap of the free electrons [2]. Varying the distance between the electrodes in the MCBJ affects the coupling strength and varying the gate voltage in the EMBJ affects the energy level alignment with the Fermi level of the electrodes. Thus, by mechanical manipulation and electrostatic gating the spin signature of the molecule can be adjusted and controlled. This study provides new insight on the interplay between magnetic fingerprints of all-organic molecules embedded in solid-state devices.

[1] Baum, T. Y., Fernández, S., Peña, D., van der Zant, H. S. J, Nano Lett. 22, 20, 8086–8092.

[2] Ternes, M., New J. Phys. 17

MON 33

Individualization of bulk synthesized Graphene Nanoribbons by Chemical Exfoliation

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We report a facile, low-cost, and scalable intercalation/exfoliation method to individualize graphene nanoribbons (GNRs) with hundreds of microns' in length. In-situ intercalation of alkali metals by vapor transfer was conducted in a glass ampoule under high vacuum. Sodium and potassium intercalation compounds with GNRs were formed (GNRIC). The GNRIC was exposed to THF solvent inducing a chemical exfoliation reaction. The exfoliated material showed a large yield of individualized GNRs depending on the dispersion environments employed. The sample was comprehensively characterized by SEM, Raman spectroscopy, optical microscopy, and AFM techniques highlighting the existence of extra-large ($>100\ \mu\text{m}$) ribbon-like pyramidal structures. This superior morphology evinced from individualized single GNRs is unprecedented, in addition to their ease of production. The obtained GNR were deposited on a SiO_2 substrate revealing unique morphological characteristics and length. This novel GNR can serve for potential optoelectronic devices, in addition to the as-expected theoretically plasmon resonances that exist in micrometer GNRs as the ones we have synthesized here.

MON 34

Observation and mapping of strongly correlated electronic ground state in the surface flat band of rhombohedral graphite

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In crystalline solids the interactions of charge and spin can result in a rich variety of emergent quantum ground states. Correlation effects are enhanced in partially filled topological flat bands, such as in Landau levels or 'magic angle' bilayer graphene. Rhombohedral graphite (RG) is perhaps the simplest and structurally most perfect condensed matter system to host a flat band protected by symmetry, with enhanced many-body effects in thicker samples. We use scanning tunneling microscopy to measure the flat surface band of 8, 10, 14 and 17 layers of RG and find correlated behavior up to a temperature of 20 K. At charge neutrality we identify a degenerate

ground state, forming a competing domain structure between a sublattice antiferromagnetic insulator and a gapless, correlated paramagnet. Density-matrix renormalization group calculations explain this observation by revealing a degenerate ground state of the system and demonstrate the important role of correlation effects. Our work establishes RG as a platform to study many-body interactions beyond the mean-field approach, where quantum fluctuations and entanglement dominate.

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MON 35

Towards novel electronic states in graphene by non-covalent functionalization

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The electron system of graphene has been considered as prototype representative of 2D Weyl-like fermionic systems. This one has been predicted to host a multitude of exotic, non-trivial quantum states depending on the interaction type and strength between the fermions. To evoke such quantum states we use non-covalently bound molecules, such as TCNQ, for functionalization in order to tune the effective Coulomb interaction within the fermionic system. We studied our samples using micro-Raman spectroscopy as well as electrical transport measurements at room temperature, low-temperature and with applied magnetic field. Our experiments reveal signatures of novel quantum states, comprising first indications of a topological Anderson insulator state as well as the formation of magneto-induced charge density waves.

MON 36

Tuning heat transport in graphene by tension

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Heat transport by acoustic phonons in 2D materials is fundamentally different from that in 3D crystals because the out-of-plane phonons propagate in a unique way that strongly depends on tension and bending rigidity. Here, we induce tension in freestanding graphene membranes by electrostatic force and use optomechanical techniques to demonstrate that it decreases the transport time of heat by as much as 33% for an induced tension of 0.07 N/m. Using phonon scattering and Debye models, we show that these observations can be accounted for by the tension-enhanced acoustic impedance match of flexural phonons at the boundary of the graphene membrane. Thus, we experimentally elucidate the tunability of phononic

heat transport in 2D materials by tension, and open a route towards electronic devices and circuits for high-speed control of temperature at the nanoscale.

MON 37

Blinking and localization of photoluminescence hotspots in monolayer MoS₂

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We investigate the location and origin of optically active sites in monolayer MoS₂ using single-molecule localization microscopy (SMLM). This technique overcomes the diffraction limit of light and enables to localize light-emitting species with a 10 nm precision. The MoS₂ is exfoliated on gold, where the intrinsic photoluminescence (PL) of MoS₂ is quenched, while the PL from defects, bubbles and wrinkles is visible. We found that upon immersion in water, strong blinking PL originating from the optically active sites appears. The blinking is mostly localized on the edges and wrinkles of MoS₂. No such blinking is observed in dry conditions or upon immersion in ethanol or other organic solvents. It appears that hydration plays a crucial role in the activation of PL hotspots. Along with SMLM we use Raman spectroscopy and atomic force microscopy to investigate and discuss the origin of the PL. We show the potential of SMLM to quickly localize optically active sites in MoS₂ with a 10 nm precision and study their photophysical properties.

MON 38

2D-Patterning of Functional Building Blocks on Graphene

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We present two methods for structuring different building units on graphene which realized the 2D-patterning of functional groups (-CF₃, -OH) and distinct building blocks (Hamilton receptors) on graphene, respectively.

MON 39

Collective States in Organic 2D-Materials

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Organic monolayer (ML) crystals have emerged as a new material to replace conventional semiconductors. Mostly these 2D materials are grown out of dye molecules

leading to outstanding optical properties due to a strong coupling of the molecular dipole moments, forming a collective state. The photonic excitation of the collective state results in a narrow and strong emission also known as superradiance (SR). To study this collective state in dependency of the dielectric environment, MLs of MePTCDI were grown on two materials with different electronic properties, providing a perfect platform to study the fundamental mechanism of the SR. High resolution AFM was used to determine the packing density of the molecules in a ML. It showed that the ML is a highly orientated structure and contains only one molecule per unit cell, indicating a dense packing. Different optical methods were used to characterize the collective state. The characteristic SR was measured by fluorescence microscopy and spectroscopy. Additionally, the vanishing Stokes shift between absorption and emission could be measured by absorption spectroscopy, indicating the presence of a collective dipole state, too.

MON 40

Interlayer excitons in semiconductor bilayers under strong perpendicular field

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We consider structures in which bilayer TMDs are sandwiched between a layer of doping molecules and Si gate. We show that these structures allow increasing, by a factor of 2, maximum electric field achievable in this 2D material. This in turn, allows reaching electric field of > 0.25 V/nm (displacement field 2 V/nm). In MoS₂ we show avoided crossing behavior between interlayer and B excitons, and demonstrate previously unresolvable splitting of A exciton that arises from coupling to the second, higher energy interlayer. Next we present the Stark splitting in MoSe₂, that has similar spin texture. We demonstrate tunability of > 220 meV of hybrid state in electric field, and study interaction of normal and spin-dark interlayer excitons tuned in resonance with in-plane excitons.

MON 41

Fabrication and characterization of lithium-doped few-layer MoS₂ films

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Few-layer MoS₂ films have huge potential in various applications, such as optoelectronic devices, energy storage and conversion, and electrode material for Li or Na batteries. However, achieving theoretically predicted properties is still challenging. Doping is a conventional method for changing the electronic properties of materials. We prepared Li-doped MoS₂ by the two-stepped method. Firstly, we prepared few-layer MoS₂ films, and subsequently annealed them in the mixture of sulfur and lithium sulfide powders. The substrates and powders were placed in the middle of the one-zone furnace together with the powders and annealed at the same temperature. Initial MoS₂ layers were prepared by two different methods – pulsed laser deposition (PLD) and sulfurization of pre-deposited Mo layers. The presence of lithium in the samples was confirmed by synchrotron-radiation X-Ray Photoelectron Spectroscopy (XPS). We compared the structural and electrical properties of both types of MoS₂ layers before and after doping.

MON 42

Magnetic field driven quantum phases in magic-angle twisted bilayer graphene

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Flat bands in magic angle twisted bilayer graphene (MATBG) have recently emerged as a rich platform to explore strong correlations, superconductivity and magnetism. However, the phases of MATBG in a magnetic field remain relatively uncharted. We report a rich sequence of wedge-like regions of quantized Hall conductance with Chern numbers $C = \pm 1, \pm 2, \pm 3$ and ± 4 , which nucleate from integer fillings of the moiré unit cell $\nu = \pm 3, \pm 2, \pm 1$ and 0, respectively. The exact sequence and correspondence of the Chern numbers and filling factors suggest that these states are directly driven by electronic interactions, which specifically break the time-reversal symmetry in the system. The analysis of Landau-level crossings from higher energy bands enables a parameter-free comparison to a newly derived magic series of level crossings in a magnetic field and provides constraints on the parameters of the Bistritzer–MacDonald MATBG Hamiltonian. Additionally, we observed the re-entrance of insulating states at $\nu = +2, \pm 3$ of the moiré unit cell of MATBG upon applying an external magnetic field close to the full flux quantum $\phi/\phi_0 = 1$ of the superlattice unit cell ($B = 25\theta^2$ T).

MON 43

Ultrafast Photoluminescence of an Electron-Hole Plasma in Semiconducting 2D Materials at Room-Temperature

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The two-dimensional (2D) transition metal dichalcogenide (TMD) materials have recently shown to be an ideal platform to investigate the excitonic Mott transition into electron-hole plasma (EHP) and liquid phases. However, the reported observations of these electronic phases were at specific conditions that involved suspended samples or low temperatures. Here, we show that pulsed laser excitation at high pump fluences can induce this exciton dissociation into an EHP in as-exfoliated mono and fewlayer TMDs (WSe_2 and MoSe_2) at room temperature leading to a broadband light emission. Our theoretical calculations revealed that the EHP photoluminescence at high energies displays an exponential decay that directly reflects the electronic temperature. Moreover, we have studied the dynamics of the electronic cooling by two-pulse correlation measurements and we revealed an ultrafast response of less than 100 fs and a slower one of few ps associated with the electron-phonon and phonon-lattice thermalizations, respectively. Our work may shed light on further studies of exciton Mott transition in other 2D materials and their heterostructures and its applications light emitting devices.

MON 44

Control over nanosheet network formation using Langmuir-type deposition techniques

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In recent years, significant progress has been made in liquid exfoliation of layered crystals into inks of nanosheets with defined size and thickness distributions and low defect density. However, when employing the nanomaterial into device architectures, their performance is often limited by the orientation of the sheets in the network. While established deposition techniques, such as spray coating or inkjet printing typically yield in porous networks of randomly oriented nanosheets, Langmuir-type deposition techniques allow a better control over the network morphology. In our approach, the nanomaterial ink is injected to a liquid/liquid interface, which in turn leads to the formation of a monolayered network of nanosheets, which can be transferred onto arbitrary substrates by draining of the liquid. In this contribution, we demonstrate the formation of tiled nanosheet networks for different nanomaterials and the fabrication of patterned multilayers and heterojunctions for gas sensing and transistor applications.

MON 45**Optoelectronic characterization of 2D heterostructures. Gr/MoS₂ and Gr/WS₂**

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Graphene (Gr) based 2D heterostructures as Gr/MoS₂ and Gr/WS₂ are obtained, deposited on quartz, and characterized by electrical conductivity at high frequency, Raman, FT-IR and UV spectroscopies. Raman spectroscopy is used to analyze the quality of the samples before and after the measurements. Terahertz time domain spectroscopy (THz-TDS) in transmission mode is used as a non-destructive technique to obtain the surface conductivity and the transmittance in the range [0.2 , 1.6] THz. The transmittance obtained for both samples is similar, whereas the surface conductivity of Gr/WS₂ is higher than the one of Gr/MoS₂ and both are higher than that obtained for individual homogeneous materials. FT-IR and UV-Vis spectroscopies are used to obtain optical transmittance and to evaluate the behavior of each layer in the ranges [90 , 180] THz and [300 , 1200] THz, respectively. In the IR range, the transmittance of the heterostructures is high and similar to that of the individual materials, as in the visible range the transmittance is totally dominated by the WS₂ or MoS₂ layers. These characteristics make these heterostructures good candidates for the fabrication of optoelectronic devices.

MON 46**Moire engineering of correlated topological systems**

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Twisted two-dimensional materials are one of the popular research topics in the field of 2D materials and condensed matter physics. Twisted stacking allows one to turn 2D materials into strongly correlated systems, providing unpretending opportunity to investigate strongly correlated physics in a relatively simple but highly tunable setup. While early research started from twisted graphene systems, using large-scale Density Functional Theory calculations, we extend the study to various other 2D materials, such as twisted BN MoS₂, GeSe, etc [1-3]. Basing on the electronic

structures and atomic symmetry of 2D materials, we can not only design twisted moiré systems to realize various strongly correlated lattice models, but also be able to engineer correlated systems with non-trivial topology [4-5]. We believe these highly tunable 2D moiré systems will provide novel platforms for the simulation of correlated quantum state of matters [6].

- [1] Nano Lett. 19, 4934 (2019)
- [2] Nat. Commun. 11, 1124 (2020)
- [3] Nat. Commun. 12, 5644 (2021)
- [4] Nat. Commun. 13, 4915 (2022)
- [5] arXiv:2207.02806 (2022)
- [6] Nat. Phys. 17(2), 155 (2021)

MON 47

Surface-Sensitive Raman Scattering by Transferable Nanoporous Plasmonic Membranes

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Raman spectroscopy is a powerful technique to characterize materials since it reveals their chemical composition, crystallinity, defects, and strain. However, the Raman response of surfaces is often weak and obscured by dominant bulk signals. Here we overcome this limitation by placing a transferable porous gold membrane (PAuM) on top of the surface of interest. Slit-like nanopores in the membrane act as plasmonic antennas and enhance the Raman response of the surface underneath. Simultaneously, the PAuM suppresses the bulk Raman signal. Using graphene as a model surface, we show that these two effects increase the surface-to-bulk Raman signal ratio by up to 3 orders of magnitude. We find that 90% of the Raman enhancement occurs within the top 2.5 of the material, demonstrating truly surface-sensitive Raman scattering. To show that our approach is useful, we analyze the surface of a LaNiO₃-thin-film, and find a Raman mode splitting for the LaNiO₃-surface layer which indicates that the surface structure differs from bulk. This shows that PAuM give direct access to Raman signatures of surfaces and their structural properties.

R. Wyss et al. submitted (2023)

MON 48**Transition Metal Dichalcogenide 2D crystals grown using Salt Assisted CVT method and investigated for their properties.**

Kevon Kadiwala¹, Andrejs Ogurcovs¹, Edgars Butanovs¹, Boris Polyakov¹

¹Institute of Solid State Physics, University of Latvia, Riga, Latvia

van der-Waals TMDs materials, such as WSe₂ and WS₂ have some unique and intriguing properties when reduced to a few layers such as layer dependent band gap, strong spin-orbit splitting, large exciton binding energy, strong photoluminescence etc. which provides us a distinctive platform to explore fundamental condensed matter phenomena as well as use them in various applications including transistors, diodes, photodetectors and so on. In this work, WS₂ and WSe₂ materials are synthesized using salt assisted CVT and are investigated for their material composition, thickness, electrical properties and photoresponse. Characterization of the materials involves micro-Raman, photoluminescence, AFM, SEM and EDX. Furthermore, these crystals are tested for p-n junction with nanowires to form a 1D-2D hetero-junction and their results are presented.

MON 49**Electrochromic device using SSAIL technology and polymeric electrochromic substance**

Evaldas Kvietkauskas¹, Karolis Ratautas¹, Šarūnas Mickus¹, Gediminas Račiukaitis¹

¹Center for Physical Sciences and Technology, Vilnius

Today smart glasses are dependant on ITO(Indium-tin oxide) but it has many disadvantages. For instance, equipment required to deposit ITO on glass needs vacuum, there is limited indium quantity and cannot be deposited on flexible films due to its fragileness and brittleness. To solve these problems, SSAIL offers selective electroless copper deposition on dielectrics. SSAIL can be applied to ceramics(like glass) and polymers(like PET). With this process, lines with diameter less than 20 nm can be made and electroless copper deposition applied which can replace standard need for ITO. Polymeric electrochromic substances can be easily synthesised in large quantities and later be applied to the made material with deposited copper lines creating electrochromic device. Used polymer in this device was acrylamide and bisacrylamide copolymer. By changing initial concentration of these monomers, the result of the polymer phase of matter can vary from liquid to gel to solid.

HÜBNER Photonics
Coherence Matters.



08:30 – 09:00	T. Weitz, Göttingen <i>Quantum Phases in Natural Bilayer Graphene Accessed by Control of Bandstructure and Screening</i>
09:00 – 09:30	A. Knothe, Regensburg <i>Microscopic Modelling of Electrostatically Induced Quantum Nanostructures in Gapped Bilayer Graphene</i>
09:30 – 10:00	J. Mangeney, Paris <i>Large Graphene Quantum Dots for THz Technology</i>
10:00 – 10:30	Coffee Break
10:30 – 11:00	R. Krupke, Karlsruhe <i>Electroluminescence from Single-Walled Carbon Nanotubes with Quantum Defects</i>
11:00 – 11:30	S. Maruyama, Tokyo <i>Optical Properties of One-Dimensional vdW Heterostructures Based on Single-Walled Carbon Nanotubes</i>
11:30 – 12:00	H. Cheng, Shenzhen <i>Inorganic Liquid Crystals Based on 2D Materials</i>
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	X. Ma, Argonne National <i>Exploring Electronic Spins in Chemically Modified Carbon Nanotubes</i>
19:00 – 19:30	V. Skakalova, Bratislava <i>Simple Chemical Approach to Two-Dimensional Metal Iodides/Graphene Heterostructures</i>
19:30 – 20:00	A. Boghossian, Lausanne <i>A NanoBioengineering Frontier for Next-Generation Optical Devices</i>
20:00	Poster Session II

08:30**Quantum phases in natural bilayer graphene accessed by control of band-structure and screening**Thomas Weitz¹¹Physical Institute, Georg-August-University of Göttingen, Göttingen, Germany

The exchange interaction can lead to correlated states in low dimensional systems such as the graphene family. Regions of large density of states are especially prone to correlation effects, an example that will be discussed is the recently identified exchange driven quantum anomalous Hall (QAH) $\nu=2$ state that exhibits quantized charge Hall conductance close to zero magnetic field as well as spin, valley and spin-valley anomalous quantum Hall effects and out-of-plane ferroelectricity in suspended bilayer graphene [1]. In the case that bilayers are encapsulated in h-BN, a large displacement field can be applied allowing the opening of a gap in the density of states with a concomitant van-Hove-singularity close to the band edges. We will discuss our recent measurements [2] in such device structures that indicate that close to the band edges novel states appear that are distinct from Stoner [3,4] and other single particle physics. For example, one identified state is consistent with a Chern insulating state at finite density in the valence band.

[1] Nature 598, 53 (2021)

[2] Nature 608, (2022) 298

[3] Science 375 (2022)77

[4] Nature Physics 18, (2022) 771

09:00**Microscopic modelling of electrostatically induced quantum nanostructures in gapped bilayer graphene**Angelika Knothe¹¹Institut für Theoretische Physik, Universität Regensburg, Regensburg

Quantum nanostructures, e.g., quantum wires and quantum dots, are needed for applications in quantum information processing devices, such as transistors or qubits. In gapped bilayer graphene, one can confine charge carriers purely electrostatically, inducing smooth confinement potentials and thereby limiting edge-induced perturbances while allowing gate-defined control of the confined structure. In this research lecture, I will give a pedagogical overview of our contributions toward the theoretical modelling of gate-defined nanostructures in bilayer graphene. I will discuss how accounting for microscopic features of the material characteristics and the confinement is crucial for a detailed understanding of bilayer graphene quantum wires, dots, and all-electronic gate-defined cavities.

09:30**Large graphene quantum dots for THz technology**Juliette Mangeney¹¹Paris, France

Graphene quantum dots (GQDs) are very attractive for quantum optoelectronic devices owing to their high flexibility in electronic states engineering through their size, shape, and edges. Room-temperature single optical photon emission in the visible range has been recently demonstrated from GQDs of a few nanometers in diameter. In the THz domain, the demonstration of sensitive detection of THz waves in large GQDs has recently been reported based on classical effects such as bolometric effects and photogating effects. Probing the quantum response of GQDs to THz light is crucial to pave the way for the development of new THz quantum devices. Here, we present results of transport measurements under coherent THz illumination for a single GQD in the Coulomb blockade regime at low temperature, demonstrating a large interaction between a single GQD and a THz electric field in the quantum regime. In particular, we determine a value of the THz electric dipole as long as $d \approx 230$ nm, which is very promising for the ultrastrong THz light-matter coupling physics at the single-electron level. We will also provide a description of the optical properties of large GQDs at THz frequencies.

10:30**Electroluminescence from single-walled carbon nanotubes with quantum defects**Ralph Krupke^{1,2,3}¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany²Institute of Quantum Materials and Technologies, Karlsruhe Institute of Technology, Germany³Institute of Materials Science, Technical University of Darmstadt, Germany

Individual single-walled carbon nanotubes with covalent sidewall defects have emerged as a new class of photon sources whose photoluminescence spectra can be tailored by the carbon nanotube chirality and the attached functional group/molecule. I will present electroluminescence spectroscopy data from carbon nanotubes, functionalized with dichlorobenzene molecules, and wired to graphene electrodes. We observe electrically generated, defect-induced emissions that are controllable by electrostatic gating and strongly red-shifted compared to emissions from pristine nanotubes. The defect-induced emissions are assigned to excitonic and trionic recombination processes by correlating electroluminescence excitation maps with electrical transport and photoluminescence data. At cryogenic conditions additional, gate-dependent emission lines appear which are assigned to phonon-assisted hot-exciton electroluminescence from quasi-levels. Electroluminescence excitation is selective toward neutral defect-state configurations with the lowest transition energy, which in combination with gate-control leads to high spectral purity.

Li et al., ACS Nano 16 (2022) 11742; 10.1021/acsnano.2c03083

11:00**Optical Properties of One-Dimensional vdW Heterostructures Based on Single-Walled Carbon Nanotubes**Shigeo Maruyama¹¹Department of Mechanical Engineering, The University of Tokyo, Tokyo

The coaxially nested one-dimensional (1D) vdW heterostructure based on single-walled carbon nanotubes (SWCNTs) can expand the board application possibilities of 1D materials [1]. Semiconductor SWCNT or chirality-sorted SWCNT wrapped with BNNT can be regarded as the ideal building blocks of field-effect transistors (FET). By comparing the optical properties of films of BNNT@MoS₂NT and SWCNT@BNNT@MoS₂NT, we found strong photoluminescence (PL) from monolayer MoS₂NT and quenching of PL by coupling to SWCNT through thin BNNT [2]. The inter-tube excitons are demonstrated by ultrafast optical spectroscopy [3]. The inter-tube excitons, the counterpart of inter-layer excitons for 2D heterostructures, suggest a possibility of efficient photovoltaic applications of the 1D heterostructure. More specific optical properties are studied for semiconductor SWCNTs and chirality-sorted SWCNTs [4,5].

[1] R. Xiang et al., Science 367, 537 (2020).

[2] M. Liu et al., ACS Nano 15, 8418 (2021).

[3] M. G. Burdanova et al., Adv. Funct. Mater. 32, 2104969 (2022).

[4] R. Zhang et al., Carbon 199, 407 (2022).

[5] C. Zhang et al., ACS Nano 16, 18630 (2022).

11:30**Inorganic Liquid Crystals Based On 2D Materials**Hui-Ming Cheng^{1,2}¹Institute of Technology for Carbon Neutrality, Shenzhen Institute of Advanced Technology, CAS, Shenzhen, China²Shenyang National Lab for Materials Science, Institute of Metal Research, CAS, Shenyang, China

Liquid crystals (LCs) provide tunable birefringence via external stimuli. In this talk, I will present our recent discovery of a new type of LCs based on inorganic 2D materials. Due to the close interplay among anisotropies in magnetism, optics and shape, we observed a giant magneto-optic Cotton-Mouton coefficient in a magnetic 2D material with a wide bandgap. Its coefficient is three orders of magnitude larger than that of all reported transparent birefringent media. With the development of a solvent-only size-sorting method, we found a quadratic dependence of the magneto-optic coefficient with the lateral size of 2D materials. Such a large coefficient can be further doubled by introducing the collective behavior into the colloidal system of 2D materials. The large magneto-optic coefficient and wide transmission windows cooperatively enable the first observation of transmissive magneto-colouration effect as well as the first fabrication of see-through colour-tunable hydrogel and deep ultraviolet birefringent modulator. Our finding provides an entry point for using wide-bandgap 2D materials as next-generation optical LCs.

18:30

Exploring electronic spins in chemically modified carbon nanotubes

Xuedan Ma¹

¹Nanoscience and Technology Division, Argonne National Laboratory

Great strides have been made in the understanding of electronic and optical properties of single walled carbon nanotubes (SWCNTs) in the past two decades. The creation of bright quantum defects in SWCNTs reported by the seminal works in the early 2010s have rekindled interests in controlled chemical modification of SWCNTs. In contrast to these exciting developments in the excitonic frontier, electron spins, which are ubiquitous in solid state materials and highly relevant to spintronic and quantum information science, in SWCNTs are relatively less understood. In this talk, I will discuss our recent exploration of electron spins in SWCNTs. We discover that controlled chemical modification can serve as an effective approach in engendering long-lived electron spins that are localized at the defect sites.

19:00**Simple chemical approach to two-dimensional metal iodides/graphene heterostructures**

Viera Skakalova^{1,2,3}, Kimmo Mustonen¹, Peter Kotrusz^{2,3}, Christoph Hofer^{1,4}, Karol Hricovini⁵, Christine Richter⁵

¹Physics of Nanostructured Materials, University of Vienna, Vienna

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³Institute of Electrical Engineering and CEMEA SAS, Bratislava, Slovakia

⁴University of Antwerp, EMAT, Antwerp, Belgium

⁵Laboratoire de Physique des Matériaux et Surfaces, CY Cergy Paris Université, Cergy-Pontoise, France

The inertness and impermeability of its atomic structure makes graphene a suitable envelop to stabilizing less obvious two-dimensional (2D) structures. We invented a synthesis of 2D metal iodides, some of them nonexistent at ambient conditions, embedded in graphene. The 2D materials are grown by wet-chemical process at ambient conditions, directly within the space between two graphene oxide layers, while reducing the oxide groups in the same reaction step. This way, the newly formed 2D materials stay tightly encapsulated in graphene. Besides copper iodide, 2D-CuI, a material that normally only occurs at elevated temperatures [1], a number of 2D structure like AgI, AuI₃, NiI₂, BiI₃ and EuI₂ have also been demonstrated. These 2D metal iodides are predicted to differ by their optical, magnetic and electrical properties relevant for novel quantum technologies. Here, transmission electron microscopy images of the atomic structure of 2D metal iodides complemented by electron energy loss and X-ray absorption spectroscopies as well as additional characterization methods will be presented.

[1] Adv. Mater. 2022, 2106922; DOI: 10.1002/adma.202106922

19:30**A NanoBioengineering Frontier for Next-Generation Optical Devices**Ardemis A. Boghossian¹¹Ecole Polytechnique Federale de Lausanne (EPFL)

The ongoing expansion of synthetic biology has led to explosive developments in the field of materials science. Armed with ability to manipulate biology, materials scientists are engineering a new generation of biological or even living technologies. These skills inspire not only new technologies but also new approaches for tackling long-standing bottlenecks in materials engineering. This synergy is especially amplified at the nanoscale – the length scale where life and nanomaterials meet.

This presentation highlights applications in optical sensing and light-harvesting energy technologies that exploit the synergistic coupling of bio-hybrid nanotechnologies. We discuss the development of bio-conjugated single-walled carbon nanotubes (SWCNTs) for optical sensing. These sensors couple the optical tunability of nanomaterials with bioengineering strategies for molecular recognition. We further explore the development of living photovoltaics based on nanobionic cells. These cells are augmented with capabilities enabled by nanomaterials. The applications herein illustrate but a few of the many technologies that can be unlocked using this hybrid engineering approach.

TUE 1**3D-imaging of Printed Nanostructured Networks using High-resolution FIB-SEM Nanotomography**

Cian Gabbett¹, Luke Doolan¹, Kevin Synnatschke¹, Adam Kelly¹, Jonathan Coleman¹

¹School of Physics, Trinity College Dublin, Dublin

While it is known that network morphology plays a dominant role in determining the physical properties of printed devices, methods to quantitatively assess this remain limited. Here, we utilise focused ion beam and scanning electron microscope nanotomography (FIB-SEM NT) to characterise the morphology of printed nanostructured networks with nanoscale resolution. Through serial milling and imaging hundreds of network cross-sections, high-fidelity 3D reconstructions of graphene, WS₂, silver nanoplatelet and silver nanowire networks were produced and analysed. Critical morphological characteristics, including network porosity, tortuosity, pore surface area and nanosheet alignment and connectivity were measured as a function of nanosheet and nanowire size.

TUE 2**Photo-Ferroelectric Van der Waals Neuromorphic Device**

Mohamed Soliman¹, Krishna Maity¹, Arnaud Gloppe¹, Bernard Doudin^{1,2}, Bohdan Kundys¹, Jean-Francois Dayen^{1,2}

¹Universite De Strasbourg, Strasbourg

²Institut Universitaire de France (IUF), Paris, France

Here, we demonstrate the non-volatile electrical and optical control of the ferroelectric polarization in all-VdW ferroelectric/semiconductor heterostructures. We perform a wavelength-dependent study unveiling ferroelectric polarization control and decoupling the mechanisms driven by photogenerated carriers for each material. The constructed Ferroelectric field-effect transistors show On/Off ratios exceeding 10^7 , large hysteresis memory windows, and multiple remanent states, sorting them as good artificial synapse candidates. Following, long-term potentiation/depression, and spike rate-dependent plasticity were shown using electrical control. Moreover, the synaptic functionalities were complemented by the unique dual optical and electrical control, enabling optically stimulated and optically assisted synaptic devices. We benchmark our device with a simulated artificial neural network and achieve an excellent accuracy level of 91%, close to the ideal synaptic case (96%). The combination of the Photo-Ferroelectric functionalities and the shown synaptic characteristics put all-VdW ferroelectric/semiconductor heterostructures on the roadmap for novel computing architectures.

TUE 3**Temperature-dependent electric transport in thin polycrystalline layers of TMD semimetals**

Martin Hulman¹, Lenka Pribusová-Slušná¹, Tatiana Vojteková¹, Jana Hrdá¹, Jozef Kačmarčík², Michaela Sojková¹, Martin Moško¹

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Topological materials (TMs) are a new material category that has appeared in condensed matter physics. Weyl and Dirac topological semimetals (WSM, DSM) possess nontrivial band structures. In a DSM, a Dirac cone is formed at the cross point of bands with linear dispersion in the Brillouin zone. Either broken time-reversal or spatial inversion symmetry splits the Dirac cone into two Weyl cones. Some 2D materials from the family of transition metal dichalcogenides can host DSM or WSM states. Weyl fermions were proposed in 1T'-WTe₂ and Td-MoTe₂, and 1T-PtSe₂ is considered a Dirac semimetal. In our contribution, we show the results of electric transport measurements at low temperatures and high magnetic fields performed on thin layers of MoTe₂, WTe₂ and PtSe₂. A common feature of all samples is that they were prepared by chalcogenisation of the respective metallic films. The layers are polycrystalline with a thickness of about 10 nm. We observed indications of strong electron coupling, quantum interference and disorder-induced effects in some of these layers.

TUE 4**Ultra-clean van der Waals heterostructures.**

Roman Gorbachev¹

¹School of Physics and Astronomy, University of Manchester, Manchester, UK

All current 2D material transfer techniques rely on the use of polymers which limits the cleanliness, ultimate electronic performance, and their potential for optoelectronic applications of the heterostructures. I will present a novel polymer-free platform for rapid and facile heterostructure assembly which utilises flexible silicon nitride membranes. We demonstrate that this allows fast and reproducible production 2D heterostructures using both exfoliated and CVD-grown materials with perfect interfaces free from interlayer contamination and correspondingly excellent electronic behaviour, limited only by the size of the crystals used. In addition, our technology removes the limitations induced by use of polymeric carriers, allowing for vdW heterostructure assembly at high temperatures up to 600°C, various solvents and in ultra-high vacuum (UHV). The UHV transfer synthesis approach employed here for the first time, can reliably create graphene moiré superlattices with significant improvement in their structural homogeneity.

TUE 5**Strain distribution in nanoindented monolayer WSe₂ membranes**

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Tunable optical and electronic properties make transition metal dichalcogenides (TMDCs) an excellent building material for different applications in many fields. When in free-standing form, mono- and few-layers of TMDCs exhibit the ability to withstand large mechanical deformations before rupture. Their highly-localized deformation can be used for tailoring their optoelectronic properties, and, generates various phenomena, such as carrier funneling. Furthermore, tungsten-based TMDCs are predicted to have long-living dark excitons, which are, however, optically active only under limited conditions. We present nanoindentation of monolayer WSe₂ membranes by an AFM tip coupled to in-situ monitoring of their optoelectronic properties through photoluminescence (PL) spectroscopy and local photocurrent measurements. Strain distribution across the deformed membranes is investigated by combining the results from indentation curves and PL shifts with ab-initio calculations of the band structure under biaxial strain of a small lattice unit, molecular dynamics simulations, and finite elements modelling of the real-size membranes, taking also into account the finite size of the indenting tip.

TUE 6**Tailoring spin and electronic structure of MoS₂ monolayer via interaction with substrate**

Vladimir Voroshnin¹

¹Helmholtz Zentrum Berlin, Berlin

MoS₂ monolayer is a direct band semiconductor. The band gap is 1.8eV and located at K and K' points in the Brillouin zone. In our study, we manipulate the electronic and spin structure of MoS₂ via interaction with a substrate to gain control over MoS₂ optical properties. We demonstrate the Rashba effect in the MoS₂ in-plane spin structure in the MoS₂/Au(111) system. Due to symmetry reasons, the Rashba effect does not influence the regions of K and K' points, which are interesting from the point of view of optical implementation. To manipulate the MoS₂ spin structure in the K and K' points regions, we use the magnetic proximity effect between the MoS₂ monolayer and the cobalt thin film in the MoS₂/graphene/Co(0001) system. We place graphene between MoS₂ and Co(0001) to prevent possible excitons, potentially able to mediate spin-flipping effects in the MoS₂ monolayer, from dissipating to the metallic substrate. We demonstrate that the magnetic proximity effect causes

the Zeeman splitting into MoS_2 valence band states in the region of Γ point and a spin tilt toward in-plane direction of the conduction band states in the regions of K and K' valleys.

TUE 7

Family behavior and Dirac bands in armchair nanoribbons with 4-8 defect lines

Roland Gillen¹, Janina Maultzsch¹

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Bottom-up synthesis from molecular precursors is a powerful route for the creation of novel synthetic carbon-based low-dimensional materials. The wealth of conceivable precursor molecules introduces a significant number of degrees-of-freedom for the design of materials with defined physical properties. In this context, a priori knowledge of the electronic, vibrational and optical properties provided by modern ab initio simulation methods can act as a valuable guide for the design of novel synthetic carbon-based building blocks.

Using show density functional theory, we performed simulations of the electronic and optical properties of armchair-edged graphene nanoribbons (AGNR) with a bisecting 4-8 ring defect line. We show that the electronic structures of the defective nanoribbons of increasing width can be classified into distinct three families of semiconductors, similar to the case of pristine AGNR. In contrast to the latter, we find that every third nanoribbon is a zero-gap semiconductor with Dirac-type crossing of linear bands at the Fermi energy, which we trace back to a partial decoupling of the nanoribbon halves by the defect line.

TUE 8

Dynamically Twisted 2D Materials

Francisco Selles¹, Roman Gorbachev¹

¹Physics and Astronomy, University of Manchester, Manchester

Moiré systems, resulting from layers of twisted 2D materials, can host exotic quantum phases, not intrinsic to the parent materials. Currently, the most widely implemented techniques for the fabrication of twisted devices do not allow dynamic control of the twist angle. Thus, there is a priority to develop experimental approaches which can accelerate the process of exploring the remaining twisted 2D material parameter space.

In this work, molybdenum disulphide (MoS_2) crystals are patterned, transferred onto monolayer MoS_2 and nanomechanically manipulated using an atomic force microscope tip. Through a two-step lithography process, indentations are etched into the patterned flakes, allowing for precise twist angle control while ensuring the underlying monolayer remains pristine. To enhance the quality of the heterostructures, transferring of flakes is carried out with a novel polymer-free approach, which utilises flexible silicon nitride membranes.

TUE 9**Covalent 2D Patterning of Graphene**Tamara Nagel¹¹Lehrstuhl für Organische Chemie II, Friedrich-Alexander-Universität Erlangen, Fürth

The poster will be about the patterned covalent functionalization of graphene using laser or electron beam irradiation as an activation source. Different kinds of reactive species have been successfully attached to graphene using this technique.

TUE 10**Designing Vertically Aligned MoS₂ flakes using Ultramicrotomy for Electrocatalysis of Hydrogen Evolution Reaction**Ankit Bhardwaj^{1,2}, Abdulghani Ismail^{1,2}, Robert A.W. Dryfe^{3,4}, Radha Boya^{1,2}¹Physics and Astronomy, The University of Manchester, Manchester²National Graphene Institute, University of Manchester, United Kingdom³Henry Royce Institute for Advanced Materials, University of Manchester, United Kingdom⁴Department of Chemistry, University of Manchester, United Kingdom

Designing and developing inexpensive and highly efficient electrocatalysts is a key component of many emerging clean-energy technologies. MoS₂ is well known to show catalytic hydrogen evolution reaction (HER) activity. Designing vertically aligned MoS₂ was envisaged to increase its electrocatalytic activity, where the activity mainly comes from the edges. However, the existing methods are not well controlled and a mixture of MoS₂ forms (basal planes and edges) is usually present. Herein, a new method based on ultramicrotomy is presented to fabricate vertically aligned MoS₂ which contains only controlled edges exclusively. The main finding is the confirmation of the higher activity of the edges compared to the basal plane MoS₂. Indeed, this method showed superior catalytic activity compared to other methods that uses similar crystals of 2H MoS₂. A Tafel slope down to 77 mVdec⁻¹ with an overpotential of 180 mV vs standard hydrogen electrode (SHE) is obtained. The main advantages of the method are its simplicity, speed and versatility which gives it the possibility to be applied to study the edge-activity of other types of 2D materials.

TUE 11**Symmetry Broken Josephson Junctions in Magic Angle Twisted Bilayer Graphene**Jaime Díez-Mérida^{1,2}, Andrés Díez-Carlón^{1,2}, Shuoying Yang¹, Yingming Xie³, Xuejian Gao³, Kenji Watanabe⁴, Takashi Taniguchi⁴, Xiaobo Lu¹, Kam Tuen Law³, Dmitri K. Efetov^{1,2}¹ICFO - Institut de Ciències Fotoniques, The Barcelona Institute of Science and Technology, Barcelona, Spain²Fakultät für Physik - Ludwig Maximilians Universität, München, Germany

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The simultaneous co-existence and tunability of the superconducting, magnetic and topological orders in magic angle twisted bilayer graphene (MATBG) open up new possibilities for the creation of complex hybrid Josephson junctions. Here we report on the creation of gate-defined magnetic Josephson junctions in MATBG, where the weak link is gate tuned closed to the correlated state at a moiré filling factor of $\nu = -2$. A highly unconventional Fraunhofer pattern emerges, in which supercurrent is carried by edge states, it is phase-shifted and asymmetric with respect to the current and magnetic field directions, and shows a pronounced magnetic hysteresis. The combination of magnetization and its current induced switching allows us to realize a programmable zero field superconducting diode, a major building block for a new generation of superconducting electronics.

TUE 12

Plasmonic metasurface fabricated with a facile and scalable process using plasma etching for sensitive molecular detection

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Nanoscale plasmonic metasurfaces and structures can dramatically enhance electromagnetic fields relative to the incoming light. The enhancement is primarily due to the charge separation of free electrons at resonant oscillations and has been extensively applied in various applications, such as surface-enhanced Raman spectroscopy (SERS), chemical- and biomedical sensors, photocatalysis, and photovoltaic cells. Metasurfaces containing plasmonic nanostructures can be fabricated through several techniques, including electron beam lithography, laser interference lithography, focused ion beam milling, wet chemical synthesis, embossing, and annealing of thin films and patterns. Each technique has strengths and limitations. In general, the fabrication of uniform nanostructured metasurfaces is a complicated and costly procedure, which mitigates the widespread use of this technique in ubiquitous applications. Here, we present an active nanoplasmonic metasurface in gold fabricated by a facile and scalable method based on plasma etching technology. The novel metasurface is tested for sensitive molecular detection using SERS and fluorescence-based systems.

TUE 13

The tunable optoelectronic properties of polyynes probed by synchrotron-based UV resonance Raman spectroscopy

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Polyynes are the finite realization of 1D linear chains made of alternated triple and single sp-hybridized CC bonds with appealing structure-dependent optoelectronic properties [1]. Raman spectroscopy is a powerful tool to analyze polyynes' properties from which it is possible to extract information about their bandgap, structure, and electron-phonon coupling [2].

We demonstrated how the optoelectronic properties of polyynes can be inferred from their synchrotron-based UV resonance Raman spectra. From the analysis of the intensity and frequency modulations of the fundamental normal mode of polyynes (i.e. a collective in-phase stretching of all the CC bonds in the chain) and its overtones, it is possible to understand the fine structure of the vibrational energy levels and the anharmonicity of the potential energy surfaces [3]. Moreover, we found that the Huang-Rhys factor, a marker of the electron-phonon coupling, grows for increasing chain length and varies depending on the termination [3].

[1] C. S. Casari et al., *Nanoscale*, 2016, 8, 4414–4435

[2] A. Milani et al., *Beilstein J. Nanotechnol.*, 2015, 6, 480–491

[3] P. Marabotti et al., *Nat. Commun.*, 2022, 13, 5052

TUE 14

Preparation and characterization of MoTe₂, WTe₂ and PtTe₂

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Research in thin-film materials has significantly increased, especially in a group of transition metal dichalcogenides (TMDs), including MoTe₂, WTe₂, and PtTe₂. These materials have unique optoelectronic properties that vary due to the thickness of the layer and the crystal structure. Electrical properties vary depending on structures, from semiconducting to metallic. The preparation of films by tellurization of molybdenum/molybdenum trioxide, tungsten, and platinum is more complex than sulfurization or selenization due to the weaker redox properties of tellurium. The challenge in thin films is the controlled preparation of the required crystal structure of homogeneous large-area layers. We prepared hexagonal and monoclinic MoTe₂, orthorhombic WTe₂, and hexagonal PtTe₂ by a chemical vapor deposition method. Films were characterized by Raman spectroscopy (also low-temperature), X-ray diffraction, and GIWAXS to confirm the structures of thin films. The aim is to contribute to the preparation of tellurides and their characterization, which is necessary for using materials in applied practice.

TUE 15**Interfacial ferroelectricity in marginally twisted 2D semiconductors studied via KPFM**

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Here, we present our most recent results in which we further study the physical properties of the ferroelectric domains formed in 3R-MoS₂ bilayers by employing two-pass phase modulated Kelvin probe force microscope (PM-KPFM) in high vacuum environments (1E-6 mbar). PM-KPFM is a technique that allows the characterization of the contact potential difference of a sample in a non-destructive and non-invasive manner, achieving spatial and electronic resolutions down to 20 nm and 20 mV, respectively. Although no major features are observed in the topography map, the contact potential difference map shows the presence of ferroelectric domains on top of the 3R-MoS₂ homo-bilayer. Different patterns can be seen, from the triangular commensurate region to areas with more irregular patterns. These differences are attributed to variations of the twisting angle between the regions as a result of the fabrication process. Besides imaging the domain structure, we employed this data to calculate quantitatively the potential difference between the domains, which resulted to be $2V = 100 + 20 \text{ mV}$, in agreement with the theoretical calculations.

TUE 16**Anti-Stokes Photoluminescence in WSe₂ Activated by Plasmonic Cavities through Resonant Excitation of Dark Excitons**

Niclas S. Mueller¹, Rakesh Arul¹, Ashley P. Saunders², Amalya C. Johnson², Ana Sánchez-Iglesias³, Shu Hu¹, Lukas Jakob¹, Junyang Huang¹, Angela Demetriadou⁴, Luis M. Liz-Marzán³, Fang Liu², Jeremy J. Baumberg¹

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Anti-Stokes photoluminescence (PL) is light emission at a larger energy than the excitation laser, with applications in optical cooling, bioimaging and lasing. Here, we show how plasmonic nano-cavities activate anti-Stokes PL in WSe_2 monolayers through resonant excitation of a dark exciton. The tightly confined plasmonic fields couple to the out-of-plane transition dipole of the dark exciton in WSe_2 , which serves as the excitation channel. Light is emitted at larger energy by the bright exciton. Through a statistical analysis of hundreds of plasmonic cavities we show that an efficient coupling to the dark exciton leads to a hundred-fold enhancement of the upconverted PL. This is further corroborated by experiments in which we tune the excitation wavelength. Finally, we show that the anti-Stokes PL can be further increased by non-linear mixing of two red detuned lasers that resonantly excite the dark and bright excitons.

TUE 17

Probing the Ultrafast Dynamics of Excitons in Single Semiconducting Carbon Nanotubes

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We investigate the exciton decay dynamics in single (6,5) single-walled carbon nanotubes (SWCNTs) using transient interferometric scattering and time-resolved photoluminescence (PL) microscopy with few-exciton detection sensitivity [1]. Observing the same single SWCNT at the same experimental conditions avoids ambiguities arising from ensemble averaging, which may hinder the development and testing of model descriptions for the excited state dynamics. We can describe both PL and pump-probe transients with the same model function and parameters that combine EEA with exponential exciton decay [2]. Pump-probe transients detected when increasing the average number of excitons from about 2 to 16 within a nanotube segment length of 600 nm reveal ultrafast annihilation of excitons on a time-scale reaching down to 200 fs. The power dependence of the diffusional times can be very well described using the initial average exciton-exciton distance and reported values of the diffusion coefficient of (6,5) SWCNTs.

[1] K. Birkmeier, T. Hertel, A. Hartschuh, Nat. Commun. 13, 6290 (2022).

[2] A. Srivastava, J. Kono, Phys. Rev. B 79, 205407 (2009).

TUE 18**The electrical conductivity of solution-processed nanosheet networks**Adam Kelly¹¹Trinity College Dublin, Dublin

Solution-processed networks of 2D nanosheets are increasingly promising for a range of applications in the field of printed electronics. However, the electrical performance of these networks is almost always inferior to that of the individual nanosheets owing to variations at the junctions where the nanosheets come into contact. These junctions are influenced by many interacting factors such as the dispersion/ink formulation, deposition method, post-treatment techniques, and the dimensionality of the nanosheets themselves. Each of these can modify the morphology of the printed network which in turn significantly affects the conduction properties through the junction resistance. Here, I discuss the role that each of these factors play in influencing the junction resistance by using reported electrical data to analyse the relationship between morphology and network conductivity. This analysis allows us to propose several conduction regimes where the conductivity can be limited by the junctions, the material, or a combination of both. I also present a simple method for rapid analysis of the junction resistance itself.

TUE 19**Circularly polarized near-infrared light-emitting transistors with enantiomer-sorted single-wall carbon nanotubes**Yohei Yomogida¹, Finn L. Sebastian², Yuuya Hosokawa¹, Nicolas F. Zorn², Sonja Wieland², Kazuhiro Yanagi¹, Jana Zaumseil¹¹Tokyo Metropolitan University²Heidelberg University

Near-infrared (NIR) circularly polarized light-emitting devices have potential applications in spintronics, optical communications, and bioimaging. Especially, the NIR-II region above 1000 nm is important for optical diagnostics. Various emitter materials have been developed, but so far they show only weak circular polarization in the NIR region. One strategy to achieve strong circular polarization is to use tubular structures that are expected to enhance the magnetic dipole moment related to the magnitude of the circular polarization. Here we use enantiomer-sorted (6,5) and (11,-5) single-wall carbon nanotubes (SWCNTs) that exhibit circularly polarized absorption and photoluminescence around 1000 nm with high dissymmetry values. These properties were maintained in thin films that were integrated in light-emitting transistor structures and showed circularly polarized electroluminescence.

TUE 20**Microscopic picture of interlayer exciton-phonon coupling**Muralidhar Nalabothula¹, Ludger Wirtz¹, Sven Reichardt¹¹Department of Physics and Materials Science, University of Luxembourg, Luxem-

bourg.

Excitons play a key role for opto-electronic applications of 2D heterostructures. They also can strongly couple to phonons as evidenced by their imprint on resonant Raman scattering intensities. In 2D heterostructures, this sort of strong coupling and its signature in Raman scattering offers an ideal setting to learn about exciton-phonon (exc.-ph.) coupling across material layers. Here we focus on the example of monolayer WSe₂ and hBN. Its Raman spectrum features the normally silent out-of-plane optical phonon mode of hBN that becomes active due to symmetry breaking and very strongly enhanced due to resonant exc.-ph. scattering. While the resonant scattering pathways have been identified as involving excitons in WSe₂ that couple to the phonons in hBN, a microscopic understanding of this interlayer exc.-ph. coupling is still missing. We provide such understanding using the state-of-the-art method for the computation of resonant Raman intensities, which allows a detailed atomistic and quantum mechanical dissection of the Raman scattering process. Supplemented by a classical picture, our work sheds light on the microscopic mechanism behind exc.-ph. coupling in 2D heterostructures.

TUE 21

WiFi energy harvesting system for low-power applications manufactured using the SSAIL method

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Energy harvesting refers to the process of collecting and storing energy from various sources, such as solar, thermal, kinetic, and electromagnetic, to power electronic devices. The goal of energy harvesting is to create self-sustaining systems that can operate indefinitely without the need for external power sources. In recent years, research in energy harvesting has been focused on developing new materials and techniques to increase the efficiency and reliability of energy harvesting systems. Additionally, there has been increasing interest in integrating energy harvesting into wireless sensor networks (WSN) and the Internet of Things (IoT) to power these devices. We propose a WiFi energy harvesting system for low-power applications manufactured using the Selective Surface Activation Induced by Laser (SSAIL) technology. One of the key advantages of Wi-Fi energy harvesting is that it utilizes a ubiquitous source of energy, which means that it has the potential to be used in a wide range of locations. Additionally, Wi-Fi energy harvesting does not require any additional infrastructure, as it can be harvested from existing Wi-Fi signals using specialized antennas and rectifiers.

TUE 22**Spin-orbit proximity effects in carbon nanotubes.**Marcin Kurpas¹¹Institute of Physics, University of Silesia in Katowice, Chorzow

We study proximity spin-orbit effects in heterostructures made of a 1D carbon nanotube and a 2D material. In contrast to periodic 2D systems, in which the crystal potential across the interface is rather smooth, in 1D/2D heterostructures it displays a substantial in-plane variation due to the finite size of the nanotube. This leads to the emergence of new types of effective spin-orbit fields absent in 2D systems [1]. In effect, the Dirac cone bands of the nanotube split off in a similar way as in the case coexisting external electric and magnetic fields [2]. Our results show that proximized carbon nanotubes can realize interesting physical phenomena, such as helical modes, and are promising systems in spintronics applications. In effect, the Dirac cone bands of the nanotube split off in a similar way as in the case coexisting external electric and magnetic fields [2].

[1] M. Kurpas, in preparation (2022).

[2] J. Klinovaja et al. Phys. Rev. B 84, 085452 (2011).

TUE 23**Direct-growth of outer carbon nanotubes surrounding single-walled carbon nanotubes**Koki Kozaki¹, Kenta Kusakabe¹, Hodaka Nishimura¹, Ryotaro Kaneda¹, Keigo Otsuka¹, Shigeo Maruyama¹, Shohei Chiashi¹¹Department of mechanical engineering, the University of Tokyo

First, single-walled carbon nanotubes (SWCNTs) suspended on a sapphire slit substrate were synthesized by gas-flow CVD method, at 900 degrees, using mixture of ethanol, hydrogen and Ar at atmospheric pressure. Then outer carbon nanotubes (CNTs) surrounding the suspended SWCNTs were synthesized by acetylene CVD method, at 1350 degrees, 5 kPa, with hydrogen and Ar buffer gases. The acetylene CVD directly synthesized graphene on graphite or hexagonal boron nitride, without metal catalysts. After the synthesis, the intensity of the D-band and 2D-band in Raman scattering spectra were increased. This increase could be due to defects of the outer carbon layers, suggesting that the outer CNTs are composed of multiple domains. The down-shift of the G-band was also observed and it might be caused by thermal strain in the nanotubes. In this study, the outer CNTs were synthesized at higher temperature than the inner SWCNTs.

TUE 24**Anharmonicity in higher order Raman modes of confined carbyne**Johannes Lechner¹, Pietro Marabotti², Lei Shi³, Thomas Pichler⁴, Sebastian Heeg¹¹Institut für Physik und IRIS Adlershof, Humboldt Universität zu Berlin, Berlin

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Confined carbyne consists of long linear carbon chains (>100 atoms) inside carbon nanotubes and is considered a close, stable analogue to the truly 1-dimensional carbon allotrope carbyne. Here we investigate the higher order modes of the Raman active C-mode of single confined carbyne chains by confocal resonant Raman spectroscopy. We observe large frequency shifts which imply strongly anharmonic properties. Comparative analysis of confined carbyne chains with different C-mode frequencies provides further evidence that the properties of long carbon chains confined inside carbon nanotubes do not depend on their length. We further observe an unusual relationship in the relative intensities of Raman peaks of different orders and the excitation wavelength, enabling further insight into the structural properties of confined carbyne as a material system.

TUE 25

Polymer-Free Transfer Platform for the Fabrication of Graphene Liquid Cells.

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Graphene liquid cells are traditionally fabricated with polymer transfer layers but these unavoidably introduce hydrocarbon contamination which is challenging to remove. Here we present our method for the fabrication of ultra clean engineered graphene liquid cells (GLCs) with controlled liquid volumes, through the application of our novel polymer-free 2D heterostructure assembly process using flexible SiNx cantilevers. The GLC structure involves encapsulating hBN – which has etched cavities containing the liquid samples – between the two few-layer graphene (FLG) windows. The GLC is fabricated by picking up 2D crystals sequentially to cover a hole in the cantilever. The end of the cantilever can then be detached by fracture along a perforated edge and mounted upon a silicon chip for loading in the TEM. Through our cantilever based GLC fabrication process we have shown the clean and facile fabrication of heterostructure stack-based GLCs, using a ‘peel on and peel off’ technique with our cantilevers. High angle annular dark field scanning transmission electron microscopy (HAADF STEM) imaging of the sample reveals atomic resolution imaging of specimens in the liquid cell.

TUE 26**Ultrafast spin-polarized charge transfer at a ferromagnet-semiconductor interface**

Nele Stetzuhn^{1,2}, Abhijeet Kumar¹, Denis Iagodka¹, Sviatoslav Kovalchuk¹, Cornelius Gahl¹, Kirill I. Bolotin¹

¹Freie Universität, Berlin

²Max-Born-Institut, Berlin

Two-dimensional ferromagnetic materials are an exciting platform for easily tunable spintronic devices. Here, we combine the prototypical 2d ferromagnet CrI₃ with a monolayer of WSe₂. Their type-II band structure alignment leads to the transfer of spin-polarized electrons and holes across the interface on a femtosecond timescale. We observe this tunneling process and the subsequent decay of carriers and spins using two-color time-resolved Kerr spectroscopy.

TUE 27**Hybridization of fabric fibers with functionalized carbon nanomaterial-carriers of enhanced qualities against critical operational conditions**

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Hybridization of carbon nanostructures with fabric fibers enables the realization of multipurpose textiles featured in various applications.[1] Herein, we strategically chemically modified carbon nanostructures to give them desired properties for their subsequent physisorption onto Kevlar, Nomex and VAR fibers. In detail, chitosan was utilized to provide antibacterial properties, benzotriazole for enhanced UV resistance and thiourea for flame retardancy. Following their complete characterization, the samples were tested for the aforementioned properties, validating our initial approach.[2] This work provides insights to the fabric industry in its quest to fulfil the current technical expectations on protective clothing and can bridge the gap between research and real life applications.

[1] I. K. Sideri and N. Tagmatarchis, Mater. Horiz. 8, 3187 (2021).

[2] Manuscript in preparation.

TUE 28**Collective Vibrations in Homogeneous Carbon Nanotube Bundles**

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The spectra of isolated carbon nanotubes (CNTs) have been extensively studied, particularly the radial breathing mode (RBM) region because of its singular peak frequency inversely proportional to the tube's diameter. When identical CNTs are packed into bundles their vibrational properties were predicted to change and additional low-frequency modes were expected in the Raman spectrum. However, the experimental study of collective vibrations has been limited due to the difficulty in obtaining homogeneous chirality bundles. Here, we present a Raman study of the collective vibrational modes arising from homogeneous bundles formed by a SWCNT coil. In such coils, we observe two breathing-like modes, in contrast to the single RBM characteristic for isolated tubes. We investigate the exciton-phonon coupling for these modes with resonant Raman spectroscopy. Further, we study the diameter dependence by analyzing different coils and other bundling geometries and compare them with theoretical lattice dynamics of infinite bundles of identical nanotubes. These results provide an insight into intratube lattice dynamics in CNTs for a better understanding of collective vibrational effects.

TUE 29

Charge carrier localization and delocalization in p-doped SWNTs

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Doping of low-dimensional semiconductors and the ability to quantify doping levels as well controlling the distribution of excess charges represent essential technological challenges for the development of new semiconductor-based technologies.

Here, we present a room temperature investigation of intrinsic and doped semiconducting single-wall carbon nanotubes (s-SWNTs) using stationary and time-resolved spectroscopies [1-3]. Specifically, we address the question if and under what conditions, charge carriers in doped s-SWNTs may become delocalized or localized. Nanotube samples used here are chirality-enriched and polymer-wrapped (6,5) s-SWNTs, p-doped by redox chemical reduction of AuCl₃. At low doping levels, experimental data indicates a localization of carriers, most likely by interaction with exohedral Cl⁻ impurities. However, such localization appears to be lifted when approaching the degenerate doping regime.

[1] K.H. Eckstein, et al., J. Phys. Chem. C, 2021, 125(10), 5700-5707.

[2] K.H. Eckstein, et al., J. Phys. Chem. C, 2019, 123(49), 30001-30006.

[3] K.H. Eckstein, et al., ACS Nano, 2017, 11(10), 10401-10408.

TUE 30**Device Applications of One-Dimensional Heterostructure Nanotubes**

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To fabricate functional devices of one-dimensional heterostructure nanotubes, namely coaxial combination of single walled carbon nanotube, boron nitride nanotube, or further coating by other materials, such as molybdenum disulfide nanotube, the template individual suspended single walled carbon nanotubes were produced over silicon poles, and the confined cobalt on silicon pole top was the catalyst. Thereafter, boron nitride nanotubes and molybdenum disulfide nanotubes were sequentially coated outside of the template carbon nanotubes by chemical vapor deposition. The as-grown suspended heterostructure nanotubes were characterized by AES and Raman, and they can be facilely transferred onto target substrate assisted by water vapor. Top-gated heterostructure nanotube transistor and metal-insulator-semiconductor heterojunction diode will be presented.

TUE 31**Exciton optics and dynamics in organic and organic/TMD heterostructures.**

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Organic semiconductors are exciting candidates for photovoltaic and biosensor technologies. Currently however there are limitations preventing these materials reaching the level of efficiency of competing devices. These limitations can be overcome by interfacing organic crystals with TMDs. In this joint theory-experiment work, we study the exciton landscape in organic molecular crystals as well as organic/TMD heterostructures, with a particular emphasis on their optical response. We demonstrate both theoretically and experimentally that the low-temperature PL is dominated by the formation of interlayer excitons, with the electron and hole located on the TMD and molecule layer, respectively. We find that additional sidebands emerge as a result of the indirect recombination of excitons. We study the exciton landscape within an organic crystal and find a unique polarisation- and temperature-dependence of optical spectra. We describe the exciton dynamics in these crystals, and predict phonon-bottlenecks in the exciton relaxation. We study energy trans-

fer processes in organic/TMD heterostructures, governed by the Förster interaction, and predict the effect on the optical spectra.

TUE 32

High carrier mobility PtSe₂ Films Grown by One Zone Selenization

Michaela Sojková¹, Jana Hrdá¹, Peter Hutár¹, Tatiana Vojteková¹, Lenka Pribusová Slušná¹, Dagmar Gregušová¹, Ondrej Pohorelec¹, Martin Hulman¹

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PtSe₂ has attracted interest due to its physical properties. The substrate plays an important role in the film growth. The final alignment strongly influences its electrical properties, especially charge carrier mobility. Here, we present fabrication of PtSe₂ thin films on different substrates (c-plane sapphire, Si, Si/SiO₂ and annealed Si/SiO₂). One zone selenization of magnetron sputtered Pt layers was used for the film growth. We studied the influence of the substrate, synthesis conditions and an initial Pt thickness on the structural and electrical properties of as-prepared PtSe₂ films. The films grown on c-plane sapphire exhibit signatures for a long-range in-plane ordering resembling an epitaxial growth and increased values of the charge carrier mobility. Films grown on the non-crystalline substrates showed low crystallinity and reduced carrier mobility while films prepared on annealed Si/SiO₂ are comparable with those prepared on the sapphire. The decrease of heating ramp led to the growth of films with bigger grains and increased carrier.

TUE 33

Ultrafast Photocurrent to Probe the Formation of Dark Interlayer Excitons in a MoS₂/MoSe₂ Heterostructure

Denis Yagodkin¹, Elias Ankerhold¹, Abhijeet Kumar¹, Johanna Richter¹, Kenji Watanabe¹, Takashi Taniguchi¹, Cornelius Gahl¹, Kirill I Bolotin¹

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Optically dark excitons determine a wide range of properties of photoexcited semiconductors yet are hard to access via conventional spectroscopies. Here, we develop a time-resolved ultrafast photocurrent technique (trPC) to probe the formation dynamics of optically dark excitons. The nonlinear nature of the trPC makes it particularly sensitive to the formation of excitons occurring at the femtosecond timescale after the excitation. As proof of principle, we extract the interlayer exciton formation time 0.4 ps at 160 $\mu\text{J}/\text{cm}^2$ fluence in a MoS₂/MoSe₂ heterostructure and show that this time increases with fluence. In addition, our approach provides access to the dynamics of carriers and their interlayer transport. Overall, our work establishes trPC as a technique to study dark excitons in various systems that are hard to probe by other approaches.

TUE 34**Strongly enhancing the interaction of Pt nanoclusters with 2D MoS₂ crystals for efficient hydrogen evolution**

Tamas Ollar¹, Antal Koos¹, Peter Vancsó¹, Peter Kun¹, Peter Nemes-Incze¹, Jozsef Sandor Pap¹, Levente Tapasztó¹

¹Centre for Energy Research, Budapest, Hungary

While platinum is one of the most efficient and widely studied catalysts, from bulk to single atom level, further improving its activity and stability is still needed, to enable large-scale applications, such as the cost-efficient, mass-production of green hydrogen. Here, we show that by fully exploiting the interaction of small Pt clusters with 2D MoS₂ crystals, the intrinsic activity of Pt clusters can be substantially increased. The strong Pt-MoS₂ interaction impacts about every aspect of Pt structures related to their catalytic performance, resulting in a quasi-flat morphology, sizeable band gap, substantial strain and doping, as well as interfacial sites of outstanding hydrogen adsorption properties. These factors together enable the simultaneous enhancement of activity and stability of small Pt clusters. Such strongly interacting Pt/MoS₂ catalysts can be prepared by a simple and scalable room-temperature electrochemical deposition technique, and are able to reach the activity of commercial Pt-C catalysts at orders of magnitude lower Pt loadings.

TUE 35**Higher-indexed Moiré patterns in MoTe₂/graphene heterostructure**

Péter Vancsó¹, Trung T. Pham², Márton Szendrő¹, Krisztián Palotás^{3,4}, Roshan Castelino², Mehdi Bouatou⁵, Cyril Chacon⁵, Luc Henrard², Jérôme Lagoute⁵, Robert Sporken²

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In van der Waals heterostructures, Moiré patterns have important consequences on the physical properties of the systems. A prime example is the particular electronic behavior of bilayer graphene with a small magic angle [1], which has opened a new area of research. In this work, we provide a study of single layer of 2H-MoTe₂ grown on graphene by MBE and present scanning tunneling microscopy (STM) investigations combined with density functional theory (DFT) calculations. Our results show that the STM images of the MoTe₂/graphene heterostructure exhibit unusually rich

and complex Moiré structures with the appearance of unique higher-indexed Moiré patterns. DFT calculations and STM simulations have explained these Moiré patterns by revealing the importance of the electronic coupling between the layers in the heterostructure even for weaker Moiré potential modulations [2]. The experimentally observed higher-indexed patterns, which are predicted by Moiré theory, further expand the possibilities of Moiré physics in the field of vdW heterostructures.

[1] Y. Cao et al., Nature 556, 43-50 (2018).

[2] T. T. Pham et al., NPJ 2D Mater. Appl. 6, 48 (2022).

TUE 36

Unravelling interactions between TMDCs and metals

Matěj Velický¹, Luka Pirker¹, Otakar Frank¹

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Strong interactions between 2D materials and gold have attracted a wide interest recently, leading to a reliable production of large monolayers of different 2D materials, in particular TMDCs, and appearance of intriguing phenomena in optical spectroscopy, electron spectroscopy, and electrochemistry.[1] Other metals should theoretically exhibit even stronger interaction with TMDCs than Au, however, experimental observations suggest that their susceptibility to oxidation prevents this in air-prepared samples.[2]

Herein, we exfoliate TMDCs on a range of different metals under an inert atmosphere and characterize the resulting monolayers using different techniques, in particular Raman spectroscopy. The resulting Raman spectra show significant differences between different metals in the positions, shapes, and intensities of the E and A₁ modes. We rationalize the observed Raman spectra based on differences between the TMDCs and metal lattices, work functions, and morphology.

1. Velický et al., ACS Nano 12, 2018, 10463-10472

2. Velický et al., Adv. Mater. Interfaces 7, 2020, 2001324

TUE 37

Valley polarization of trions in TMDC interfaced with magnetic dielectric

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²Department of Physics and Engineering, ITMO University, Saint Petersburg

³Moscow Institute of Physics and Technology, Dolgoprudny

⁴Department of Physics and Astronomy, University of Sheffield, Sheffield

One of the promising approaches to control the transition metal dichalcogenides (TMDs) excitonic valley properties is via interfacing the layer with magnetic materials. It allows, for example, lifting the energy degeneracy at the K and K' points

through proximity effects and eliminating the need for large external magnetic fields. In this work we study circularly polarized photoluminescence of trions in MoSe₂ monolayers interfaced with thin films of bismuth iron garnet (BIG). Due to the out-of-plane magnetization in the BIG film, these systems exhibit contrast in the co-polarized photoluminescence of trions under right and left circularly polarized excitation. Importantly, the extracted magnitude of the effective magnetic field is almost an order of magnitude larger than the saturation magnetization of BIG. This indicates the emergence of proximity effects at the MoSe₂/BIG interface and suggests that interfacing TMDs with thin magnetic films gives an access to large effective magnetic fields even in the absence of strong external fields [1].

[1] Vasily Kravtsov et al. 2022 2D Mater. 9 015019.

TUE 38

Interfacial ferroelectricity in marginally twisted 2D semiconductors

Astrid Weston^{1,2}, Eli Castanon^{1,2,3}, Vladimir Enaldiev^{1,2,4}, Fabio Ferreira^{1,2}, Shubhadeep Bhattacharjee^{1,2}, Shuigang Xu^{1,2}, Hector Corte-Leon³, Zefei Wu^{1,2}, Nick Clark^{2,5}, Teruo Hashimoto^{2,5}, Sarah J. Haigh^{2,5}, Olga Kazakova³, Andre Geim^{1,2}, Roman Gorbachev^{1,2,6}

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⁵Department of Materials, University of Manchester, UK

⁶Henry Royce Institute for Advanced Materials, University of Manchester, UK

We demonstrate room-temperature ferroelectricity in 3R-twisted bilayer MoS₂. Below a critical angle, twisted bilayers of MoS₂ atomically reconstruct to generate an energetically favourable triangular domain structure in the case of the 3R-stacking polytype. These heterostructures feature broken inversion symmetry, which, together with the asymmetry of atomic arrangement at the interface of the vertically stacked layers, enables ferroelectric domains with alternating out-of-plane polarisation arranged into a twist-controlled network. Through the mechanism of domain wall sliding, the polarised states can be 'switched' by applying out-of-plane electrical fields as visualized in-situ using channelling contrast electron microscopy. The polarisation-dependent electrical potential distribution of the observed ferroelectric domains was quantified using Kelvin probe force microscopy and agrees well with theoretical calculations. Our results show that adding a twist between two adjacent monolayers has the potential for room temperature electronic and optoelectronic semiconductor devices with built-in ferroelectric memory functions.

TUE 39**Hydrocarbon Contamination in Angstrom-scale Channels**Ravalika Sajja¹¹Department of Physics and Astronomy, School of Natural Sciences, The University of Manchester, United Kingdom

Nonspecific molecular adsorption like airborne contamination occurs on most surfaces including 2D materials and alters their properties. While the surface contamination is well studied, the effect of contamination in a confined system such as nanochannels/pores leading to their clogging is still lacking. We report a systematic investigation of hydrocarbon adsorption in the angstrom(Å) slit channels of varied heights where hexane is chosen to mimic the hydrocarbon contamination. A dynamic transition of the clogging and revival process is shown in sub-2 nm thin channels and longterm storage and stability of our Å-channels is demonstrated. This study highlights the importance of the nanochannels' stability and demonstrates self-cleansing nature of sub-2 nm thin channels enabling a robust platform for molecular transport and separation studies. We provide a method to assess the cleanliness of the nanoporous membranes, vital for the practical applications of nanofluidics in various fields like molecular sensing, separation and power generation.

TUE 40**In-plane Excitation for Near-Field Microscopy**Patryk Kusch¹, Jose Arcos¹, Aleksei Tsarapkin³, Victor Deinhart², Katja Höflich³, Stephanie Reich¹¹Freie Universität Berlin - Institut für Experimentalphysik, Berlin²Helmholtz Zentrum Berlin³Ferdinand Braun Institut Berlin

Implementing metallic single tips in atomic force microscopes led to the development of nanoimaging techniques and setups like tip-enhanced Raman spectroscopy (TERS), and scattering-type scanning near-field microscopy (s-SNOM). We introduce new tip structures for in-plane excitation in TERS and s-SNOM experiments by applying double tips. The double tips comprise two single tips that point to each other and are grown by electron beam-induced deposition. Illuminating such tips with s-polarized, i.e., perpendicular to the tip axis, allows exciting a strongly enhanced near-field between the two tips that is oriented in-plane. We demonstrate the capabilities of the double tips by TERS and s-SNOM experiments on various samples. We take near-field images of graphene and WS₂ and nanoimage their edge by TERS and tip-enhanced photoluminescence. We succeed even in the observation of the defect band of graphene at its edge. We record images of single one-dimensional boron nitride nanotubes by s-SNOM and excite propagating waveguided modes in MoS₂. For comparison, we repeat the experiments with conventional single tips and support our findings by numerical calculations.

TUE 41**Spatially-Resolved Surface Plasmon Modes in the Topological Insulator Bi_2Te_3 from Energy-Gain Spectroscopy**

Helena La¹, Abel Brokkelkamp¹, Stijn van der Lippe¹, Jaco Ter Hoeve^{2,3}, Juan Rojo^{2,3}, Sonia Conesa-Boj¹

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Topological insulator materials provide an ideal platform for unveiling collective plasmonic excitations at optical frequencies. Establishing the onset and properties of such plasmonic resonances as a function of local structure at the nanoscale is key for the development of novel tunable plasmonics in the THz frequency range for applications from quantum computing, and terahertz detectors, to spintronic devices. Here, we present a comprehensive electron energy-gain spectroscopy study of Bi_2Te_3 that identifies with nanoscale resolution the spatial and energetic distributions of energy-gain resonances corresponding to surface plasmon modes in the visible spectral region. We detect energy-gain peaks at 1.1 eV, 2.1 eV, and 3.1 eV, and find that the 1.1 eV is mainly confined at the edges. Our results illustrate the potential of electron energy-gain spectroscopy to the direct mapping of collective plasmonic excitations in 2D materials which would be beneficial for the design of novel applications in tunable plasmonic devices in the THz and mid-infrared frequency range.

TUE 42**The Impact of Inert Conditions During the Fabrication Process on the Optical Properties of MoS_2 Monolayers**

Alina Schubert¹, Michael Kempf¹, Rico Schwartz¹, Patricia Gant², Felix Carrascoso², Carmen Munuera², Andres Castellanos-Gomez², Tobias Korn¹

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²Instituto de Ciencia de los Materiales de Madrid, Madrid

Transition-metal dichalcogenides (TMDCs) are layered materials that can be thinned down to monolayers. The optical properties of these flakes depend strongly on the cleanliness of the surfaces. Transferring TMDCs with PDMS is simple to perform and allows the fabrication of large monolayers [1]. The objective of this work was to improve the methodology so that sample quality is enhanced without reducing the yield or increasing the effort required for production. For this purpose, a statistic of 20 MoS_2 monolayers was set up, which were half transferred to a SiO_2 substrate at ambient conditions and half transferred in a glovebox [2]. All samples were characterised by photoluminescence (PL) spectroscopy at room temperature and ~ 4 K. By examining the exciton and trion features in the spectra, it could be shown that only the small difference in the transfer process results in changes of the optical properties that can be attributed to a higher sample quality of the samples fabricated in the

glovebox.

[1] Castellanos-Gomez, A. et al. 2D Mater. 1 (2014)

[2] Gant, P. et al. 2D Mater. 7 (2020)

TUE 43

Visible-frequency graphene plasmons in nanocorrugated graphene

Gergely Dobrik¹, Péter Nemes-Incze¹, Bruno Majérus², Péter Vancsó¹, Gábor Piszter¹, Miklós Menyhárd¹, Benjámin Kalas¹, Péter Petrik¹, Luc Henrard², Levente Tapasztó¹

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The nanoscale confinement of charge carriers is an effective approach for engineering the properties of materials. We demonstrate [1] that amplifying the random nanoscale corrugation of graphene, can realize the edge-free lateral confinement of its electrons. This enables the low-loss (edge-free) ultra-confinement of graphene plasmons into sub-5nm graphene areas, scaling up the plasmon resonance frequency to the commercially relevant visible range. Moreover, we found that propagating visible plasmon modes also exist in nanocorrugated graphene. We were able to image their interference patterns by SNOM measurements at visible ($\lambda = 488$ nm) frequencies. Visible graphene plasmons also manifest themselves through mediating several orders of magnitude stronger Raman enhancement than previously achieved with graphene, enabling the optical detection of specific molecules from femtomolar solutions or even ambient air.

[1] Dobrik, G., et al., Nature Nanotechnology 17, 61 (2022)

TUE 44

Biofunctionalization of graphene and carbon nanotubes for reversible site-specific protein immobilization

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The surface immobilization of biomolecules is indispensable for most characterization techniques and therefore a goal in structure analysis. Graphene and carbon nanotubes emerge as electrical biosensors due to their extraordinary transport properties. Fundamental understanding of the effects of immobilization on proteins functionalized to these conductive carbon nanomaterials thus enables the development of new types of electronic biosensors.

Here, we present functionalization by a pyrene-linker and by a lipid-linker binding reversibly to a tagged Green Fluorescent Protein (GFP) as a well characterized protein exemplary for a wide range of proteins [1]. Reflectance interference spectroscopy (RIfS) and total internal reflectance fluorescence spectroscopy (TIRFS) on graphene and CNT coated RIfS-chips reveal the binding-kinetics involved as well as a specific and reversible protein binding. Fluorescence quenching is used to determine the distance between the GFP-fluorophore and the graphene. In addition, fluorescence lifetime measurements in solution indicate fluorescence quenching caused by CNTs.

[1] Jorde et al, JAP 129, 094302 (2021).

TUE 45

Electrically probing the spin-texture of few-layer MoTe₂

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¹University of Groningen, Groningen

The realization of two-dimensional spintronics devices relies on three key processes: spin-charge conversion, spin manipulation and transport. 2D crystals with large spin-orbit coupling have been widely studied, as their spin-momentum locking allows for the manipulation of the spin. In particular, MoTe₂ provides interesting effects arising from its (potential) Weyl semimetal properties: such as surface-state Fermi arcs, unusual spin-orbit torques and non-linear Hall effect. To understand the mechanisms behind these effects, it is important to get information on their spin-dependent band structure.

Here, we study the spin texture of few-layer MoTe₂ by electrical means, using the bilinear magnetoelectric resistance effect, which gives us quantitative information on the spin-dependent electronic structure of thin flakes as a function of temperature. We observe a sinusoidal behavior of the resistance, as expected by a Rashba-like spin-orbit coupling, with a change in sign of the amplitude under 150 K. Our studies provide evidence on the control of the spin texture in MoTe₂ thin flakes, opening new doors for the use of this material on controllable atomically-thin spintronic devices.

TUE 46

Electron-phonon coupling in doped single-wall carbon nanotubes

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Electron-phonon coupling plays a key role for understanding physical phenomena such as carrier transport and superconductivity [1]. The Fano-like line shape of vibrational resonance signals in the mid infrared, sheds light on the interactions of lattice vibrations with low-energy states of the electronic absorption continuum in doped semiconducting single-wall carbon nanotubes (s-SWNTs) [2,3].

Here, we present a systematic investigation of such Fano resonances in intrinsic and

doped polymer-wrapped monochiral s-SWNT thin-films. We observe distinct resonance signals for the Raman active D- and G-phonons, which acquire IR oscillator strength via coupling to the dipole-allowed Drude-like intraband continuum in doped s-SWNTs [2]. We also observe two IR-active bands in the 800 cm^{-1} range which are discussed in terms of the coherent superposition of coupled, harmonic oscillations.

[1] M. Lazzeri et al., Phys. Rev. B, 2006, 73(15), 155426

[2] K. H. Eckstein et al., J. Phys. Chem C, 2021, 125(10), 5700-5707

[3] U. Fano, Phys. Rev. 1961, 124, 1866-1878

TUE 47

Two-dimensional cuprate nanodetector with single telecom photon sensitivity at $T = 20\text{ K}$

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²Fakultät für Physik, Ludwig-Maximilians-Universität, München, Germany

³Institute of Physics, Faculty of Electrical Engineering and Information Technology (EIT 2), Universität der Bundeswehr München, Germany

⁴Catalan Institute of Nanoscience and Nanotechnology (ICN2), BIST and CSIC, Barcelona, Spain

⁵James Watt School of Engineering, University of Glasgow, UK

Superconducting single-photon detectors constitute a key enabling technology for quantum photonics, both in free-space and on-chip architectures. Still, the low critical temperature ($T_C \sim 5\text{ K}$) of the commercial films precludes their application in a wider range of fields. High-temperature superconductors, such as the cuprates, offer the prospect of detecting single photons at moderate cryogenic temperatures. Here, we report single-photon detection in exfoliated flakes of the 2D cuprate superconductor $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\epsilon}$ at a record temperature of 20 K for telecom wavelengths ($\lambda = 1550\text{ nm}$). We combine van der Waals fabrication techniques with novel non-destructive nanopatterning to define 2D cuprate nanowires. These nanowires exhibit sharp current-voltage characteristics and non-bolometric response up to 30 K. We achieve single and multi-photon detection regimes at 20 K tuning the bias conditions of the nanowire. Such detectors are prime candidates for next generation quantum photonics with relaxed cryogenic constraints.

[1] Luque Merino, R. et al, arXiv:2208.05044

[2] Seifert, P. et al, 2D Materials, 8, 035053 (2021)

TUE 48**Absolute quantification of sp^3 defects in carbon nanotubes by Raman spectroscopy**

Finn L. Sebastian¹, Nicolas F. Zorn¹, Simon Settele¹, Sebastian Lindenthal¹, Felix J. Berger¹, Christoph Bendel¹, Han Li², Benjamin Flavel², Jana Zaumseil¹

¹Institute for Physical Chemistry, Heidelberg University, Germany

²Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

The covalent functionalization of single-wall carbon nanotubes (SWCNTs) with luminescent sp^3 defects modifies their optical properties and boosts their photoluminescence quantum yields (PLQYs) by creation of red-shifted emission features in the near-infrared. Many synthetic routes for the selective introduction of sp^3 defects with distinct binding configurations are available, however, no convenient metric to precisely quantify their density on the SWCNT lattice exists. In general, the intensity of the D mode in Raman spectra of sp^2 -hybridized carbon materials serves as a relative measure of defects and disorder. For graphene, a quantitative relation between the density of defects and the ratio of the Raman D mode intensity to the G mode intensity (D/G ratio) is well-established but nothing similar exists for carbon nanotubes. Here, we report an absolute quantification method for sp^3 defects in semiconducting SWCNTs directly based on the integrated differential Raman D/G⁺ ratios and their correlation to defect densities extracted from PLQY measurements, corroborated by a statistical analysis of single-nanotube emission spectra at 4 K.

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08:30 – 09:30	TUTORIAL: R. Riberio, Palaiseau <i>Non-Identical Moiré Twins in Bilayer Graphene</i>
09:30 – 10:00	A. Jorio, Belo Horizonte <i>Homojunctions, Topological Points, Strain Solitons and Kohn Anomaly in Graphene Systems</i>
10:00 – 10:30	Coffee Break
10:30 – 11:00	K. Bolotin, Berlin <i>Generating and Exploring the Effects of Ultrastrong Electric Field in 2D Materials via Molecular Gating</i>
11:00 – 11:30	F. Alijani, Delft <i>Nonlinear and Noisy Dynamics of 2D Materials</i>
11:30 – 12:00	C. Draxel, Berlin <i>Level Alignment and Excitations at Heterointerfaces</i>
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	E. Gaufrès, Bordeaux <i>1D Heterostructures : Periodically Encoded Dipolar Chains based on BNNT Template</i>
19:00 – 19:30	B. Flavel, Karlsruhe <i>The Alignment of Single Wall Carbon Nanotubes by Filtration</i>
19:30 – 20:00	L. Cognet, Bordeaux <i>Super-Resolution Microscopy of Excitonic Photoluminescence in SWIR Emitting Single Wall Carbon Nanotubes</i>
20:00	Poster Session III

08:30**Non-identical moiré twins in bilayer graphene**Rebeca Ribeiro-Palau¹¹Center for Nanoscience and Nanotechnology, Palaiseau

The relative angular alignment between 2D layers of a van der Waals (vdW) heterostructure can dramatically alter its fundamental properties. A striking example is the recent observation of strongly correlated states and intrinsic superconductivity in twisted bilayer graphene. Another remarkable effect of angular layer alignment, predicted for certain vdW heterostructures, is the emergence of phases of matter with non-trivial topological properties, where charge carriers flow without dissipation, being protected against perturbations. In graphene aligned with boron nitride (BN), such a phase has been predicted, with topological protection linked not to the spin, as commonly observed, but rather to the valley degree of freedom.

The experimental observations of these topological valley currents has been largely put in question by theorist, results of numerical simulation and recent scanning SQUID results. In these, the observed non-local signal has been attributed mostly to localized states on the edge of graphene. In this talk, we will show how these two pictures are not incompatible and can be re-conciliated if we take the angular layer alignment into account.

09:30**Homojunctions, topological points, strain solitons and Kohn anomaly in graphene systems**Ado Jorio¹¹Physics, UFMG, Belo Horizonte, Brazil

Graphene studies using micro- and nano-Raman spectroscopies are reported here. The nano-Raman spectroscopy is implemented in the tip-enhanced Raman spectroscopy (TERS) configuration. By applying the tip-approach technique on single-layer graphene devices, we demonstrate variations in the phonon coherence length and group velocity for the optical phonons at the Γ point. Gate dependent micro-Raman experiments show unique electron-phonon coupling behavior at the magic angle [1,2]. With the nano-Raman, we were able to measure the depletion region in graphene homojunctions [3], and strain solitons and topological points generated by atomic reconstruction in twisted bi-layer graphene with rotation angles below 1 degree [4]. The results are rationalized by an atomistic model that enables evaluation of the local density of the electronic and vibrational states of the superlattices [1,4].

[1] A. C. Gadelha et al. Nano letters 22(15), 6069 (2022)

[2] T. C. Barbosa et al. 2D Materials 9(2), 025007 (2022)

[3] A. C. Gadelha et al. J. Phys. Chem. Lett. 12, 7625 (2021)

[4] A. C. Gadelha et al. Nature 590, 405 (2021)

10:30**Generating and exploring the effects of ultrastrong electric field in 2D materials via molecular gating**Kirill I. Bolotin¹¹FU Berlin

We consider a new type of heterostructure: a 2D material with donor molecules on one side and acceptor molecules on the other. The charge transfer between the molecules generates an electrical field inside the 2D material. We experimentally measure the field produced by this “molecular gating” and show that it reaches $> 4\text{V/m}$, the highest field measured in a solid-state device. We then explore the effect of this intense field. First, we demonstrate that the field suffices to modify and eventually completely close the bandgap in bilayer 2D semiconductors driving a semiconductor-to-metal transition. Second, we show that the field lifts degeneracies between excitons in semiconductor 2D bilayer and brings different excitons into resonance. Finally, we demonstrate new types of excitonic states that arise because of that.

11:00**Nonlinear and noisy dynamics of 2D materials**Farbod Alijani¹¹Precision and Microsystems Engineering, TU Delft, Delft

The advent of graphene, and the ability to fabricate single-atom thick membranes, have made it possible to reach the ultimate sensing capabilities that not so long ago were only dreamed of. But this revolutionary downscaling has been associated with severe constraints on the linear dynamic operation of these devices since signatures of nonlinearities already emerge at excitation amplitudes of only a few pN. In this talk, I will present theory and experiments for using nonlinear and noisy dynamics of 2D materials to sense the nanomechanical properties of ultrathin materials and detect very weak signals. By fitting experimental data with nonlinear models and relating nonlinear parameters to membrane mechanics, I first propose a contactless method for extracting material properties of 2D materials. I will then discuss the interrelation between mode coupling and nonlinear mechanical losses, and show how by engineering nonlinear damping mechanical frequency combs can be generated. Finally, I will discuss the use of noisy dynamics in 2D materials for detecting nanomechanical motion of micro-organisms, and show how this rich and complex dynamics can be used to detect antibiotic resistance

11:30**Level alignment and excitations at heterointerfaces**Claudia Draxl¹¹Physics Department and IRIS Adlershof, HU Berlin, Berlin

Most fascinating phenomena are observed in materials where various interactions happen on the same energy scale. Among them are organic-inorganic hybrid systems or interfaces between 2D materials. Another example is provided by combinations of polar and nonpolar building blocks where 2D electron gases (2DEG) form at their interface. For an *ab initio* description of their electronic excitations, all these materials are critical examples, being governed by the interplay between electron-electron interaction, electron-phonon coupling, electron-hole correlations, and potentially also spin-orbit coupling (SOC). A particular role is also played by the mutual dynamical screening of the interface constituents. With selected examples I will show how hybrid and charge transfer excitations can form at such interfaces, or how a 2DEG can be obtained and then manipulated by an electric field. I will also discuss the importance of forefront many-body methodology since density-functional theory (DFT) may well fail in predicting the level alignment and consequently optical and transport properties.

18:30**1D heterostructures : Periodically Encoded Dipolar Chains based on BNNT template**Etienne Gaufres¹¹Laboratoire Photonique Numérique et Nanosciences, Institut d'Optique, Université de Bordeaux, Talence, France

Single walled carbon nanotubes (SWCNTs) have been used as a 1D template for assembling various organic and inorganic compounds. In the context of fluorescent molecules assembly, it was unfortunately demonstrated that the nanotubes readily quench the dyes fluorescence.[1,2] As an alternative, boron nitride nanotubes (BNNTs) have been identified as a promising dielectric host for the design of fluorescent nano-hybrids.[3]

In this presentation we will first focus the polarization properties of the fluorescence from the 6Ts confined inside BNNT. We will show that the fluorescence from the 6T assembly is stable and strongly polarized with extinction ratios as high as 700. We will also demonstrate that this polarization property can be expanded in transparent thin films loaded with 6T@BNNTs.[4]

Finally, we will present the surprising capability of BNNTs to rearrange the confined dyes along the nanotube axis under mechanical stretching. We will show that this mechanism produces periodic luminescent chains of aligned molecules.[5]

[1] S Van Bezouw, ACS Nano 2018

[2] E Gaufres ACS Nano 2016

[3] C Allard et al, Adv. Mater. 2020

[4] A Badon, JB Marceau et al, Mat. Horiz. 2023

[5] JB Marceau, in prep.

19:00**The Alignment of Single Wall Carbon Nanotubes by Filtration**Benjamin Flavel¹¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe

Dead-end filtration on polyvinylpyrrolidone-coated polycarbonate track-etched membranes has proven to be an effective method to prepare macroscopically aligned thin films from solution-based single-wall carbon nanotubes (SWCNTs). However, the key question of what drives the SWCNTs to align in this process remains a matter of debate and the reported conditions required to achieve it are narrow. In this work, a custom microfluidic setup capable of precise control and measurement of the volume rate, trans-membrane pressure and the filtration resistance is used to follow SWCNT film formation. Conditions associated with the formation of SWCNT crystallites or their global alignment are identified and these are discussed in terms of membrane fouling and the interaction potential between the surface of the membrane and nanotubes. Furthermore, the role of SWCNT length and diameter on the alignment process is investigated and films with an area of $A=3.81 \text{ cm}^2$ and a thickness of 40 nm are prepared from two series of length sorted fractions comprised of small (0.78 nm) and large (1.4 nm) diameter SWCNTs. Finally, radially symmetric patterns are shown to be possible via hot embossing.

19:30**Super-Resolution Microscopy of excitonic photoluminescence in SWIR Emitting Single Wall Carbon Nanotubes**Laurent Cognet¹¹Institute of Optics, CNRS, University of Bordeaux, Bordeaux-Talence, France

Single-molecule super-resolution localization microscopy has established a new paradigm in optical imaging by providing super-resolution images, i.e., with a resolution much better than the diffraction limit. On the other hand, single-walled carbon nanotubes exhibit bright and stable excitonic photoluminescence in the SWIR, a wavelength range with great promise in quantum optics or bioimaging for example. At the same time, long wavelengths are for high resolution imaging and limit our capacity to directly study exciton localization or to reach high-resolution in imaging applications.

The application of concepts developed in super-resolution imaging to design and study the basic photophysics of carbon nanotubes or to design new nanoprobe thus represents an interesting opportunity. I will present our current efforts in this quest and their application to understand basic excitonic processes in carbon nanotubes, including direct visualization of excitonic localization (including after color center implantation), generation of ultrashort fluorescent nanotubes, or creation of optical molecular switches based on carbon nanotube nano-hybrids.

WED 1**Strain control of hybridization between dark and localized excitons in a 2D semiconductor**

Pablo Hernández López¹, Sebastian Heeg¹, Christoph Schattauer², Sviatoslav Kovalchuk³, Abhijeet Kumar³, Douglas J. Bock³, Jan N. Kirchhof³, Bianca Höfer³, Kyrylo Greben³, Denis Yagodkin³, Lukas Linhart², Florian Libisch², Kirill I. Bolotin³

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Mechanical strain is a powerful tuning knob for excitons, Coulomb-bound electron-hole complexes dominating optical properties of two-dimensional semiconductors. While the strain response of bright free excitons is broadly understood, the behaviour of dark free excitons (long-lived excitations that generally do not couple to light due to spin and momentum conservation) or localized excitons related to defects remains mostly unexplored. Here, we study the strain behaviour of these fragile many-body states on pristine suspended WSe₂ kept at cryogenic temperatures. We find that upon straining, dark and localized excitons in monolayer WSe₂ are brought into energetic resonance, forming a new hybrid state that inherits the properties of the constituent species. The characteristics of the hybridized state, including an order-of-magnitude enhanced light/matter coupling, avoided-crossing energy shifts, and strain tunability of many-body interactions, are all supported by first-principles calculations. The hybridized exciton reported here may play a critical role in the operation of single quantum emitters based on WSe₂.

Hernández López, P. et al. accepted in Nat. Comm.

WED 2**Determining the optical bandgap of graphene nanoribbons inside SWCNTs using optical absorption techniques**

Dido Denier van der Gon¹, Valeria Milotti¹, Claudia Berkman¹, Lukas Perner¹, Joselyn Benalcázar¹, Jorge Laranjeira², Manuel Melle-Franco², Thomas Pichler¹, Oliver Heckl¹, Paola Ayala¹,

¹University of Vienna, Austria

²University of Aveiro, Portugal

Semiconducting nano-structures such as single wall carbon nanotubes (SWCNTs) and graphene nanoribbons (GNRs) are becoming more and more important for nanoelectronics and other technologies but to use them to their full potential we need to be able to properly control and understand their electronic and optical properties. GNRs are 1-dimensional strips of graphene with a defined width and edge structure which determine their characteristics.

In order to synthesize these GNRs, we have used endohedral functionalization of SWCNTs by inserting the terrylene dye molecule. Like this, we have synthesized

ultra-narrow graphene armchair nanoribbons (5-AGNRs) inside SWCNTs. These 5-AGNRs are expected to have small but non-vanishing bandgaps making them ideal for electronic applications. The bandgap of this material inside SWCNTs has, to the best of our knowledge not been measured using optical characterization techniques. To better understand the properties of this 1d material we have performed Fourier Transform Spectroscopy (FTS) on a broad energy range. We have determined the GNR bandgap to be around 0.19 eV close to theoretical predictions of a bandgap around 100 meV for long GNRs.

WED 3

Bimetallic nanowires NiCo as a efficient catalyst support in ORR: structure and electrochemical properties.

Dariusz Łukowiec¹

¹Silesian University of Technology, Gliwice

Because of the great social and economic importance of the energy deficit problem, scientists are conducting a broad and very intensive search for new catalysts that are being evaluated for their performance. Current work is focused on the preparation of efficient and stable support for metal catalysts (Pd, Pt, Ru) working in fuel cells but requiring the use of smaller amounts of noble metals. The use of support in the form of nanowires (1D) can contribute to faster diffusion through liquid, reduction of surface energy (better control over agglomeration and solubility), and consequently improve electron transport and optimize the use of the noble metal. The second thing worth noting is the oxophilic nature of Ni and Co which increases the tolerance to poisoning of the noble metal by CO and thus increases its catalytic efficiency. Different supports in the form of NiCo nanowires with changing ratio of metals (5:5, 3:7, 1:9, 7:3, 9:1) with deposited Pd or Pt were synthesized. Herein, the structure and morphology of obtained nanocomposites was studied in detail. Cyclic voltammetry tests demonstrate that the obtained materials is a promising catalyst towards oxygen reduction reactions.

WED 4

Modulation of Far-Infrared Phonon Polaritons in AlAs/GaAs Heterostructures via Photoinjection of Charge Carriers

Giulia Carini¹, Nazmul Alam², Martin Wolf¹, Joshua D. Caldwell³, Stephanie Law², Alexander Paarmann¹

¹Fritz Haber Institute, Berlin

²University of Delaware

³Vanderbilt University

In the past decade, significant efforts have been made to investigate surface phonon polaritons (SPhPs), quasiparticles stemming from the hybridization of phonon resonances with infrared light on the interface of polar crystals. In particular, polar dielectric heterostructures enabled thickness-dependent strong coupling between

the phonon polaritonic modes emerging in the reststrahlen bands (RBs) of the different layers[1]. Furthermore, active modulation of the SPhP resonances via photo-injection of free charge carriers allowed hybridization with the photo-induced plasmons[2]. In our contribution, we make use of photodoping in AIAs/GaAs heterostructures, to switch between phonon polaritons and plasmon-phonon coupled polaritons. We observe photo-induced hybridization between the AIAs-thin film's Epsilon-Near-Zero mode and the upper branch of the plasmon-phonon coupled mode of the photo-excited GaAs substrate. The ability to control the optical response of III-V semiconductor heterostructures via photodoping paves the way for interesting far-infrared nanophotonic devices.

1. Passler, et al., Nano Letters 18, 4285 (2018).
2. Dunkelberger, et al., Nature Photonics 12, 50 (2018).

WED 5

Sectioning of Two-Dimensional Materials: An Innovative Approach for Scalable Fabrication of Nano-fluidic Channels

Raj Kumar Gogoi¹, Ankit Bhardwaj¹, Radha Boya¹

¹Condensed Matter Physics Group, The University of Manchester, UK

Confined channels made from 2D materials have emerged as unique fluidic platforms to study the unusual physics of ultra-confined space. The major bottleneck in the fabrication process of such channels is either low-throughput or compromise with the high precision of channel dimensions. To overcome these hurdles, we developed an innovative method using ultramicrotomy by embedding the desired 2D channels in a suitable resin followed by slicing it into ultra-thin membranes. Membranes prepared by this method are used to study ion-transport through the free space between the interlayers of layered materials preserving their natural occurrence. The method also enables efficient and robust use of in-plane fluidic channels in reconstructed laminate membranes, with short channel lengths and increased mechanical stability. Moreover, with this method, thousands of 2D channels can be prepared from a single pre-made slit-shaped 2D channel without any compromise in their precise dimensions. The slit-shaped 2D channels are ideal candidates to explore the unexpected fluid-transport phenomena, but fabricating a single device requires time-consuming and highly sophisticated fabrication techniques.

WED 6

Temperature dependent intercalation of molten 1-hexadecanol into Brodie graphite oxide

Andreas Nordenström¹, Artem Iakunkov¹, Nicolas Boulanger¹, Gui Li¹, Christoph Hennig^{2,3}, Igor Baburin⁴, Mads Jørgensen^{5,6}, Innokenty Kantor^{6,7}, Alexandr Talyzin¹

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⁴Theoretische Chemie, Technische Universität Dresden, Germany⁵Department of Chemistry and iNANO, Aarhus University, Aarhus, Denmark⁶MAX-IV Laboratory, Lund University, Lund, Sweden⁷Department of Physics, The Technical University of Denmark, Lyngby, Denmark

Intercalation of 1-hexadecanol (C16) into the structure of multi-layered graphene oxide was studied. Brodie graphite oxide (BGO) immersed in excess of liquid C16 just above the melting point shows expansion of c-unit cell parameter from $\sim 6 \text{ \AA}$ to $\sim 48.76 \text{ \AA}$, forming a structure with two densely packed layers of C16 molecules in a perpendicular orientation relative to the graphene oxide planes (α -phase). Heating of the BGO-C16 α -phase in excess of C16 melt results in reversible phase transition into β -phase at 336 - 342 K. The β -phase shows much smaller c-unit cell parameter 29.83 \AA and change in orientation of alcohol molecules, from perpendicular to parallel relative to GO planes. Cooling of the β -phase in absence of C16 melt resulted in the formation of a new (γ) phase with inter-layer distance of 26.5 \AA . Surprisingly rich variety of structures revealed in the BGO-C16 system provides opportunities to create materials with precisely controlled GO inter-layer distance.

WED 7**Metal grid-type transparent conductive electrode fabricated by laser-induced selective metal deposition**

Karolis Ratautas¹, Modestas Sadauskas¹, Evaldas Kvietkauskas¹, Šarūnas Mickus¹, Gediminas Račiukaitis¹

¹Laser technologies, Center for Physical Sciences and Technology, Vilnius

The current transparent conductive film market is dominated by expensive and fragile Indium-tin oxide electrodes, also known as ITO. However, ITO made from the rare metal Indium. It results in a high-cost and brittle technology. There is a huge demand for alternative technologies to the ITO transparent electrode. New materials like carbon nanotubes, silver nanowires are still in the research stage and expensive as well. Another alternative could be a metallic mesh with metal wires less than 5 micrometers in diameter to be invisible but still electro-conductive. We propose our Selective Surface Activation Induced by Laser (SSAIL) technology which utilizes laser writing and electroless copper plating. SSAIL technology allows forming electrically conductive circuit tracks on various dielectric surfaces. The method technology can be applied on transparent dielectric materials – glass, fused silica or transparent polymers like Polyethylene terephthalate (PET). In this study we will present metal mesh formation on transparent and flexible PET.

WED 8 **\AA -scale ion transport: beyond steric selectivity and dehydration**

Goutham Solleti^{1,2}, Ashok Keerthi^{2,3}, Abdulghani Ismail^{1,2}, Ankit Bhardwaj^{1,2}, Hossein Jalali⁴, Yi You^{1,2}, Yiheng Li⁵, Nassim Hassani⁴, Haoke Peng⁵, Fengchao Wang⁵,

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⁴Department of Physics, Shahid Rajaee University, Lavizan, Tehran, Iran

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⁶Department of Physics, University of Antwerp, Belgium

Ion-selective biological channels play a vital role in physiological processes, which necessitates their use in many technologies. While biological channels can efficiently separate same-charge ions with similar hydration shells, it remains a challenge to mimic such exquisite selectivity using artificial solid-state channels. Such exceptional performance of the biological channels is attributable to their unique architecture which is close to the size of the ion and dehydration mechanism. There is a need to rationalize the design of artificial channels to make them as competent as biological channels, which in turn requires understanding of why and how such selectivity occurs. Here we show that the studied 2D Å-scale capillaries can distinguish between same-charge ions with similar hydrated diameters. The selectivity is attributed to the different positions of ions within the layered structure of nanoconfined water, which in turn depends on the ion-core size and it differs for anions and cations. The revealed mechanism points at the possibility of ion separation beyond the simple steric sieving.

WED 9

Twisted bilayer antimonene

Stefan Wolff¹, Roland Gillen¹, Janina Maultzsch¹

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Antimony has proven to be a promising candidate for two-dimensional (2D) mono-elemental materials. In bulk form, it is a layered crystal comprising sheets of antimony atoms arranged in a hexagonal buckled honeycomb lattice called antimonene. Other than many other 2D materials, the interlayer bonds in few-layer antimonene show partially covalent character. Due to this covalent character, changes of the local stacking order via rotation and translation may lead to new interesting features and properties of the material. Density functional theory (DFT) is used to simulate twisted bilayer antimonene structures with different rotation angles and to investigate their physical properties. Our analysis of the charge density shows how the overlap of atomic orbitals in certain areas changes, depending on the proximity of atoms from neighboring layers. A comprehensive understanding of how the properties of twisted bilayer antimonene are modified compared to naturally stacked bilayer antimonene may lead to future applications making use of well-constructed, favorable stacking orders in layered materials.

WED 10**Noble gas clusters in a graphene sandwich**

Manuel Längle^{1,2}, Christian Pesenhofer¹, Kenichiro Mizohata³, Alberto Trentino^{1,2}, Clemens Mangler¹, Kimmo Mustonen¹, Harriet E. Åhlgren¹, Jani Kotakoski¹

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Due to their chemical inertness, noble gases are in gas phase under normal conditions. When trapped between two graphene sheets, however, the exerted pressure presses noble gas atoms together leading to the formation of clusters [1]. We create such clusters by implanting singly charged low energy ions into suspended bi- and double layer graphene, which allows their direct imaging through (scanning) transmission electron microscopy inside the graphene sandwich [2]. While all small clusters (up to at least 14 atoms) remain solid, larger clusters can exhibit either solid- or liquid-like structures depending on their size, chemical element and possibly local microscopic environment.

[1] Längle, M., Mizohata, K., Åhlgren, E., Trentino, A., Mustonen, K., & Kotakoski, J., *Microscopy and Microanalysis*, 26(S2), 1086-1089

[2] Rasim Mirzayev, Kimmo Mustonen, Mohammad R. A. Monazam, Andreas Mittelberger, Timothy J. Pennycook, Clemens Mangler, Toma Susi, Jani Kotakoski, Jannik C. Meyer, *Science Advances* 3, e1700176 (2017)

WED 11**Combined electron excitation and knock-on damage in monolayer MoS₂**

Carsten Speckmann^{1,2}, Julia Lang¹, Jacob Madsen¹, Clemens Mangler¹, Toma Susi¹, Jani Kotakoski¹

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The advent of aberration-corrected (scanning) transmission electron microscopy and 2D materials over a decade ago made it possible to quantify electron irradiation-induced damage at the atomic scale [1]. This has led to an improved understanding of the interaction of energetic electrons with target atoms, while also opening a pathway for controlled defect creation. It was shown that damage in graphene can be solely explained by knock-on damage due to elastic scattering. However, this does not hold for semiconductors such as MoS₂ for which inelastic scattering also plays a role [2,3]. Here, we measured the displacement cross section for sulfur atoms in MoS₂ with energies between 55-90 keV, and compared the results with the literature [2,3]. Our data reveals that the displacement process can occur from the ground state, or with a single or multiple excitations, caused by the same electron. These results bring us closer to a complete description of electron-irradiation dam-

age in a semiconducting material.

[1] T. Susi et al., Nat. Rev. Phys. 1, 397 (2019)

[2] S. Kretschmer et al., Nano Lett. 20, 2865 (2020)

[3] A. Yoshimura et al., Nanoscale, (2022). DOI: 10.1039/D2NR01018F

WED 12

Optical properties of plasmonic supercrystals

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Plasmonic supercrystals are novel materials formed by metallic nanoparticles arranged in a face-centered cubic lattice (Schulz 2020). In these crystals, light is confined into hotspots between nanoparticles, which enhances light matter interaction and leads to plasmon-polaritons in the deep-strong light-matter coupling regime (Mueller 2020). This makes this material the first system to exhibit coupling between light and a continuum of states in the deep-strong regime at ambient conditions. In this work we further explore the optical properties of plasmonic supercrystals, this time on top of a gold substrate and for the first time on (111) and (100) crystal surfaces. To do this we perform reflection as well as near field measurements and compare our results with FDTD simulations.

WED 13

Strain-induced transitions between different Moiré-morphologies in twisted 2D heterostructures

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2D materials layered on top of each other form Moiré-patterns, which host a large variety of exciting physical phenomena e.g.: Mott-insulation, flat bands, superconductivity. However, the behavior of the surface topography stemming from the out-of-plane deformations of such patterns is still a largely unexplored field and lacking a comprehensive theoretical description, even so, they can highly influence the properties of such systems. Here we found by the systematic lattice relaxation of a vast number (~8000) of different Moiré-superstructures using Classical Molecular Simulations, that under different homogenous biaxial strain conditions three types of topographic Moiré-phases can be realized. We demonstrated, that by tuning the twist angle, phase transitions can be induced between them, giving rise to more complex behavior of superlattice corrugation as a function of twist angle. One of the surprising findings is the emergence of corrugation-free morphologies located on the phase boundaries, which can be present even under mild strains and at ar-

bitrarily small twist angles. Possible experimental realizations are revealed by STM investigations of the graphene/graphite system

WED 14

2D Materials at the atomic scale: visualization and design

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The realization of novel TMD-based devices relies heavily on understanding the relation between structural and electrical properties at the nanoscale. The ultimate goal is that of crafting TMD nanostructures in a way that makes possible the tailored control of their properties. Here, recent studies illustrating novel fabrication approaches of TMD nanostructures based on combining top-down and bottom-up methods will be presented. These allow to control the resulting geometries and material combinations, making possible the realization of novel functionalities such as metallic edge states arising in MoS₂ nanowalls and nanowires, enhanced non-linear response in vertically-oriented MoS₂ nanostructures, and surface and edge plasmons in WS₂ nanostructures. I will emphasize the crucial role that cutting-edge transmission electron microscopy techniques play in these studies, together with recent developments where machine learning techniques are used to realize a spatially-resolved determination of the bandgap and dielectric function in nanostructured TMD materials.

WED 15

Measuring the bolometric response of superconducting magic-angle twisted bilayer graphene

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To date the most sensitive detectors for electro-magnetic radiation are based on superconducting materials and exploit local photo-induced heating across their strongly temperature dependent superconducting transition. The allegedly unconventional superconducting phase of magic-angle twisted bilayer graphene (MATBG) has been predicted to possess extraordinary thermal properties, as it is formed from a highly

diluted electron ensemble with both a record-low carrier density $n \sim 10^{11} \text{ cm}^{-2}$ and electronic heat capacity $C_e < 100k_B$. While these attributes position MATBG as a ground-breaking material platform for revolutionary bolometric applications, these thermal properties have so far not been experimentally shown. In this study, we measure the bolometric response of MATBG and extract from it the thermal conductance (G_{th}) in the superconducting state which in the low temperature limit is consistent with a power law dependence, as expected for nodal superconductors. Our work lays the foundation for future thermal transport studies on this system.

WED 16

Chemical modification of carbon nanostructures with enhanced qualities for fabrics performing under critical operating conditions

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The introduction of carbon nanostructures and 2D nanomaterials in everyday life applications is essential to fully exploit their novel characteristics. Chemical modification allows 2D nanomaterials to be used as carriers of customized properties and counterparts to fabric fibers.[1] So, we strategically modified carbon nanostructures to give them wanted properties, i.e. with Ag nanoparticles for antibacterial use, with triazine for UV resistance and with melamine for flame retardancy, for their subsequent physisorption onto Kevlar, Nomex and VAR fibers. Samples were tested for limited flame spread and blocking ultraviolet radiation with excellent results, while their antibacterial activity was verified[2]. This work will bridge the gap between industry and real life applications.

[1] I. K. Sideri, N. Tagmatarchis, Mater. Horiz.2021, 8, 3187-3200.

[2] Manuscript in preparation.

WED 17

Tunable excitons in bilayer graphene for on-chip infrared spectroscopy

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In AB-stacked bilayer graphene (BLG), the optical absorption spectrum is dominated by excitonic resonances, which can be tuned by an out-of-plane electric field in a dual-gated field effect transistor device configuration. Firstly, I will show the basic exciton properties by using an FTIR-photocurrent spectroscopy technique,

which feature a narrow linewidth and a peak infrared absorption of more than 40%. Then I will demonstrate the concept of on-chip spectroscopy using these graphene devices as tunable infrared detectors. By electrically scanning the exciton resonance across the infrared spectral range, sharp absorption features corresponding to molecular fingerprints can be readily resolved in both the DC detection mode and AC-modulated detection mode. These on-chip spectrometers avoid conventional grating-based and FTIR spectrometers—opening up new routes for infrared detection and spectroscopy.

WED 18

Hexagonal hybrid bismuthene by molecular interface engineering

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In this contribution, we present a purely chemical approach towards a new two-dimensional pnictogen: a sandwiched, covalently functionalized bismuth/bismuthene hybrid. The colloidal synthesis is based on a light-catalyzed redox reaction of the Bi (III) precursor bismuthneodecanoate and dodecanethiol, leading to the crystallisation of single-crystalline bismuth hexagons, encapsulated in sulfur functionalized bismuthene capping layers. Due to the covalent functionalization of the terminating planes, Bi atoms arrange as flat hexagons with a calculated in-plane lattice parameter of 0.75 nm (vs. 0.45 nm for rhombohedral Bi). The graphene-like structure leads to a metallic behaviour of the terminating layers, as evident from rt single-particle transport measurements. We characterized the complex new compound by TEM, XRD, XPS, spectroscopy, electrical transport and ab initio calculations. The obtained technological platform will enable the use of this pnictogen for applications ranging from medicine, chemistry and probably even quantum computing. The spin orbit coupling of the heaviest stable chemical element is expected to play a decisive role in future quantum devices.

WED 19

Covalent Laser Patterning of Graphene

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Covalently patterned Janus-functionalized graphene featuring a spatially defined asymmetric bifacial addend binding motif remains a challenging synthetic target. Here, a facile and universal laser writing approach for a one-step covalent Janus patterning of graphene is reported, leading to the formation of up to now elusive graphene architectures, solely consisting of antaratopically functionalized superlattices. The structurally defined covalent functionalization procedure is based on laser-triggered concurrent photolysis of two different photosensitizers situated on both sides of the graphene plane, generating radicals and subsequent addend binding in the laser-irradiated areas only. Careful structure analysis was performed by Raman spectroscopy and Kelvin probe force microscopy. In terms of the advantages of our newly established concept, including a simple/easy-to-operate patterning procedure, arbitrary pattern availability, and a high degree of addend binding, an easy access to tailor-designed Janus-functionalized graphene devices with spatially resolved functional entities can be envisaged.

WED 20

Direct Growth of Holey Graphene by Low-Pressure Chemical Vapor Deposition using Non-Halogenated Precursors

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Graphene, a two-dimensional material, has extraordinary physical properties, which make it a promising candidate for future nanoelectronics. However, its near-zero bandgap restricts its application in optoelectronics. A bandgap in graphene can be readily introduced by external manipulators such as electric field, doping, chemical treatment, etc., or by producing defects/holes. Still, these approaches are not feasible for large-scale operation/production of graphene owing to the complexity of manipulation. To date, numerous top-down and bottom-up tactics have been implemented to yield holey graphene (hG), but they necessitate lithography, making growth a multi-step process. Herein, we utilize a cost-effective method for the direct growth of hG using non-halogenated aromatic precursor *p*-terphenyl in low-pressure chemical vapor deposition (LPCVD). Quantifying holes/defects via Raman spectroscopy of our preliminary samples calculates the point defect distance (L_D) up to ~ 7 nm. Further optimization of CVD process parameters would produce hG with L_D up to ~ 1 nm, resulting in a gapped semiconductor.

WED 21

Strongly Anharmonic Octahedral Tilting in 2D Hybrid Halide Perovskites

Matan Menahem¹, Zhenbang Dai², Sigalit Aharon¹, Rituraj Sharma¹, Maor Asher¹, Yael Diskin-Posner³, Roman Korobko¹, Andrew M. Rapp², Omer Yaffe¹

¹Chemical and Biological Physics, Weizmann Institute of Science

²Chemistry, University of Pennsylvania

³Chemical Research Support, Weizmann Institute of Science

Two-dimensional hybrid halide perovskites (2D HHPs) intrigue material scientists from both scientific and technological points of view. They exhibit pronounced and easily tunable excitonic properties, strongly coupled to thermal fluctuations. In this presentation, I will show a study of the structural dynamics of the prototypical 2D HHP $(CH_3(CH_2)_3NH_3)_2PbI_4$ (BAPF) by comparing it to its 3D counterpart $CH_3NH_3PbI_3$ (MAPF) and aromatic counterpart $(C_6H_5 - (CH_2)_2NH_3)_2PbI_4$. Using temperature-dependent XRD, polarization-orientation Raman scattering, and DFPT calculations we show the strong similarities between the structural dynamics of 2D HHPs and their 3D counterparts. By doing so, we uncover the mechanism of the order-disorder phase transition in BAPF, which preserves the crystal symmetry due to a skewed double-well potential, biased by the hydrogen bonding between the organic amine and the inorganic scaffold. The phase transition involves unlocking an anharmonic octahedral tilting motion which increases the anharmonicity of the lattice dynamics and decreases other phonons' lifetime. These anharmonic fluctuations are essential for technological applications.

WED 22

Position-Controlled Fabrication of Vertically-Aligned Mo/MoS₂ Core-Shell Nanopillar Arrays for Nanophotonic applications

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The fabrication of 2D materials, such as transition metal dichalcogenides (TMDs), in geometries beyond the standard platelet-like configuration exhibits significant challenges, severely limiting the range of available morphologies. These challenges arise due to the anisotropic character of their bonding van der Waals out-of-plane while covalent in-plane. Moreover, industrial applications based on TMDs nanostructures with non-standard morphologies require full control on the size, morphology and position on the wafer scale. Such a precise control remains an open problem of which solution would lead to the opening of novel directions in terms of optoelectronic applications. Here, we report on a novel strategy to fabricate position-controlled Mo/MoS₂ core-shell nanopillars (NPs). Transmission electron microscopy analysis reveals the core/shell nature of the NPs. We demonstrate that individual Mo/MoS₂ NPs exhibit significant nonlinear optical processes driven by the MoS₂ shell, realising a precise localisation of the nonlinear signal. Our results represent an important step towards realising 1D TMD-based nanostructures as building blocks of a new generation of nanophotonic devices.

WED 23

Photo-physical Properties of Graphene Quantum Dots on Perovskite Substrates.

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Graphene quantum dots (GQDs) are a promising platform for building quantum light emitters. We have for instance shown that single GQDs are stable and bright single photon emitters [1]. Recently, the importance of vibration in their light emission process has been shown [2,3]. In the perspective of exploiting the outstanding properties of GQDs, a path to be explored is to couple them with other active materials. In this context, lead-halide hybrid perovskites are a family of semiconductors holding great promises. In the present work, we will first present the photo-physical properties of new GQDs structures showing a high solubility and fluorescence quantum yield up to 94% [4]. Then we will report on a study of the coupling of these GQDs to micrometer-thick methylammonium lead bromide perovskite single crystals down to the single molecule.

[1] S. Zhao *et al.*, Nature Communications, 9, 3470 (2018)

[2] T. Liu *et al.*, Nanoscale, 14, 3826 – 3833 (2022)

[3] T. Liu *et al.*, Journal of Chemical Physics 156, 104302 (2022)

[4] D. Medina Lopez *et al.* In preparation

WED 24

Second- and third-order optical susceptibilities across excitons states in 2D monolayer transition metal dichalcogenides

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Semiconducting transition metal dichalcogenides have significant nonlinear optical effects. In this work, we have used second-harmonic generation and the four-wave

mixing spectroscopy in resonance with the excitons in MoS₂, MoSe₂, and WS₂ monolayers to characterize the nonlinear optical properties of these materials. We show that trions and excitons are responsible for enhancing the nonlinear optical response and determine the exciton and trion energies by comparing them with the photoluminescence spectra. Moreover, we extract the second- and third-order optical sheet susceptibility (χ^2 and χ^3) across exciton energies and compare them with values found in the literature. We also demonstrate the ability to generate different nonlinear effects in a wide spectral range in the visible region for monolayer MoS₂, opening the possibility of using two-dimensional materials for nonlinear optoelectronic and photonic applications.

WED 25

Local Raman spectroscopic fingerprints of MoS₂-Au interactions

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Metal-mediated exfoliation of TMDCs has recently attracted considerable interest due to high yields of large size monolayer flakes [1]. The van der Waals interaction between metals and TMDCs enables the exfoliation of large size monolayers but also alters their properties due to strain and charge doping. An in-depth study of the strain and charge doping fingerprints of the strong interaction between monolayer MoS₂ and Au will be presented [2]. The interaction with different types of Au substrates was studied with AFM, Kelvin probe force microscopy, micro- and tip enhanced Raman spectroscopy (TERS). The heterogeneity of the MoS₂-Au interaction, depends on the type of Au substrate, which was investigated with nanoscale TERS and correlation analysis of micro Raman spectroscopy mappings. The strong MoS₂-Au interaction is also evidenced by the appearance of additional, otherwise forbidden Raman modes, and it can be modulated by the force set-point of the TERS tip [3].

[1] ACS nano, 12, no. 10 (2018): 10463-10472.

[2] The journal of physical chemistry letters, 11, no. 15 (2020): 6112-6118.

[3] Physical Review B, 105, no. 19 (2022): 195413.

WED 26

Towards Patterned Functionalization of Graphene and Black Phosphorus Heterostructures

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The poster will be about the fabrication and the covalent, laser-induced functional-

ization of a graphene and black phosphorus heterostructure, as well as a novel formation of a stacked heterostructure including graphene, black phosphorus and organic PDIs.

WED 27

Mapping quantum Hall edge states in graphene by scanning tunneling microscopy

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Quantum Hall edge states are the paradigmatic example of the bulk-boundary correspondence. They are prone to intricate reconstructions calling for their detailed investigation at high spatial resolution. Here, we map quantum Hall edge states of monolayer graphene at a magnetic field of 7 T with scanning tunneling microscopy. Our graphene sample features a gate-tunable lateral interface between areas of different filling factor. We compare the results with detailed tight-binding calculations quantitatively accounting for the perturbation by the tip of the microscope. We find that an adequate choice of gate voltage allows for mapping the edge state pattern with little perturbation. We observe extended compressible regions, the antinodal structure of edge states that is slightly influenced by the potential gradient at the interface and their meandering along the lateral interface.

WED 28

The Cryogenic Quantum Twisting Microscope

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Measuring the energy-momentum dispersion relation in quantum materials can provide key insights into their strongly correlated electronic phenomena. We have recently demonstrated a new type of a scanning probe microscope – the Quantum Twisting Microscope (QTM) – capable of measuring electrons in momentum space in a similar way to the way a scanning tunneling microscope (STM) measures electrons in real-space. The QTM is based on a van-der-Waals (vdW) heterostructure on a tip, which, when brought into contact with another vdW sample, allows electrons to tunnel into it at many locations simultaneously, and quantum coherently. This makes the QTM tip a scanning electronic interferometer. With an extra twist degree of freedom, this microscope becomes a momentum-resolving local scanning probe.

The first version of our microscope operated at room temperature, and already there demonstrated quantum coherence at its tip, and the ability to image the dispersions of monolayer and twisted bilayer graphene. Yet, even more exciting physics can emerge if the QTM could be generalized to cryogenic temperatures. We will present our advances in cryo-QTM momentum-resolved imaging.

WED 29

Raman and photoluminescence studies on twisted bilayer CVD-grown MoS₂

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Twisting two monolayers of MoS₂ on top of each other gives a new tuning parameter to the system, namely the twist angle. Depending on the twist angle we observe characteristic optical features with Raman and photoluminescence spectroscopy such as the appearance of moiré phonon modes and energy shifts of the excitonic transitions. Chemical vapor deposition (CVD) was used to produce clearly separated, triangular shaped MoS₂ monolayers. Using such CVD-grown monolayers, twisted bilayers are manufactured with twist angles between 0° and 60°. Here the fabrication of such twisted bilayers and their optical features shall be presented.

WED 30

Exposing spin states at zigzag edges of armchair graphene nanoribbon

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The zigzag edges of arm-chair graphene nanoribbon (GNR) offer unique advantages such as selective site functionalization, quantum magnetism and to tune the bonding of ribbon to external electrical leads. In the pristine form, these edges are expected to be spin active thus naturally giving a nontrivial topological character to the ribbon without the need for elaborate chemical modifications. However, due to its high reactivity, the edges are passivated by atom abstraction and radical recombination reactions which in turn destroy their magnetic properties. To revive edge magnetism and explore the topological properties there is a need for a non-invasive bottom-up method that preserves the structural integrity and protect spin states from interacting with microenvironment. In this work we describe a facial method for addressing these issues in addition to decoupling the physisorbed nanoribbon from the underlying substrate.

WED 31**Structural and chemical changes in a Si nanoparticle-based anode for LIBs during the first (de)lithiation cycle studied by in situ Raman spectroelectrochemistry**

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Anodes prepared from Si nanoparticles (10 nm) mixed into a conductive carbon-based matrix for Li-ion batteries were studied by in situ Raman spectroelectrochemistry, which gives information on the crystal lattice changes and possible degradation / amorphization of Si nanocrystals, as well as the solid electrolyte interphase (SEI) layer formation on the electrode surface within the charge/discharge cycles. The shift of the first-order Raman peak of Si at 521 cm⁻¹ which is assigned to crystalline silicon is related to the stress evolution in nanoparticles caused by the (de)lithiation (tensile-to-compressive transition) in Si nanoparticles and the native oxide on their surface. Additionally, the detailed in situ Raman measurement of the first lithiation cycle allowed us to detect the decomposition of the electrolyte (LiPF₆ in EC/DMC) associated with SEI layer formation. A decrease in the intensity of the Raman C=O and C-O vibrational modes in the region between 700–1050 cm⁻¹ of EC/DMC was observed at reduction potentials of 0.8 V and 0.3 V vs. Li/Li⁺.

WED 32**Electrical tuning of moiré excitons in MoSe₂ bilayers**

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¹Physics, Chalmers University of Technology, Göteborg

²Physics, Philipps-Universität Marburg, Marburg

Recent advances in the field of vertically stacked 2D materials have revealed a rich exciton landscape. In particular, it has been demonstrated that out-of-plane electrical fields can be used to tune the spectral position of spatially separated interlayer excitons. Other studies have shown that there is a strong hybridization of exciton states, resulting from the mixing of electronic states in both layers. However, the connection between the twist-angle dependent hybridization and field-induced energy shifts has remained in the dark. Here, we investigate on a microscopic footing the interplay of electrical and twist-angle tuning of moiré excitons in MoSe₂ homobilayers. We reveal distinct energy regions in PL spectra that are clearly dominated by either intralayer or interlayer excitons, or even dark excitons. Consequently, we predict twist-angle-dependent critical electrical fields at which the material is being transformed from a direct into an indirect semiconductor. Our work provides new microscopic insights into experimentally accessible knobs to significantly tune the moiré exciton physics in atomically thin nanomaterials.

WED 33**Local strain and interaction in TMDC heterobilayers**Alvaro Rodriguez^{1,3}, Javier Varillas^{1,2}, Martin Kalbáč¹, Otakar Frank¹¹J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic²Institute of Thermomechanics, Prague, Czech Republic³ICMM-CSIC, Madrid, Spain

Van der Waals heterostructures based on TMDCs have recently attracted tremendous interest due to their exotic excitonic features, e.g. the presence of interlayer or Moiré excitons. Lattice reconstruction leads to complex strain patterns, which also aid in confinement of quasiparticles. SPM methods are commonly used for their characterization; however, the information they can provide is very limited. In the present work, we show distinct spectral fingerprints, both on the micro- and nanometer scales, of these heterostructures. MicroRaman spectroscopy, together with molecular dynamics simulations was used to reveal the presence of complex strains in reconstructed Moiré superlattices of TMDC heterobilayers. Depending on the twist angle, varying levels and contributions of biaxial, uniaxial, and shear strains determine the resulting shift and shape of the Raman peaks. Apart from the periodic strain distribution, highly localized deformation takes place in ubiquitous nanobubbles and blisters forming due to the trapped contamination between the layers, as evidenced by tip-enhanced PL, which is also used to trace the absence of interlayer exciton emission from such features.

WED 34**Sealing of single-walled carbon nanotubes encapsulating water molecules**Ryotaro Kaneda¹, Koki Kozaki¹, Shu Sato¹, Keigo Otsuka¹, Shigeo Maruyama¹, Shohei Chiashi¹¹Department of Mechanical Engineering, The University of Tokyo, Tokyo

Single-walled carbon nanotube (SWCNT) is a nanomaterial with a hollow structure. Water molecule encapsulation into SWCNT has been investigated by several optical analysis such as Raman scattering and photoluminescence. Although the chirality that can be detected by these methods is limited, Rayleigh scattering spectroscopy can measure SWCNTs of all chirality. There are no reports about sealing the SWCNT encapsulating water molecules. In this study, we observed water encapsulation in opened SWCNT by Rayleigh scattering spectroscopy and performed opening and closing SWCNT by a pulse laser.

After opening, the peak energy red-shifted in water vapor and no red-shift was observed in vacuum. The red shift was caused by water molecule encapsulation and the water molecule went out when the SWCNT were in vacuum. Pulse laser irradiation with higher power density in water vapor was performed to close the end of the SWCNT. The red-shift was observed even in vacuum. This suggests that the pulse laser irradiation with higher power density caused the partially melting of SiO₂ layer and sealing the open-end of SWCNT.

In conclusion, we succeeded in sealing the SWCNT encapsulating water molecules.

WED 35

C-WAVE™ a widely tunable laser like source for resonant Tip-Enhanced Raman Spectroscopy

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Nanomaterials and in particular carbon nanotubes (CNTs) exhibit interesting optical, electronic and vibronic properties. Since these CNTs typically are present as an ensemble, techniques need to be employed to overcome the influence of inhomogeneous broadening of the underlying transitions and to study individual CNTs. Tip enhanced resonant Raman Spectroscopy (TERS) which is derived from atomic force microscopy enables to gather spectroscopic information from individual CNTs with the help of an optical near field tailored by a nanoscale tip. As the Raman signals of individual CNTs are too weak for detection, the authors [J. Phys. Chem C 2018, 122, 28273-28279] used the C-WAVE™ tunable optical parametric oscillator to perform resonant excitation. The unique wavelength coverage of the C-WAVE™ from 450 nm to 750 nm in the visible wavelength range and 0.9 - 3.5 μm in the near-infrared spectrum provides access to a variety of Raman active transitions accompanied by excellent beam-pointing stability.

WED 36

Negative exciton polarization by trion-trion annihilation in encapsulated MoSe₂ monolayers

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We investigate the carrier dynamics in encapsulated, high-quality MoSe₂ monolayers with ultrafast pump probe, cw and pulsed-excitation photoluminescence (PL) measurements.

In transient reflectivity pump-probe experiments, we find that resonant excitation of trions leads to a long-lived occupation and negative polarization of the neutral A exciton. This is surprising, since the trion is at lower energy than the neutral A exciton. A power series with pulsed as well as cw illumination reveals a quadratic power law for low excitation intensities but saturates at higher excitation intensities. This strengthens our hypothesis that a trion-trion annihilation process is responsible for the generation of neutral A excitons.

Contrary to an intuitive understanding, we find a negative valley polarization of the so generated neutral excitons. Using a pulsed laser for trion pumping, we achieve a negative polarization of up to 60%. This is by about an order of magnitude larger than what is typically reached as positive polarizations in PL experiments at near-resonant pumping.

WED 37**New local pseudopotential for wave packet dynamical calculations for multi-layer carbon materials**Géza I. Márk¹, Péter Vancsó¹, Alexandre Mayer²¹Nanostructures Departement, Centre of Energy Research, Budapest, Hungary²Department of Physics, University of Namur, Belgium

Wave packet dynamics (WPD) is an efficient method of computational quantum mechanics. The time-dependent dynamics is available through the solution of the time-dependent Schrödinger equation and the energy-dependent dynamics can be calculated by the time-energy Fourier transform. Our WPD method has two input quantities: i) the Ψ_0 initial wave function and ii) the $V(r)$ potential describing the system. Formerly we created such a one-electron local pseudopotential [1] which proved suitable to study transport phenomena in various sp^2 carbon nanosystems, e.g. graphene grain boundaries [2] and nanotube networks [3]. In this work, we present an extended version of the local pseudopotential which correctly describes Van der Waals stacks of carbon sheets, e.g. AA, AB, and ABC graphite and graphene. We utilized this potential to study the hopping dynamics of wave packets between the graphene sheets in multilayer systems, also with- and without defects.

[1] A. Mayer, Carbon 42(2004)2057.

[2] P. Nemes-Incze et al, Appl.Phys.Lett. 99(2011)023104.

[3] D.G. Kvashnin et al, Nano Res. 8(2015)1250.

WED 38**Coherent Charge Oscillations in a Bilayer Graphene Double Quantum Dot**Katrin Hecker^{1,2}, Luca Banszerus^{1,2}, Aaron Schäpers¹, Anton Peters¹, Samuel Möller^{1,2}, Eike Icking^{1,2}, Takashi Taniguchi³, Kenji Watanabe⁴, Christian Volk^{1,2}, Christoph Stampfer^{1,2}¹JARA-Fit and 2nd Institute of Physics, RWTH Aachen University, Germany²Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany³International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan⁴Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan

Landau-Zehner-Stückelberg (LZS) interference, which was first used to describe atomic collisions, is a powerful tool to study the dynamics of artificially designed quantum mechanical two-level systems (TLSs) in many solid state platforms. One field of application is the investigation of charge noise and charge decoherence in a semiconductor double quantum dot (DQD). Recently, bilayer graphene (BLG), due to its gate-tunable band gap and low spin-orbit and hyperfine interaction, arised as a promising host material for spin qubits in highly tunable quantum dots (QDs). So far, it has become possible to confine single electrons in BLG QDs and to understand

their spin and valley texture, but coherent evolution of a TLS and its microwave excitation have not been investigated, yet. Here, we show coherent charge oscillations in a BLG DQD using LZS interferometry. We perform photon-assisted tunneling (PAT) to explore the energy spectrum of the TLS. The PAT and LZS measurements yield a charge decoherence time, T_2^* , of about 430 ps. These measurements show the first coherent evolution of a TLS in BLG QDs and allow studying the spectral distribution of charge noise in follow-up experiments.

WED 39

Photoswitching Molecular Conjugation on Single-Walled Carbon Nanotubes

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Increased emission from the tailoring of carbon nanotubes using organic molecules have been utilized in optoelectronics, biosensing, bioimaging, etc. Our group over the past years has extensively worked on the non-destructive covalent approach to modify luminescent SWNTs using photoswitching spiropyran [1]. This hybrid nanomaterial has been used in the control of the SWNTs intrinsic luminescence in the NIR region (beyond $1\mu\text{m}$) [2]. However, the synthetic approach used to obtain this smart nanomaterial was based on a single reaction step; hence controlling the number of groups attached to the SWNTs is a challenge. Herein, the design, stepwise synthesis and characterization of a smart nano-based material functionalized with spiropyran photoswitchable molecules are reported.

[1] Setaro, A., Adeli, M., Glaeske, M. et al. Preserving pi-conjugation in covalently functionalized carbon nanotubes for optoelectronic applications. *Nat Commun.*, 2017, 8, 14281.

[2] Godin, A., Setaro, A., Gandil, M., Haag, R., Adeli, M., Reich, S., Cognet, L. Photoswitchable single-walled carbon nanotubes for super-resolution microscopy in the near-infrared. *Sci. Adv.* 2019, 5, eaax1166.

WED 40

Composite super-moiré lattices in hBN commensurate twisted bilayer graphene

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Twisted bilayer graphene hosts a plethora of correlated quantum phenomena, such as superconductivity, correlated insulators, and strange metal phases. The microscopic details of the heterostructure thereby highly influence the characteristic of the final device. Here, we present transport experiments of a hexagonal boron nitride (hBN)-commensurate twisted bilayer graphene device. We are able to observe the presence of the individual moiré lattices by magnetotransport measurements and compare our results to theoretical simulations. Band structure calculations show a super-moiré enhanced electron-hole asymmetry of the single-particle gaps which is investigated by means of finite bias spectroscopy.

WED 41

Plasma-derived multifunctional graphene quantum dots for water monitoring and purification

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A natural low-cost and biocompatible chitosan was converted in the atmospheric pressure microplasma system into graphene quantum dots (GQDs) with adjustable sizes controlled with Photoluminescence (PL) and Raman measurements. The rapid synthesis does not need the strong acids and bases, toxic solvents and chemicals, as well as high temperature and vacuum conditions [1]. The appearance of GQDs with graphene-like nuclei and diameter of 4-6 nm has been confirmed by a high resolution transmission electronic microscopy (HRTEM) measurements. The PL maps (emission vs excitation) have demonstrated a size-dependent position of resonant PL signal. The size-dependent Raman signals were selectively registered under excitation by radiation of He-Cd laser(325 nm), which was higher in energy than the PL peak maximum. The bright PL of GQDs was used as indicator of presence and amount of heavy metals in aqueous suspensions. The GQDs were used even as the filters for purification of such suspensions from heavy metals[2].

[1] D. Kurniawan, W.-H. Chiang, Carbon 167 (2020) 675-684.

[2] D. Kurniawan, Chem. Eng. Journ. 451(2023) 139083(1-12).

WED 42

Tunable graphene phononic crystal

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Periodic patterning of a material induces a band structure for phonons, in analogy to an electronic band structure in solids created by a periodically varied atomic potential. A phononic band gap is controlled by the patterning design. Such a bandgap may enable applications toward mechanical qubits, efficient waveguides and advanced sensing. High-quality phononic crystals have been fabricated using materials such as Si, SiN or hBN. However, the tunability of material strain and phononic states limit the progress toward the applications listed above. To address this challenge, we experimentally realized a tunable phononic crystal by graphene, an ultra-thin two-dimensional material with highly out-of-plane flexibility. We experimentally found a band gap from 28 MHz to 32 MHz and showed its strain tunability by ~5 MHz. This suggests a highly tunable mechanical phononic crystal.

WED 43

Strain-induced bandgap modifications in twisted two-dimensional WS₂ nanostructures

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The local electronic properties of 2D materials, such as WS₂, depend closely on the details of their underlying atomic arrangements. Twisted 2D flakes benefit from a high degree of tunability, where the relevant degree of freedom is the twisting angle. Additionally, the onset of local strain fields, induced by the twisting, have been predicted to markedly influence resultant electronic properties such as the bandgap or dielectric function. However, experimental studies of local strain-induced bandgap modifications in TMD nanostructures are usually limited by the spatial resolution of spectroscopic techniques, which prevents accessing the relevant information at the nanoscale. Here we combine high-resolution Electron Energy-Loss Spectroscopy (EELS) and with 4D Electron Microscopy Pixel Array Detector (EMPAD) to carry out an extensive investigation of the impact of local strain fields on the bandgap modulations of WS₂ twisted flakes. The combined analysis reveals strain-dependent bandgap modifications in WS₂ nanostructures, demonstrating the unique potential

of our approach to scrutinise the subtle interplay between strain fields and local electronic properties in WS₂ nanomaterials.

WED 44

Non-destructive low-temperature contacts to MoS₂ nanoribbon and nanotube quantum dots

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Planar TMDCs are at the center of manifold research efforts due to their two dimensional nature and outstanding electronic and optical properties. Despite detailed studies of their optical response, worldwide efforts to reach single level transport in lithographically designed quantum dots have so far been mostly unsuccessful. This is due to the requirement for very small confinement potentials as well as disorder from dangling bonds at the edges of nanoflakes.

As-grown MoS₂ nanotubes and nanoribbons can circumvent these issues due to their intrinsic narrow confinement. Our first Coulomb blockade measurements on a MoS₂ nanotube [1] were so far limited by disorder below the metallic scandium contacts. Here, we present low temperature transport measurements on MoS₂ nanotubes and nanoribbons contacted with the semimetal bismuth. [2] We demonstrate the non-destructive and transparent nature of the contacts to our quantum dots and indicators of quantum confinement in our device. [3]

[1] S. Reinhardt et al., pssRRL 13, 1900251 (2019)

[2] P. C. Shen et al., Nature 593, 211 (2021)

[3] R. T. K. Schock et al., arXiv:2209.15515 (2022)

WED 45

Structure-imposed electronic topology in graphene nanoribbons

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Zigzag graphene nanoribbons (ZGNR) can be transformed into new structure types by removing terminal carbon atoms in a regular pattern. When a single atom is removed on each zigzag edge so-called cove-edged ZGNR (ZGNR-C) are created, while removing multiple atoms results in gulf-edged ZGNR (ZGNR-G). In our seminal work, we demonstrated the direct structure-electronic structure relation based on the structural parameters that unambiguously characterize ZGNR-C. This allowed to create a scheme that classifies their electronic state, i.e., if they are metallic, topological insulators or trivial semiconductors, and to find an empirical formula for the

band gap of the semiconducting ribbons. Since then, we were able to expand this description to ZGNR-G systems where the chemical space of possible structures increases further due to the variable size of the gulf edges. With this, we give guidance to realize new graphene nanoribbon heterojunctions hosting topological states and investigate the transport properties of exemplary systems.

WED 46

Relation between the quantum volume and the topology of Euler insulator

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To understand the relation between the quantum volume and topological invariant is an important problem in the topological state research. In this work we investigate if the quantum volume could also detect topology induced by the Euler class. We establish an inequality between the quantum volume and the Euler number. Exploiting this inequality we investigate when quantum volume can be a good measure to infer the Euler number. We discovered that quantum volume calculated in Brillouin zone can also be a good measure of Euler number transition during the topological phase transition.

WED 47

Second harmonic generation of enantiomer-separated, aligned single chirality chiral carbon nanotubes

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Single-wall carbon nanotubes (SWNTs) have been predicted to have chiral nonlinear optical behavior due to their chiral symmetry and corresponding optical selection rules[1]. Theoretical investigations predict that chiral CNTs have second-order susceptibility consisting of only chiral terms χ_{xyz}^2 , while achiral CNTs prohibit second-order susceptibility. In particular, since $\chi_{xyz}^2(\text{left-handed CNT}) = -\chi_{xyz}^2(\text{right-handed CNT})$ [2], enantiomer-separated, single chirality chiral CNT is needed to get SHG signals, which makes the observation difficult.

Recently, we have observed SHG signal by enantiomer-separated, aligned CNTs with single chirality (11,-5). In order to understand the spectra, we have developed a tight-binding method to calculate SHG spectra as a function of incident photon energy, polarization, and sample orientation[3]. The theoretical results are consistent with the recently made measurement. For more detail, please come to the presentation.

[1]. G. Y. Guo, et al., Phys. Rev. B 69, 205416, (2004).

[2]. R. W. Boyd, Nonlinear optics. Academic Press, London, 2020.

[3]. R Xu, Y. Tian, et al, in preparation

WED 48

Graphdiynes as 2D carbon materials beyond graphene: from theory to experiments

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³ETSF and Dipartimento di Fisica "Aldo Pontremoli", Università degli Studi di Milano, Milano, Italy

Novel carbon nanostructures can be produced by properly combining carbon atoms with sp and sp² hybridization. Among these systems, graphdiynes represent a class of 2D carbon materials beyond graphene [1]. Here, we present a combined experimental and theoretical investigation of different 1D and 2D structures produced by on-surface synthesis on Au(111) [2-5]. We investigated the formation of graphdiyne nanoribbons [2,5] and 2D graphdiyne-like extended networks [3,4] by scanning tunneling microscopy STM, Raman spectroscopy, and density functional theory (DFT) simulations. DFT calculations show how the metal surface has a relevant effect on the electronic and vibrational properties [4]. In anthracene derivatives, we show how the formation of packed linear structures and the occurrence of homocoupling reactions are affected by the steric hindrance of neighboring sp² structures [5].

[1] P. Serafini et al. J. Phys Chem C 125, 33, 18456 (2021)

[2] A. Rabia et al. Nanoscale, 11, 18191 (2019)

[3] A. Rabia et al. ACS Appl. Nano Mater. 3, 2178 (2020)

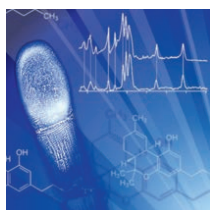
[4] S. Achilli et al. 2D Materials 8 044014 (2021)

[5] S. Achilli et al. Phys. Chem. Chem. Phys. 24, 13616 (2022)



Introducing nano-FTIR

Imaging & Spectroscopy @ 10 nm Spatial Resolution



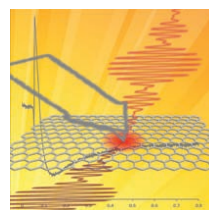
Chemical nano-ID

Molecular spectroscopy
@ 10 nm spatial resolution
(nano-FTIR)



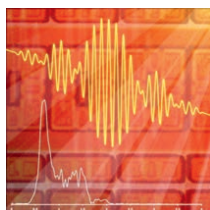
Synchrotron nanospectroscopy

IR-Synchrotron compatible
for ultra-broadband
nano-FTIR spectroscopy



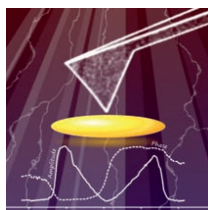
Ultrafast nanospectroscopy

Femtosecond pump-probe
spectroscopy @ 10 nm
spatial resolution



Terahertz nanospectroscopy

Far-infrared / THz imaging &
spectroscopy < $\lambda/20'000$
spatial resolution



Nano-plasmonic field mapping

Real space imaging
of the local electric field
e.g. nano-antennas



Cryogenic nanoscopy

The only commercial cryogenic
near-field microscope
operating < 10 K

- 08:30 – 09:00 G. Abellán, Valencia
Hexagonal Hybrid Bismuthene by Molecular Interface Engineering
- 09:00 – 09:30 X. Feng, Halle
Advances in Organic 2D Crystals - From On-Water Surface Chemistry to Functional Applications
- 09:30 – 10:00 L. Schue, Palaiseau
Optical Signatures of the 3D Anisotropy in Black Phosphorus
- 10:00 – 10:30 Coffee Break
- 10:30 – 11:00 P. Ayala, Vienna
On the Interaction Between Single-Walled Carbon Nanotubes and Encapsulated Nanostructures
- 11:00 – 11:30 T. Wei, Erlangen
Spatially Resolved Molecular Engineering of Graphene
- 11:30 – 12:00 E. Vázquez, Ciudad Real
2D Materials for 3D Smart Soft Structures
- 12:00 – 17:00 Mini Workshops
- 17:00 – 17:30 A. Mannix, Standford
Automated Assembly of Synthetic van der Waals Solids
- 17:30 – 18:00 C. Schönenberger, Basel
Search for the Fractional Josephson Effect in Topological and Nontopological Materials
- 18:00 – 18:30 SUMMARY
Kirchberg 2023 - Conference Summary
- 18:30 – 20:00 Break
- 20:00 – 22:00 Bauernbuffet – Farewell Dinner

08:30**Hexagonal hybrid bismuthene by molecular interface engineering**Gonzalo Abellán¹¹Institute of Molecular Science (ICMol), University of Valencia, Valencia

Novel, high quality devices, based on layered heterostructures are typically built from materials obtained by complex solid-state physical approaches or laborious mechanical exfoliation and transfer, as wet-chemically synthesized materials commonly suffer from surface residuals and intrinsic defects. Here, we introduce a new 2D member to the pnictogen family, synthesized by a colloidal approach, that consists of a coherent sandwich of beta-bismuth, encapsulated by sulfur-alkyl-functionalized flat bismuthene interfaces. While an unprecedented degree of structural quality is demonstrated, an altered atomic arrangement of the outermost, functionalized bismuthene layers leads to a drastic changes in the chemical reactivity and electronic structure. The metallic nature is evidenced by room temperature transport measurements of individual nanoflakes. Our data proof that surface reconstructions in 2D systems can promote unexpected new states that can pave the way to new functionalities and devices. Last but not least, a large scale production strategy will be introduced.

09:00**Advances in Organic 2D Crystals - From On-Water Surface Chemistry to Functional Applications**Xinliang Feng^{1,2}¹Dept. SMFD, MPI of Microstructure Physics, Halle²cfaed, Faculty of Chemistry and Food Chemistry, Technische Universitaet Dresden

A central chemical challenge is to realize a controlled polymerization in two distinct dimensions under thermodynamic/kinetic control in solution and at the surface/interface. Here, we present our recent efforts in bottom-up synthetic approaches towards novel organic 2D crystals with structural control at the atomic/molecular level. On-water surface synthesis provides a powerful synthetic platform by exploiting surface confinement and enhanced chemical reactivity and selectivity. We present a surfactant-monolayer assisted interfacial synthesis (SMAIS) method that is highly efficient in promoting a 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. Its 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 very promising for a range of applications in electronics, optoelectronics and spintronics. Other physicochemical phenomena and application potentials of organic 2D crystals are also discussed.

09:30**Optical signatures of the 3D anisotropy in black phosphorus**Leonard Schue^{1,2}¹Université de Montréal, Canada²CNRS/Ecole Polytechnique, Palaiseau, France

After reports of high mobility and a tunable bandgap covering a wide spectral range from the visible to the mid-IR region, black phosphorus (BP) has emerged as a promising 2D material for high performance optoelectronic devices. Owing to its orthorhombic structure, BP expresses strong anisotropic properties. While recent investigations on few-layers crystals have extensively explored the in-plane anisotropy, much less attention has been given to the out-of-plane direction.

In this work, we use polarization-resolved photoluminescence and Raman spectroscopies to investigate the band structure anisotropy of bulk BP along the zigzag, armchair and out-of-plane directions. Polarization selection rules and DFT calculations of the complex dielectric permittivity are used to understand the origin of the strongly polarized optical response and demonstrate the remarkable extent to which the anisotropy influences the optical properties and carrier dynamics in black phosphorus.

10:30**On the interaction between single-walled carbon nanotubes and encapsulated nanostructures**Paola Ayala¹¹Faculty of Physics, University of Vienna, Vienna, Austria

The fabrication of single-walled carbon nanotubes (SWCNT) within the last decades has achieved materials approaching the theoretical predictions. The electronic and optical properties of pristine SWCNT can be unraveled with more than one spectroscopy technique. However, working with hybrids of SWCNT still embraces significant challenges because controlling and modifying those properties implies understanding interactions of the SWCNTs with other structures or molecules. For instance, their photoluminescence (PL) is modified clearly changes in filled SWCNTs. In this context, small diameter tubes can form novel hybrids confining linear carbon chains (LCC) or graphene nanoribbons (GNR) that offer extremely attractive new insights. I will show how our efforts towards identifying the charge transfer from encapsulated nanostructures to SWCNT hosts on hybrids confining LCC and GNR. We will discuss the extraction of SWCNT-carbon chain-hybrids from their double-walled counterparts, and a plausible diameter-dependent enhancement of the PL by energy transfer. Further, I will focus on how to discern specific Raman active modes independently from other fragments of ribbon-like molecules.

11:00**Spatially Resolved Molecular Engineering of Graphene**Tao Wei¹, Frank Hauke¹, Andreas Hirsch¹¹Organische Chemie II, Friedrich-Alexander-Universität, Erlangen

Exploring the tailored physical/chemical properties is at the forefront of graphene research. The emerging development of covalent molecular engineering represents a rather promising tactic for this purpose carrying several unique advantages. In this line, we have developed two scenarios, including reduction-mediated lithography and laser writing, for spatially resolved covalent 2D-patterning of graphene, affording a variety of well-structured graphene architectures. Furthermore, based on the combination of 2D-patterning techniques and post-functionalization approaches, more promising hierarchically ordered multifunctional graphene architectures were facilely constructed. We further demonstrated that the chemical information of these built 2D-systems can be finely manipulated by establishing complete write/read/erase circles.

11:30**2D Materials for 3D Smart Soft Structures**Ester Vázquez¹¹Universidad de Castilla-la Mancha, Ciudad Real

The synthesis of different hydrophilic polymeric networks, by in situ radical polymerization in the presence of graphene derivatives, gives rise to three-dimensional nanocomposite soft scaffolds. The role of the nanomaterial within the polymer network is primarily intended for the reinforcing (i.e., increasing the stiffness and toughness). However, we have shown that the presence of graphene can also enhance features such as biocompatibility, sensing, or self-healing ability, giving rise to truly hybrid composites. In addition, the ability of these materials to respond to different stimuli, such as electric fields, and the possibility of preparation following 3D printing methodologies, paves the way for applications in soft robotics and on-off drug delivery. These materials require the production of large quantities of graphene easily dispersible in water, and for this reason, ball milling approaches developed in our laboratories have proven to be a method of choice for the preparation of 2D starting materials.

17:00**Automated assembly of synthetic van der Waals solids**Andrew Mannix¹¹Stanford University

Synthetic van der Waals (vdW) solids assembled from 2D materials yield unprecedented opportunities via atomic-scale composition control and the interlayer twist or lattice mismatch-induce moiré. However, the production of vdW solids remains a largely artisanal process, limited in the size of the source material and the throughput. In this talk, I will discuss recent efforts to enhance the quality and speed of vdW solid fabrication. Our core approach, Robotic 4D Pixel Assembly, enables rapid manufacturing of vdW solids with unprecedented speed, area, patternability, and angle control. We use a high-vacuum robot to assemble prepatterned pixels made from 2D materials grown at the wafer scale. We fabricated vdW solids of up to 80 individual layers, consisting of (10 to 1000 μm)² areas with pre-designed patterned shapes, laterally/vertically programmed composition, and controlled interlayer angle. This enabled efficient spectroscopic assays of vdW solids and fabrication of twisted n-layer assemblies. To conclude, I will outline ongoing efforts in my lab to understand and engineer electronic interfaces, moiré superlattices, and point defects within vdW solids.

17:30**Search for the Fractional Josephson Effect in Topological and Nontopological Materials**

Christian Schönenberger¹, Roy Haller¹, Artem Kononov¹, Martin Endress¹, Carlo Ciaccia¹, Minkyung Jung^{1,2}, Joost Ridderbos^{1,3}, Gergő Fülöp⁴, Dieter Weiss⁵

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²DGIST Research Institute, Daegu, Korea

³Faculty of Electrical Engineering, University of Twente, Enschede, The Netherlands

⁴Budapest Univ. of Technology and Economics, BME, Budapest, Hungary

⁵Univ. of Regensburg, Regensburg, Germany

We report on an extensive search of the AC Josephson effect of superconducting junctions and weak links obtained from various materials in a “low-ohmic” environment allowing for DC bias. The materials are two-dimensional graphene, Al proximitized InAs quantum wells, the Dirac semimetal cadmium arsenide, the Weyl semimetal tungsten telluride WTe₂, the 3D topological insulator HgTe, InAs nanowires and carbon nanotubes, as well as conventional Al-based reference Josephson junctions. We have studied AC Josephson emission, Shapiro steps, current-phase relations and Fraunhofer patterns to address the current distribution. We can observe missing Shapiro steps, but there is no AC Josephson signal appearing concurrently at frequency eV/h , as expected for topological junctions. However, we find strong higher order Josephson terms that go with frequency as $2neV/h$ with $n=1,2,3...$. These terms stem from simultaneous inelastic tunneling of n Cooper-pairs. The relation to the skewness of the CPR will be addressed.

18:00

Kirchberg 2023 - Summary

Christoph Stampfer^{1, 2}

¹JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Germany

²Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Germany

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