

XXXVIIth
International Winterschool
on Electronic Properties
of Novel Materials

Molecular Nanostructures

Program



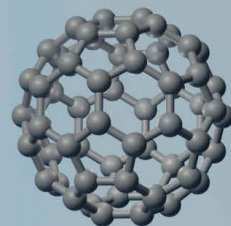
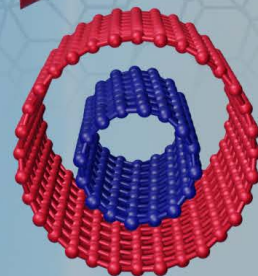
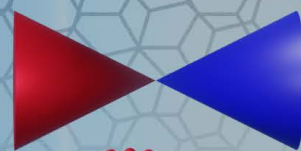
Hotel Sonnalp
Kirchberg/Tirol
Austria

08 - 14 March, 2025



Kirchberg

IWEPNM 2025



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

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This year's logo of the IWEPNM shows elements of the conference logos of the past 40 years.

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Financial assistance from the sponsors and supporters is greatly acknowledged.

Dear Friend:

Welcome to the 37th International Winterschool on:

Electronic Properties of Novel Materials!

This Winterschool is a sequel of thirty-six 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 |
| Accommodation | Tobias Dierke, Eileen Schneider & Mira Kreßler |
| Finances | Antonio Setaro |
| Accommodation Finances | Kati G.-Hubmann |
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| Announcements | Stefan Wolff |
| Daily Information Poster | Gabriela Luna Amador |
| Conference Publications | Antonio Setaro |
| Visa | Angelin See |

Also the manager of the hotel, Carina Mayer, and her 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

Chairpersons

J. Maultzsch (Erlangen)

S. Reich (Berlin)

A. Hirsch (Erlangen)

C. Stampfer (Aachen)

Program Committee

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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 2025 starts on Saturday, 8 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Friday, 14 March, breakfast. The welcome reception takes place in the Sonnalp hotel lobby on Saturday evening at 9.00 pm. On Tuesday night we will celebrate the 40 years anniversary of the Kirchberg Winterschool by a special session and a reception with sparkling wine and finger food. On the last evening (Thursday) we will have a farewell dinner in the seminar hall at 7.30 pm with music and a quiz on the history of the Winterschool and excellent prizes.

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 2025 Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria

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

All questions concerning the IWEPNM 2025 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 2025 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 Michaela Kisch (michaela@kitzkids.com). 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 Sunday, Monday, and Wednesday. Poster awards are kindly provided by Wiley VCH.

Conference Publication

Invited and contributed presentations from IWEPM 2025 are scheduled for publication as a special issue in *physica status solidi* (pss) (b). **Manuscript submission is due on Mai 31st.** 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.

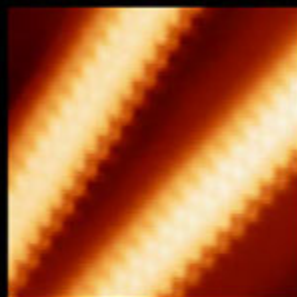
Please **submit one complete PDF- or Word-file for review** (Word or Latex source files are required after acceptance for production). The submission system can be found here: <http://www.editorialmanager.com/pssb-journal>

Please select article type "Original Paper" of the journal of your choice and subsequently the section "IWEPM: 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 iwepm-publication@physik.fu-berlin.de.

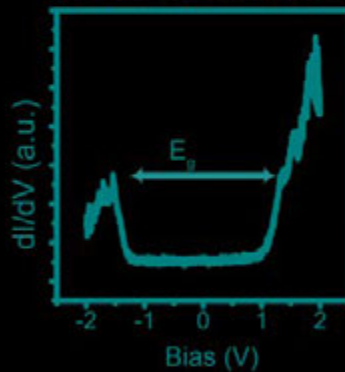
**Robust Contact by Direct
Formation of C—Au Bond
in Suspended Armchair
Graphene Nanoribbon**

Abdou Hassanien

STM IMAGING WITH GNR-TIP



INTRINSIC BAND GAP



IWEPNM 2025
CHAIRPERSONS FOR THE ORAL SESSIONS

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

| | | |
|-------------------|---|--|
| Sunday, 09.03. | morning morning, after coffee break evening | Stephanie Reich Claudia Backes Ute Kaiser |
| Monday, 10.03. | morning morning, after coffee break evening | Hans Kuzmany Iris Niehues Andreas Hirsch |
| Tuesday, 11.03. | morning morning, after coffee break evening | Janina Maultzsch Annick Loiseau Christoph Stampfer |
| Wednesday, 12.03. | morning morning, after coffee break evening | Viera Skakalova Thomas Pichler Alexander Soldatov |
| Thursday, 13.03. | morning morning, after coffee break evening | Florian Libisch Sebastian Heeg Ralph Krupke |

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

DAILY PROGRAM

AND

ABSTRACTS

Sunday, March 9th

- 08:30 – 09:00 H. Kataura, Tokyo
Defect-Free Dispersion of Single-Wall Carbon Nanotubes
- 09:00 – 09:30 S. Maruyama, Tokyo
New Kinds of 1D vdW Heterostructures Based on Single-Walled Carbon Nanotubes
- 09:30 – 10:00 S. Heeg, Berlin
Anharmonicity and Confinement Effects in Carbyne-Like Materials
- 10:00 – 10:30 Coffee Break
- 10:30 – 11:00 M. Prato, Trieste
Carbon Nanotubes for Nerve Injury Repair
- 11:00 – 11:30 H. Hölzel, Giessen
Energy Management of Functional Molecular Material
- 11:30 – 12:00 S. Hecht, Berlin
2D Covalent Framework Materials by On-Surface Polymerization
- 12:00 – 17:00 Mini Workshops
- 17:00 – 18:30 Dinner
- 18:30 – 19:00 D. Lungerich, Seoul
Evolution of Molecules Under the Electron Beam
- 19:00 – 19:30 J. Zhao, Hong Kong
Phase Transition and Ferroelectricity in Two-Dimensional Chalcogenides
- 19:30 – 20:00 M. Lozada-Hidalgo, Manchester
Field Effects in Proton Transport and Hydrogenation in Graphene
- 20:00 Poster I

Sunday, March 9th

08:30

Defect-free dispersion of single-wall carbon nanotubes

Hiromichi Kataura¹, Mariko Kubota¹, Maymi Tsuzuki¹, Takeshi Tanaka¹

¹Nanomaterials Res. Inst., Nat. Inst. of AIST, Tsukuba

For the application of single-wall carbon nanotubes (SWCNTs) in electronic devices, it is not enough to separate high-purity semiconductors; low defect dispersion before separation is critical to take advantage of their high mobility. To date, sonication has been widely used for dispersion, but sonication causes significant defects that degrade device performance. To address this issue, Sofie et al. [1] used magnetic stirrer for a low defect dispersion prior to separation, but even magnetic stirrers have been found to induce minor defects. In this study, we demonstrated that a different type of stirrer can be used to disperse SWCNTs with almost no defects. Furthermore, we found that by controlling the concentration of surfactant, SWCNTs with fewer defects could be selected. These findings resulted in an isolated dispersion of extremely defect-free SWCNTs that exhibited $G/D > 300$ at 488 nm. This G/D is higher than that of the raw SWCNT, EC1.5-P (Meijo). Furthermore, the G/D improved to over 500 when high purity semiconductor separation was performed. This dispersion technique is more effective for SWCNTs with smaller diameters.

[1] Sofie Cambré et al. ACS NANO 6, 2012, 2649.

09:00

New kinds of 1D vdW heterostructures based on single-walled carbon nanotubes

Shigeo Maruyama^{1,2}, Yongjia Zheng^{1,2}, Wanyu Dai¹, Chunxia Yang², Keigo Otsuka¹, Rong Xiang^{1,2}

¹Department of Mechanical Engineering, The University of Tokyo, Tokyo

²School of Mechanical Engineering, Zhejiang University, Hangzhou

We have demonstrated the one-dimensional (1D) van der Waals (vdW) heterostructure: single-walled carbon nanotubes (SWCNTs), boron nitride nanotubes (BNNTs), and molybdenum disulfide (MoS_2) sequentially wrapped in the radial direction. We have optimized CVD conditions for various metal dichalcogenides such as tungsten disulfide (WS_2), niobium disulfide (NbS_2), and molybdenum diselenide (MoSe_2) in addition to the original MoS_2 . Furthermore, we can combine two TMDs: axial junction of such as WS_2 - MoS_2 nanotubes and alloyed nanotubes such as $\text{W}_x\text{Mo}_{(1-x)}\text{S}_2$. Then, we will discuss the various Yanus TMD nanotubes templated by SWCNT-BNNT. We employ the hydrogen plasma technique to demonstrate the single-walled Yanus MoS_2 with a diameter of around 8-10 nm, starting from MoS_2 nanotubes. Finally, weakly confined carbyne synthesized within SWCNT is combined for these 1D heterostructures.

Sunday, March 9th

09:30

Anharmonicity and confinement effects in carbyne-like materials

Sebastian Heeg¹

¹Institut für Physik, Humboldt Universität zu Berlin, Berlin

Carbyne, an infinite linear chain of carbon atoms, is the truly 1D allotrope of carbon that has remained elusive to date. While carbyne-like materials like long linear carbon chains encapsulated in carbon nanotubes or short carbon atomic wires are available for study, the transition between the two systems and common properties that can be linked to carbyne are poorly understood. In this talk, I will present our Raman spectroscopy study of the C-mode of individual confined carbyne chains up to the third overtone. We find a strong vibrational anharmonicity that increases with decreasing C-mode frequency. Upon comparison to carbon atomic wires, we find that this relation between vibrational anharmonicity and C-mode frequency is universal to carbyne-like materials. Finally, I will show that the collective LO-phonon mode of carbon atomic wires confined inside carbon nanotube approaches the frequency of confined carbyne's C-mode, suggesting that convergence to length-independent properties of long linear carbon chain inside carbon nanotubes occurs at shorter chain lengths than previously thought.

10:30

Carbon Nanotubes for Nerve Injury Repair

Maurizio Prato^{1,2}

¹Università di Trieste, Trieste

²CIC biomagune, San Sebastián, Spain

Spinal cord injury is a most devastating disease, as it causes a permanent loss of motor functions, causing enormous personal, social and economic problems. Neural regeneration has been shown to be a natural process; however, the regeneration mechanisms of the central nervous system are generally ineffective in restoring appropriate function. Therefore, there is a tremendous social and medical pressure along with research interest to discover new therapeutic strategies for the effective repair of the spinal cord injury. We have shown that carbon nanotubes can act as active substrates for neuronal growth, a field that has given so far very exciting results. Nanotubes are not only compatible with neurons, but, especially, they play a very interesting role in interneuronal communication. Improved synaptic communication is just one example. During this talk, we will discuss our most recent attempts to regenerate the electrical connection in the lesioned spinal cord, with particular emphasis on the latest and most exciting results obtained in our laboratories in this fast developing field.

Sunday, March 9th

11:00

Energy management of functional molecular materials

Helen Hölzel^{1,2}

¹Organische Chemie, JLU Giessen, Giessen

²Chemical Engineering, UPC BarcelonaTech, Barcelona

The understanding of energy management like energy harvesting, transformation, conversion, and storage, has been set into focal point demanded by the search for new functional materials for various purposes, as research nowadays is driven by the need for more sustainable and alternative strategies for energy management. Herein, we present functional molecular materials and display the behavior and energy management in these systems as energy storage materials upon photoexcitation. Further, we discuss the use of this energy employing conversion and storage in chemical bonds. We shortly dive into the preparation of the materials, however focusing on the photophysical properties and requirements for efficient energy management. Moreover, we present a method of fast quantification of photophysical properties like half-lifetimes and quantum yields using a custom-built and semi-automated setup. As extension and complementarily, proof-of-principle devices based on these molecular materials will be shown.

11:30

2D Covalent Framework Materials by On-Surface Polymerization

Filippo Fabozzi^{1,2}, Stefan Hecht^{1,2}

¹Department of Chemistry, Humboldt University, Berlin

²Center for the Science of Materials Berlin, Humboldt University, Berlin

On-surface polymerization constitutes a powerful bottom-up approach to generate new 2D materials. In this presentation, our recent activities in this area using dynamic covalent chemistry as well as light-induced covalent capture (topochemistry) will be described.

In a first study to be discussed, interfacial synthesis of a single-layer, vinylene-linked 2D covalent organic framework could be achieved. By judicious choice of the monomer building blocks and optimization of the reversible Knoevenagel polycondensation conditions, growth of an extended pi-conjugated 2D polymer was realized and the resulting structure imaged by Scanning Tunnelling Microscopy. In a second study, self-assembly of photoresponsive stilbene-based monomers was used to position neighboring reactive olefinic double bonds in close proximity to undergo UV light induced [2+2]cycloaddition reactions. Therefore, the supramolecular template structure was covalently captured to provide access to unique 1D polymer strands. Our findings highlight the possibilities to create new 2D materials with control over their electronic structure, their pore size and geometry as well as potential functionalization.

Sunday, March 9th

18:30

Evolution of molecules under the electron beam

Dominik Lungerich^{1,2}

¹Institute for Basic Science, Center for Nanomedicine, Seoul

²Advanced Science Institute, Yonsei University, Seoul

In contemporary scientific exploration, the advent of aberration-corrected transmission electron microscopy has empowered researchers to capture materials at the atomic level with unparalleled precision. The utilization of state-of-the-art single-molecule atomic resolution time-resolved electron microscopy (SMART-EM) techniques allows for the visual observation of dynamic events occurring at the smallest scale of matter – molecules and single atoms. Our specific interest lies in bridging microscopic insights with state-of-the-art chemistry knowledge and exploring their application as valuable tools for chemists. The forthcoming talk will center on recent discoveries verified through the eyes of an organic chemist, elucidating reaction mechanisms induced by the electron beam that lead to the formation of precise carbon nanostructures. The comprehension of these dynamic nanoscale processes holds paramount importance for advancing applications in nanotechnology, such as the development of precise nanoscale fabrication techniques with focused electron beams.

19:00

Phase transition and ferroelectricity in two-dimensional chalcogenides

Jiong Zhao¹

¹Applied Physics Department, The Hong Kong Polytechnic University, Hong Kong

Beyond current von Neumann systems, two-dimensional (2D) ferroelectrics (FE) with miniaturized dimension, high speed and high sensitivity, and robust ferroic order with memory functionalities, are superior candidates for next-generation in-memory computing devices. Moreover, the facile phase transition in 2D materials potentially offers another degree of freedom to manipulate the non-volatile memory states. In this presentation, we will clarify the ferroic ordering and their physical origin, and introduce how to control/manipulate the phase transition and the ferroelectricity as well as ferroelasticity in 2D and build novel devices. We applied a variety of in situ transmission electron microscopy techniques, specifically employing in situ mechanical manipulation, in situ mechanical testing, in situ electrical testing, in situ heating, and in situ electron beam control, to conduct comprehensive investigations of ferroic phase transitions and ferroic ordering in two-dimensional (2D) chalcogenides. The diverse phases observed in these ferroic 2D materials showcase unique mechanical, electrical, and other captivating physical properties.

Sunday, March 9th

19:30

Field effects in proton transport and hydrogenation in graphene

Marcelo Lozada-Hidalgo¹

¹Department of Physics and Astronomy, The University of Manchester, Manchester

Graphene's basal plane is impermeable to all atoms and ions under ambient conditions. Nevertheless, it was found to be permeable to thermal protons, opening a long-standing debate. Protons can also electrochemically adsorb on graphene, which triggers a robust conductor-insulator transition, but the mechanism for the process remains unknown. In this talk we'll discuss our recent work mapping proton transport currents in graphene with nanoscale spatial resolution, which unequivocally confirm that perfect graphene crystals are permeable to protons and settle the long-standing debate. We will also discuss our work investigating the mechanism of the electrochemical hydrogenation of graphene. Finally, we will discuss our work showing that independent control of the charge density and the electric field in double-gated graphene enables the selective acceleration of proton transport and hydrogenation, which are otherwise coupled. This represents a new way of diving electrochemical processes with applications in logic-and-memory devices and energy.

1. Wahab, O. J. et al. Nature 620, 782-786 (2023).
2. Y.C. Soong, et al. (submitted).
3. Tong, J. et al. Nature 630, 619-624 (2024).



POSTER I

SUN 1**Alternative injector/detector platform for magnons: WTe_2** Krishnaraajan Sundararajan¹, Dennis K. de Wal¹, Bart van Wees¹¹Physics of Nanodevices, University of Groningen, Groningen

The modern challenge in computing lies in Moore's law reaching its physical limits hindering further predicted exponential growth in computational power. In the frontiers of research aimed at alternative solutions to this, magnonics focuses on information transport utilizing the spin rather than the charge of the electron. Towards this, two dimensional van der Waals (vdW) materials, with weak interlayer forces, offer an intriguing platform for the study of magnonics with flexibility in the possible heterostructures from combining these atomically flat materials, opening up avenues for exploration of new physics. The electrical study of magnons have so far relied on heavy metals like platinum which makes it difficult to study the magnon transport in air unstable systems like CrI_3 , a potential topological magnon insulator.

Alternative to the traditional heavy metal electrode, WTe_2 : a topological Weyl semi-metal from the vdW family is explored. The observed signal is consistent with an excitations of magnons by the conventional spin hall effect from WTe_2 . This opens up avenues to electrically address the magnon transport in systems like CrX_3 .

SUN 2**Polarons shape the interlayer exciton emission of $MoSe_2/WSe_2$ heterobilayers**Pedro Ignacio Soubelet¹, Alex Delhomme¹, Andreas V. Stier¹, Jonathan J. Finley¹¹Walter Schottky Institut, TUM School of Natural Sciences, Garching

In this contribution, we present evidence for the strong participation of hot phonons in the photo-physics of interlayer excitons (IXs) in 2H- and 3R-stacked $MoSe_2/WSe_2$ heterobilayers. Photoluminescence (PL) excitation spectroscopy reveals that excess energy associated with relaxation of intra-layer excitons towards IXs profoundly shapes the overall IX-PL lineshape, while the energy of the spectrally narrow discrete emission lines conventionally associated with trapped moiré IXs remain unaffected. A strikingly uniform line-spacing of the discrete emission lines is observed, along with characteristic temperature and excitation level dependence. Results suggest an entirely new picture of the discrete IX emission in which non-thermal phonons play a crucial role in shaping the spectrum. Excitation power and time resolved data indicate that these features are most likely polaronic in nature. Our findings extend the understanding of the photophysics of IXs beyond current interpretations based primarily on moiré-trapped IXs.

SUN 3**Mapping the catalytic activity of 2D transition metal chalcogenide crystals with high spatial resolution**Soma Keszei¹, Gergely Dobrik¹, Tamás Ollár¹, Antal Koós¹, Levente Tapasztó¹¹HUN-REN Centre for Energy Research, Budapest

MoS₂ is known to efficiently catalyze the hydrogen evolution reaction, with the edges being considered as the catalytically active sites. However, with the rise of 2D crystals, the need for activating the basal plane has also markedly increased. In general, the pristine surface of 2D crystals is inert, while various defects and imperfections were shown to activate the basal plane. However, generally, only the average catalytic activity of the whole sample is investigated, which comprises crystallites of various morphologies, grain boundaries, point defects, wrinkles, and other lattice imperfections. To gain more insight into the nature of the most active sites, electrochemical measurements with high spatial resolution are needed. Here we present Scanning Electrochemical Cell Microscopy measurements on various 2D TMDC crystals, revealing their local charge transfer characteristics and catalytic activity with a resolution of about 100 nm. Correlating the catalytic activity with atomic resolution structural data obtained by Scanning Tunneling Microscopy measurements, will allow us to identify the true active sites of pristine and modified 2D TMDC crystals.

SUN 4**Do we need black hole physics to understand the plasmon excitations of layered “strange” metals, an EELS and RIXS study.**Jörg Hermann Fink¹¹IFF, IFW Dresden, Dresden

Conventional metals show a scattering rate of charge carriers which are quadratic in temperature or energy typical of Fermi liquids. In “strange metals”, the scattering rate is enhanced at low energies leading to a linear dependence due to correlation effects. This is possibly related to strong quantum fluctuations which are also supposed to mediate superconductivity in cuprates and Sr₂RuO₄. There are theories based on holographic calculations which predict an over-damping of plasmons due to a low-energy continuum. The results are at variance with our early EELS experiments and RIXS data on various cuprates and more recent T-EELS data on Sr₂CuO₄. In all cases we see well-defined optical plasmons which decay into particle-hole excitations only for large momentum in the range of the classical Lindhard continuum. The dispersion of the optical plasmon can be well described within the RPA using an unrenormalized effective mass at high energies. In contrast, the low energy acoustic plasmon dispersion in p-type and n-type cuprates, studied by RIXS can be explained using a mass renormalization of $m^*=2$. These conflicting results can be described by an energy dependent effective mass.

SUN 5**Electrostatics simulation of bilayer graphene devices**

Siyar Duman¹, Maximilian Klammer¹, Benedikt Thoma¹, Florian Libisch¹

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

Bilayer graphene (BLG) is a popular platform for various experiments such as quantum transport and capacitance, superconductivity and devices for manipulating individual charges with the eventual goal of BLG qubits. The property which allows precise experimental control is also the cause of significant theoretical challenges when simulating such experiments: the electrostatically tunable bandgap. In particular, the smaller number of available states compared to bulk materials and the sensitive dependence of the gap on the local electric field necessitates solving the Poisson equation and the redistribution of charge due to the electrostatic potential in parallel. We solve the resulting non-linear Poisson equation in the local density of states approximation to describe the electrostatics of such devices. We compare to recent experimental data on bilayer graphene quantum dots and suggest strategies for future device designs.

SUN 6**Carbon nanotube/protein composites for cardiac cells growth**

Ekaterina A. Obratsova^{1,2}, Alexander P. Moskalets^{1,2}, Olga P. Boychenko^{1,2}, Daria V. Goliusiva², Dmitry V. Klinov^{1,2}

¹Moscow Institute of Science and Technology, Dolgoprudny

²Federal Research and Clinical Center of Physical-Chemical Medicine of Federal Medical Biological Agency, Moscow

Unique combination of electronic, mechanical and surface properties of carbon nanotubes makes them attractive for a number of biomedical applications. In particular, it has been demonstrated that carbon nanotube-based structures act as effective substrates and scaffolds for such demanding cells as cardiomyocytes (cardiac tissue cells) cultivation [1,2]. The main limiting factor for development and extension of his domain is the proven toxicity of carbon nanotubes in pure form [1,3]. Biocompatibility of carbon nanotubes can be improved by modifying its surface. In this work we have applied a row of proteins (albumin, spidroin, fibronectin, collagen) for preparation of composites with nanotubes. Thin surface coatings and structured films were formed using this composite material for cardiomyocytes growth. Stability, electrical conductivity, possibility of oriented deposition of these composites were studied. Cytotoxicity of the obtained substrates was analysed.

1. M.Barrejon et al. Carbon, 184, 2021, 641.
 2. V.Martinelli et. al. ACS Appl Bio Mater, 1, 2018, 1530.
 3. E.A.Obratsova et al. MSU Physics Bulletin, 64, 2009, 320.
- The work was supported by GZ FSMG-2023-0015

SUN 7**Ultra-sensitive hyperspectral imaging of 2D materials with an open micro-cavity**

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Optical-fiber-based micro-resonators (micro-cavities) offer a variety of applications in research and technology. Within the spin-off company Qlibri GmbH, we work on transforming this cutting-edge technology to a standalone lab device in ambient and cryogenic conditions. Using an open scanning-cavity approach, a broad range of experimental needs can be addressed. Here, we highlight the possibilities of cavity enhanced absorption microscopy with detection sensitivities that surpass any current commercial solutions. Certain use cases are presented here which include manipulation of the decay characteristics of two-dimensional van der Waals heterostructures (MoSe₂-WSe₂). Furthermore, two-dimensional scanning capabilities are highlighted, which enable spatial correlation of polariton properties with intrinsic and extrinsic effects. Finally, the sensitivity of the scanning micro-cavity is illustrated through measurements of extinction spectra of atomistic defects in monolayer MoS₂.

SUN 8**Using Spectroscopic Imaging Ellipsometry at Cryogenic Temperatures to Demonstrate a Structural Phase Change in a 2D Polar Metal**

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Spectroscopic Imaging Ellipsometry (SIE) is a powerful optical measurement technique, combining the ability of an ellipsometer to determine layer thicknesses and optical properties of thin film samples with the lateral resolution of a microscope. This enables the investigation of the homogeneity of the dielectric response on the micrometer scale in systems such as TMDCs [1] or 2D polar metals [2].

Using a cryostat with free-beam optical access, we established a unique setup for SIE at cryogenic temperatures, allowing us to explore the temperature-dependence of the local dielectric function.

Here, we present our study on 2D polar Ga, a non-centrosymmetric bilayer metal film stabilized between SiC and graphene [3] with fascinating properties [2]. We show a transition in the dielectric response from homogenous behavior at 293 K to a heterogenous regime at low temperatures, characterized by two absorption peaks

localized to distinct surface regions [4].

[1] S. Funke et al., J. Phys.: Condens. Matter 28, 385301 (2016). [2] K. Nisi et al., Adv. Funct. Mater. 31, 2005977 (2020). [3] N. Briggs et al., Nat. Mater. 19.6, 637-643 (2020). [4] J. Henz et al. in preparation (2024).

SUN 9

CVD Growth and Characterization of High-Quality Janus SeMoS and SeWS Monolayers

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Recently, we developed a route to grow Janus SeMoS monolayers (MLs) by chemical vapor deposition (CVD). [1] In this approach MoSe₂ monolayers are firstly grown on Au foils and then sulfurized to exchange the bottom selenium layer with sulfur atoms. The formation of high-quality Janus SeMoS MLs and the growth mechanism are proven by Raman and X-ray photoelectron spectroscopy (XPS), photoluminescence measurements, transmission electron microscopy and density functional theory (DFT). Here we present an investigation down to the atomic scale of Janus SeMoS MLs grown on Au(111). From low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) measurements we determine experimentally the lattice parameters of Janus SeMoS for the first time. The obtained results are in good agreement with the respective DFT calculation. Based on the angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) study, we also obtain the spin-orbit splitting value of the valence band at the K point. Moreover, applying the same approach, we grow and characterize Janus SeWS MLs and provide a comparative analysis with the Janus SeMoS system.

[1] Z. Gan et al., Adv. Mater. 34, 2205226 (2022).

SUN 10

Double tips for in-plane polarized near-field microscopy and spectroscopy

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Near-field optical microscopy and spectroscopy provide high-resolution imaging be-

low the diffraction limit, crucial in physics, chemistry, and biology for studying molecules, nanoparticles, and viruses. These techniques use a sharp metallic tip of an atomic force microscope (AFM) to enhance incoming and scattered light by excited near-fields at the tip apex leading to high sensitivity and a spatial resolution of a few nanometers. However, this restricts the near-field orientation to out-of-plane polarization, limiting optical polarization choices. We introduce double tips that offer in-plane polarization for enhanced imaging and spectroscopy. These double tips provide superior enhancement over single tips, although with a slightly lower spatial resolution ($\approx 30\text{nm}$). They enable advanced studies of nanotubes, graphene defects, and transition metal dichalcogenides, benefiting from polarization control. The double tips allow varied polarization in tip-enhanced Raman scattering and selective excitation of transverse-electric and -magnetic polaritons, expanding the range of nanoscale samples that can be studied.

SUN 11

Gate-tunable magnons in CrSBr

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In the 2D antiferromagnet CrSBr, a femtosecond laserpulse can excite coherent acoustic and optical magnons which travel several micrometers, making them promising for future magnonic devices. Additionally, magnetic order is closely coupled to the excitation energy in CrSBr, providing easy access to magnetic dynamics using time-resolved reflectivity measurements. We study the effect of a combination of perpendicular electric field F and electron density n on magnon dynamics in three-layer CrSBr. Both magnon frequencies increase by up to 10% with doping, however, their complete gate-dependence is complex and differs for the two modes. The reason for this lies in the influence of n and F on the magnitude of the magnetic moment as well as internal effective fields governing magnon dynamics, which can be modelled using a macrospin approximation. As we detect an asymmetry in the gating behavior of top and bottom layer in photoluminescence measurements, we extend the usual bulk macrospin model to include layer-dependent internal fields. In combination with capacitor model to estimate n and F , we can qualitatively reproduce the gate-dependent behavior of the magnonic frequencies.

SUN 12**Delocalized pi-d spin 1/2 state in a single-component molecular magnet**Abdou Hassanien¹, Biao Zhou², Akiko Kobayashi²¹Department of Condensed Matter Physics, Jozef Stefan Institute, Ljubljana, Slovenia²Department of Chemistry, Nihon University, Tokyo, Japan

Interests in π -d charge transfer complexes stem from the fact that the electronic properties can be systematically manipulated by changing the type and/or the stoichiometry of donor and acceptor constituents. However, to induce strong coupling between the frontier orbitals, another design of molecular system was developed in which the charge transfer is promoted within a single molecular unit. Here we study the atomic-scale electronic properties of single component molecular magnet Au[tmdt]₂; where the ligand tmdt is Trimethylenetetra-thiafulvalenedithiolate. The atomic-scale spatial variation of Kondo resonance shows evidence of intramolecular doping as the valence electrons traffic across the frontier orbitals. By taking advantage of both orbital and spin degrees of freedom, this spin 1/2 molecule possesses robust anisotropic magnetic moment which is an essential ingredient for molecular electronics.

SUN 13**Resonance Raman and DFT analysis of structural and point defects in transparent conductive oxide SnO₂:X (X=Ta, F)**Matthias Krause¹, Carlos Romero Muñiz², Frans Munnik¹, Justus Haag¹, Ramon Escobar Galindo³¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany²Departamento de Física de la Materia Condensada, Universidad de Sevilla, Sevilla, Spain³Departamento de Física Aplicada I, Universidad de Sevilla, Sevilla, Spain

Structural and point defects have a crucial influence on the electronic and optical properties of transparent conductive oxides. In this contribution we characterize different types of defects in SnO₂:X (X=Ta, F) by the combination of laser-wavelength dependent Raman spectroscopy and state-of-the-art density functional theory (DFT) calculations using hybrid functionals.

Sn-vacancy- and O-interstitial-type point defects are found in transparent conductive SnO₂:Ta thin films grown at 575 °C. These defects are responsible for strong, fingerprint-like Raman lines out of the phonon range of SnO₂,¹ which are resonance-enhanced in the visible spectral range. The defects induce strong distortions of the electronic structure in the upper range of the valence band of Ta-doped SnO₂. Moreover, the DFT calculation reveal a localized, molecular nature of the O interstitial and a delocalized nature of the Sn vacancy defect. Secondary Sn oxide phases were identified in commercial, conductive SnO₂:F samples and in non-conductive

SnO₂:Ta thin films deposited at low temperatures.

¹ M. Krause, et al., J. Mat. Chem. A 11, 17686-17698 (2023).

SUN 14

Optical Control of Josephson Junctions towards Energy-Efficient Neuromorphic Computing

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Josephson Junctions (JJ) are intrinsically capable of replicating key neuronal behaviours, making them promising candidates for neuromorphic computing. In contrast to conventional CMOS technologies, high-T_C JJs offer an energy-efficient alternative that operates at higher speeds. We address the currently missing integrated memory element by introducing active links between superconducting materials. Therefore, semiconducting 2D materials are utilized as optically active gates, which can be tuned via light pulses as external stimuli. The ultimate goal is to achieve optical control of the critical current I_C through the controlled photodoping of 2D semiconductors. As an initial step, we prepare hybrid structures consisting of WS₂ and high-T_C JJ materials based on yttrium barium copper oxide (YBCO) by van der Waals assembly. A combination of Raman and photoluminescence spectroscopy, spectroscopic ellipsometry as well as photocurrent measurement is used to characterize those hybrid structures.

SUN 15

Bridging the gap between carbyne and carbon atomic wires

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Carbyne, the elusive 1D sp-hybridized carbon allotrope, remains unrealized in bulk form. While carbon atomic wires (CAWs), short-chain precursors to carbyne, are well-studied, carbyne has only been realized as confined carbyne within nanotubes [1 – 3]. The transition from CAW to carbyne, however, remains poorly understood. Here, we present a systematic Raman spectroscopy study of size-selected CAWs encapsulated into chirality-sorted single-walled carbon nanotubes. Encapsulation causes a redshift in CAW's collective Raman mode, indicating a bond length alternation relaxation due to confinement inside nanotubes. We observe a Raman combination mode between the nanotube and chain, absent in confined carbyne,

marking it as a feature for confined CAWs. The confined CAW's collective LO-phonon mode approaches the frequency of confined carbyne's C-mode, suggesting that convergence to length-independent properties in linear carbon wires inside carbon nanotubes occurs at shorter chain lengths than previously thought.

- [1] C. S. Casari et al., *Nanoscale*, 2016, 8, 4414–4435
- [2] J. M. Lechner et al., *Chin. Phys. B*, 2022, 31, 127801
- [3] P. Marabotti et al., *Carbon*, 2024, 216, 11850

SUN 16

Fabrication of Graphene-TMD heterostructures

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In contrast to semi-metallic graphene, some of 2D TMDs show semiconducting properties offering interesting applications in optoelectronic devices. However, state-of-the-art TMD syntheses often face poor crystallinity of the 2D layers and chemical degradation when exposed to the environment. In our study, we propose a single solution based on a simple idea to fabricate the TMD structures under graphene. These 2D heterostructures were prepared in one step, where the precursor thin metal film was covered by a graphene oxide layer and subsequently annealed in the presence of chalcogen. During annealing, the TMD layer is formed while graphene oxide is reduced to graphene. The graphene serves as a protective layer and avoids oxidation/decomposition of TMD material. We will present how the graphene layer on the top of the metal will influence the crystallinity and spatial orientation of the final TMD films.

SUN 17

Growth of CVD single layer graphene on rigid catalytic substrates

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Currently, graphene is mostly grown on flexible Cu foils. However, the low reproducibility of such substrates, as well as the challenge in achieving the desired Cu crystal orientation, has highlighted the need of exploring alternative substrates for graphene growth. In this work, we investigate the deposition of Cu onto sapphire substrates, obtaining Cu rigid thin film as the catalytic substrate with controlled crystal quality. Here, we have studied the influence of the Cu annealing parameters (temperature, gas flow and time) to optimize the production of homogeneous, large-

scale, single layer graphene. The quality of the grown graphene is morphologically and electrically evaluated and compared with the standard technology based on Cu foils. Moreover, we propose an alternative graphene transfer method, avoiding manual intervention, suitable for upscaling and semi-automatization. The use of a flat rigid surface enables the deposition of inorganic thin layers on pristine graphene, avoiding direct contact of graphene and polymer-based supporting layers and resins.

SUN 18

Supramolecular interactions in nanostructured biofilm composites

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The physical and chemical characteristics of graphene-based nanostructured hybrid biomaterials enable them to be used in a wide range of applications in both medical and industrial fields. However, there remains a gap in understanding the formation of nanocomposites made from chitosan and graphene, and their intrinsic interaction with plasmonic nanoparticles. Our study offers a comprehensive understanding of the interaction between chitosan and graphene in the formation of graphene–chitosan nanocomposites with gold or silver nanoparticles. By combining spectroscopic techniques and DFT calculations, we were able to uncover the mechanism and driving forces behind these supramolecular interactions. We demonstrate the physical/chemical interactions based on the protonation of the amine groups of chitosan. In chitosan, the proton's net charge is $+0.41e$, which makes it possible to functionalize graphene locally. The charge transfer interaction that occurs during the formation of graphene and chitosan composites can be controlled in the development of biocompatible reinforced biofilms, which are important for the material sciences and biomedical engineering fields.

SUN 19

One-dimensional graphene nanomaterials as active laser media

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One-dimensional graphene nanomaterials – single-wall carbon nanotubes (SWNTs) and narrow graphene nanoribbons (GNRs) demonstrate a high potential for using as active media in lasers [1]. They work in a wide spectral range due to the size-dependent electronic density. The quantum yield of photoluminescence (PL) for

SWNTs is about 3-7%, while for GNRs it reaches several tens of percents. PL can be observed even by naked eyes. The PL lifetime measured appeared to be of 7.1 ns.

In this work we studied 2 types of samples: the suspension of 7-armchair graphene nanoribbons (7-AGNRs) in toluene and the 7-AGNRs deposited on polystyrene microspheres (with diameter of 6 μm) serving as microresonators. The GNR films were synthesized via a CVD method based on the “bottom-up” approach from DBBA molecules on Ni foil [2]. The PL gain was measured with 3 lasers (with different pulse durations). The results obtained confirm a good prospective for one-dimensional graphene structures to serve as active laser media.

1. Jia-Shiang Chen, ACS Nano 16 (2022) 1677.
2. P.V. Fedotov, J. Phys.Chem. C 124(47)(2020) 25984.

SUN 20

Interactions Between Two-Dimensional Crystals and Molecules via Density Functional Theory

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The unique properties of two-dimensional (2D) materials can be modified through chemical functionalization, driven by interactions with functional groups or molecules. Density functional theory (DFT) calculations are used to investigate non-covalent functionalization of bilayer graphene with 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN). The interactions between the graphene layers and the HATCN molecules play a significant role in determining the functionalization behavior, which depends on the stacking arrangement. Locally stacked regions in the moiré lattice of twisted bilayer graphene (tBLG) play a crucial role for functionalization. Consequently, the moiré pattern of tBLG can serve as a template to control the degree of functionalization [1]. Laser-triggered covalent functionalization of molybdenum disulfide (MoS_2) enables the fabrication of patterned 2D heterostructures with phenyl-based interface linkers. Through DFT calculations, various potential binding motifs and their associated optical properties are predicted. Calculations of reaction energies and Raman modes provide insight into the likelihood of different reaction pathways and the structures they yield.

[1] T. Dierke, S. Wolff et al., Angew. Chem. Int. Ed. (2024).
doi: <https://doi.org/10.1002/anie.202414593>.

SUN 21**Symmetries of excitons and selection rules for optical/vibrational spectroscopy**

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We present a method to analyze the symmetry of excitons, calculated via the Bethe-Salpeter Equation. We show that the excitonic states transform as irreducible representations of the underlying crystalline point group, thereby avoiding the use of the hydrogenic notation of “s, p, and d excitons”. Symmetry enables us to analyze the selection rules for exciton-phonon couplings, which are an important ingredient for the understanding of Raman spectroscopy as well as of phonon-assisted luminescence spectroscopy.

We apply our method to the discussion of optically dark and bright excitons in layered boron nitride (BN). We furthermore discuss the selection rules in the phonon-assisted luminescence spectra of different stackings of BN (hBN, rBN, and BBN). We also emphasize the importance of selection rules for the understanding of interlayer exciton-phonon scattering, such as, e.g., observed in the resonant Raman spectra of hBN@WSe₂. [1]

The symmetry analysis of excitons is being implemented into the yambo code [2].

[1] <https://doi.org/10.48550/arXiv.2407.16111>

[2] www.yambo-code.eu

SUN 22**Polariton tuning in beta-phase gallium oxide via isotopic substitution**

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In recent years, phonon polaritons (PhPs) - hybridised modes arising from the strong coupling of infrared light to lattice vibrations - have shown great promise for harnessing light at sub-wavelength dimensions with reduced losses. In particular, low-symmetry crystals, such as uniaxial and biaxial, possess hyperbolic regimes in which PhPs become highly directional. We have shown in previous work [1,2] that 16O β -phase gallium oxide (bGO), with a monoclinic crystal structure, supports hyperbolic shear polaritons with even higher directionality due to broken mirror symmetry in the real-space propagation. Here, we report near-field microscopy scans of polaritons in isotopically substituted 18O bGO films epitaxially grown on a 16O bGO substrate, measured at the free-electron laser facility FELBE (HZDR). We experimentally prove a significant red shift of about 45 cm^{-1} of the 'polaritonic' spectral region by isotopic substitution.

[1] Passler, N.C., et al., Nature (2022)

[2] Matson, J., Wasserroth, S., et al., Nat. Comm. (2023)

SUN 23

Nano-Raman Analysis of Nanoprotuberances in MoSe₂/hBN Heterostructures

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Nanoprotuberances that emerge during the fabrication of heterostructures can affect structural and optical properties of a material. In this study, we examine their impact on a monolayer MoSe₂ sample deposited on hBN using a dry stamping technique [1]. The selected regions, where these formations range from 50 to 200 nm in diameter and reach an average height of about 15 nm, were investigated through atomic force microscopy (AFM) mapping and tip-enhanced Raman spectroscopy (TERS) [2]. By correlating topographical features with spectroscopic variations at the nanoscale and performing a statistical analysis of the nanostructures, changes in local chemical composition were observed, likely associated with contamination or trapped gases.

[1] Naito, Hibiki, et al. Nanoscale Advances 5.18 (2023): 5115-5121.

[2] Jorio, Ado, et al. 2D Materials 11.3 (2024): 033003.

SUN 24

Nitrogen-doped MoTe₂/graphene heterostructure

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Chemical doping of 2D materials is a straightforward method to tune their physical properties. Nitrogen doping of graphene is a prime example, where the n-type dopant allows the control of the band structure and the realization of p–n junctions, the building blocks of electronic devices [1]. In this work we study the structural and electronic properties of nitrogen-doped single layer MoTe₂ grown on graphene [2]. Utilizing nitrogen plasma treatment, we are able to incorporate nitrogen atoms and clusters into the top MoTe₂ layer. We investigated the doped MoTe₂/graphene heterostructure with scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. Our results show that nitrogen atoms are frequently situated in Te vacancies, where they create localized electronic states inside the band gap of MoTe₂. From our DFT calculations we found that this nitrogen defect hosts magnetic moment at charge neutrality, which vanishes at larger electrical doping. This enables us to electrically tune the magnetic properties of the heterostructures.

[1] M. Bouatou et al., *Adv. Funct. Mater.* 32, 2208048 (2022)

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

SUN 25

Photoluminescence from Silica-Coated Functionalized Single-Walled Carbon Nanotubes

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A single-photon source is a critical component for developing quantum communication and computing devices. Functionalized single-walled carbon nanotubes (f-SWCNTs) are among the promising solid-state platforms for creating these sources, with key advantages such as room-temperature operation and the ability to tune the emission wavelength. In this study, we investigate the impact of a SiO₂ protective coating on the optical properties of f-SWCNTs.

The (6,5) nanotubes were modified with aryl diazonium salt, exhibiting a PL peak in the 1150 nm area, which corresponds to the ortho⁺ geometry of the sp³ defect attachment. A SiO₂ surface shell was formed using a modified Stöber method to shield the emitter from environmental factors. This shell significantly alters the local dielectric environment, resulting in a red-shifted peak that indicates a different geometry of the sp³ defect attachment (ortho⁺⁺).

This approach enables the use of nanotubes as single-photon sources operating at room temperature and at telecommunication wavelengths, expanding their potential for practical applications.

SUN 26

Towards a Universal Assignment of Confined Carbyne's C-mode frequency to host nanotube chirality

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The experimental study of long linear carbon chains within double-walled carbon nanotubes, i.e., confined carbyne (CC), has paved the way for unraveling carbyne properties [1,2]. Elucidating how CC properties evolve with larger-diameter nanotubes, where interactions with the CC weaken, enables predictions of carbyne behavior in vacuum. Raman spectroscopy of isolated CC revealed a linear relationship between its C-mode frequency and the inner nanotube diameter [2]. However, these findings were limited to nanotubes/CCs with diameters/C-modes below 0.75 nm/1835 cm⁻¹ due to the need of overlapping optical resonances. Here, we overcome this using resonance Raman spectroscopy to independently analyze CC and host nanotubes at their respective resonances. By co-localizing their spectra's positions, we establish a correlation between CC's C-mode frequencies up to 1865 cm⁻¹ and inner nanotubes with diameters up to 0.818 nm. Our results align with prior models [2] and expand the dataset to include larger nanotubes, filling the gap toward a non-confined environment.

[1] Shi et al., Nature materials 15.6 (2016): 634-639

[2] Heeg et al., Nano letters 18.9 (2018): 5426-5431

SUN 27

A novel ultra wide bandgap semiconductor: rutile Germanium Oxide

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The realization of ultra-wide band gap material (UWBGM) based devices has been pursued in recent years as UWBGM are promising in particular for high-power applications and deep-UV electronics. In 2019, rutile Germanium oxide has been theoretically predicted as an UWBGM with excellent physical properties [1]. Yet, synthesis

has been long limited to mm-sized crystals and low consensus over many measured properties is found in literature, possibly due to limited crystal quality.

Recently, growth of large volume single crystals with high crystal perfection and high electrical conductivity has been achieved [2], allowing careful characterization of the material's properties.

In the presented study, we focus on the findings obtained by polarization resolved Raman spectroscopy, with which we are able to resolve the decade spanning discussion about the Raman active phonon's energies and determine their relative Raman tensor elements, relevant for simulation of phonon derived properties, such as heat transport or phonon mediated optical transitions. Our experimental observations are accompanied by DFPT calculations.

[1] Chae et al., APL 102104 (2019)

[2] Galazka et al., pss(b)

SUN 28

Exciton Finestructure in $(\text{PEA})_2\text{PbI}_4$

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The exceptional optoelectronic performance of Ruddlesden-Popper perovskites, despite inherent imperfections, raises fundamental questions about photophysical relaxation pathways and the origin of distinct excitonic features. Recent studies have identified multiple exciton bands in 2D perovskites, but the underlying mechanism –whether excitonic, polaronic, or Rashba-related– appears unresolved [1-3]. To address these competing hypotheses, we studied spectra of mechanically exfoliated $(\text{PEA})_2\text{PbI}_4$ using temperature-dependent photoluminescence measurements in addition to first-principles GW and Bethe-Salpeter calculations. Below 60 K, exciton bands break into individual transitions. Evidence for their excitonic nature is provided by power- and polarization-dependent PL measurements, as well as calculated transition dipole moments. Our findings offer new insights into exciton fine structure and optical transitions in 2D perovskites, deepening understanding of their photophysical properties.

[1] Do et al., Nano Lett. 2020, 20, 7, 5141–5148.

[2] Posmyk et al., Adv. Optical Mater. 2023, 2300877.

[3] Zhai et al., Sci. Adv. 2017, 3 : e1700704.

SUN 29

Short-range and long-range magnetic ordering in FeCl_3 monolayers

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Two-dimensional ionic crystals offer a compelling platform for engineering magnetic properties. In particular, molecules intercalated within graphene sheets benefit from environmental protection and charge exchange with the host graphene. Our study centers on FeCl₃ intercalated compounds, where we employ three inelastic light scattering techniques to investigate phase transitions within these heterostructures. First, quantum spin fluctuations are evidenced by a broad peak at low energies, with its intensity corresponding to the magnetic specific heat. Secondly, we detect phonon anomalies, characterized by deviations in the Raman mode shifts and broadening from classical expectations. Finally, we examine the charge transfer mechanism between graphene and FeCl₃, wherein changes in electron distribution alter graphene's doping level, resulting in Raman intensity variations as a function of temperature. By cross-analyzing these results we identify the temperature of long-range and short-range ordering.

SUN 30

Efficiently and accurately describing large-scale moiré superstructures

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Moiré superlattices strongly influence material properties, leading to several competing many-body phases in, e.g., twisted bilayer graphene close to the magic angle. However, the resulting large unit cells make a theoretical description of these superstructures challenging. Competing approximations to nevertheless efficiently model these systems include, e.g., the Bistritzer-MacDonald [1] model in momentum space, or a real-space tight-binding simulation based on density functional theory [2]. We compare these models for twisted bilayer graphene to each other as well as recent experiments [3], and suggest modifications to better include strain, local reconstructions as well as substrate effects. The resulting effective models serve as starting point for many-body descriptions.

[1] R. Bistritzer, and A. H. MacDonald, Moiré bands in twisted double-layer graphene PNAS 108, 12233 (2011)

[2] N. Giroto, L. Linhart, and F. Libisch, Coupled phonons in twisted bilayer graphene, Phys. Rev. B 108, 155415 (2023)

[3] A. Rothstein et al., Band gap formation in commensurate twisted bilayer graphene/hBN moiré lattices, Phys. Rev. B 109, 155139 (2024)

SUN 31

Electron-Phonon Interaction in Bilayer Graphene Quantum Dots

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We report progress in studying electron-phonon interactions in bilayer graphene double quantum dots (DQDs) using charge detection techniques. By operating the charge detector at a large bias, we generate non-thermal excitations in the DQD, which alter the occupation statistics of the quantum states. These changes are subsequently detected by the charge detector. Our measurements near the degeneracies of different DQD charge states reveal detector signals that can be interpreted as fingerprints of the specific excitation spectra. For selected charge states, we observe oscillatory detector signals as a function of DQD detuning, which could potentially be linked to a phonon interference effect. Although similar interference effects have been previously observed in semiconductor QDs made from other materials, such effects are expected to be particularly pronounced in 2D materials like bilayer graphene. Due to their reduced dimensionality an alignment of the DQD axis and the phonon propagation direction is more likely. Overall, our findings are expected to contribute to the understanding of the recently measured spin- and valley-relaxation rates in bilayer graphene quantum dots.

SUN 32

Intrinsic and radiative losses in plasmonic supercrystals

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Plasmonic nanoparticle crystals are novel materials formed by metallic nanoparticles arranged in a face-centered cubic lattice (Schulz 2020). Within these structures, light is confined into hotspots between the nanoparticles, significantly enhancing light-matter interaction and leading to plasmon-polaritons in the deep-strong light-matter coupling regime (Mueller 2020). In this study, we investigate the loss mechanisms and plasmon-polariton lifetime in plasmonic crystals. We measured the full width at half maximum of the absorption peaks for a crystal composed of nanoparticles with diameters of 79 nm and a thickness of up to 2 μm . We obtained transmission values up to 34%, despite the metal fraction of the crystal being 0.64 and the skin depth of gold being approximately 15 nm in this energy range. Using the Lorentz model and treating the crystal as an open cavity, we calculated the intrinsic losses of the crystal to be $\Gamma = 100$ meV. Our findings reveal that increasing the crystal thickness reduces losses below the intrinsic limit, indicating that radiative losses dominate.

SUN 33**Corrugation-dominated mechanical softening of defect-engineered graphene**Rika Saskia Windisch¹, Wael Joudi², Jani Kotakoski², Florian Libisch¹¹Theoretical Physics, Technical University of Vienna² Faculty of Physics, University of Vienna

We perform molecular dynamics simulation of a graphene membrane using a machine learned force-field in order to provide theoretical insight to the findings of [1], where the decrease of two-dimensional (2D) elastic modulus with increasing vacancy density is related to enhanced corrugation caused by vacancies. We investigate the equilibrium corrugation as a function of membrane size for different types and concentrations of vacancies. We find that double vacancies lead to a substantially increased corrugation of the membrane, while single vacancies have no effect, which is in good agreement with the model presented in [1]. A step-wise increase in supercell size simulates pulling on the membrane to determine its 2D elastic modulus. We compare the simulation results for the 2D elastic modulus with their experimental data acquired by AFM nanoindentation and confirm that the drastic decrease is primarily caused by vacancy-induced surface corrugation.

[1] Wael Joudi, Rika Saskia Windisch, Alberto Trentino, Diana Propst, Jacob Madsen, Toma Susi, Clemens Mangler, Kimmo Mustonen, Florian Libisch and Jani Kotakoski, submitted (2024)

SUN 34**Exciton transfer and interface excitons in mixed-dimensional heterostructures**N. Fang^{1,2}, Y. R. Chang¹, S. Fujii^{2,3}, D. Yamashita^{2,4}, M. Maruyama⁵, Y. Gao⁵, C. F. Fong^{1,2}, D. Kozawa^{1,2,6}, K. Otsuka^{1,7}, K. Nagashio⁸, S. Okada⁵, Y. K. Kato^{1,2}¹Nanoscale Quantum Photonics Laboratory, RIKEN Cluster for Pioneering Research, Japan²Quantum Optoelectronics Research Team, RIKEN Center for Advanced Photonics, Japan³Department of Physics, Keio University, Japan⁴Platform Photonics Research Center, National Institute of Advanced Industrial Science and Technology (AIST), Japan⁵Department of Physics, University of Tsukuba, Japan⁶Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan⁷Department of Mechanical Engineering, The University of Tokyo, Japan⁸Department of Materials Engineering, The University of Tokyo, Japan

Two-dimensional van der Waals heterostructures have introduced unconventional phenomena that emerge at atomically precise interfaces, and further development is expected in mixed-dimensional heterostructures. Here we discuss exciton physics in 1D-2D heterostructures consisting of one-dimensional carbon nanotubes and two-dimensional tungsten diselenide. Both the chirality and the layer number are

identified before assembling the heterostructures, allowing for investigation of the band alignment effects. For small band gap nanotubes corresponding to type I band alignment, exciton transfer is observed [1]. For large band gap nanotubes corresponding to type II band alignment, exciton transfer diminishes and localized interface excitons exhibiting room-temperature quantum emission is observed [2]. With mixed-dimensional van der Waals heterostructures where band alignment can be engineered, new opportunities for quantum photonics are envisioned.

[1] N. Fang *et al.*, Nature Commun. 14, 8152 (2023).

[2] N. Fang *et al.*, Nature Commun. 15, 2871 (2024).

SUN 35

Strain-tuning Moiré excitons in 2D Heterostructures

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Tunable-moiré superlattices hold potential for programmable quantum emitters, exotic quantum phases and resonant-hybridization of excitonic states. In this poster, I will discuss our results on strain-tuning interlayer and intralayer moiré excitons in 2D Transition Metal Dichalcogenides (TMDCs). Employing electrostatic actuation, we apply upto 2% controllable, tensile strain to a suspended WS₂/WSe₂ heterostructure. Photoluminescence and reflectivity measurements reveal the excitonic energies to be red-shifting with different strain gauges on the order of hundreds of meV/%, thus enabling fingerprinting of valley-character for moiré excitons. Moreover, we observe energetic resonance between inter- and intralayer moire species at higher applied strain, leading to a new hybrid, lowest-energy state for the system. The results present exciting new possibilities for strain-tunable moiré species and strongly correlated electron systems.

SUN 36

Gold Nanoparticles Electrically Coupled to Polymer-Wrapped Semiconducting Single-Walled Carbon Nanotubes for Biosensors

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Semiconducting single-walled carbon nanotubes (sc-SWCNTs) are excellent materials for electronic biosensors, due to their electrical conductivity, high specific surface area, sensitivity and ability to be functionalized with specific recognition units. Sensor performance depends on efficient signal transduction between the recognition unit and the sc-SWCNT. In this work, metallic nanoparticles (NPs) were attached to sc-SWCNTs as linker units for recognition probes and acted as signal passthroughs. We used sc-SWCNTs wrapped with poly(9,9-di-n-dodecylfluorenyl-2,7-diyl-alt-2,2'-bipyridine-5,5') (PFBPy-5,5'). The 5,5'-linkage of the BPy monomer

facilitates metal chelation and provides tight chemical anchoring. We grew AuNPs on sc-SWCNTs@PFBPY-5,5' using electrochemical reduction of Au ions. A cortisol sensor was prepared by attaching thiol-terminated cortisol aptamers to the sc-SWCNT@PFBPY-5,5'+AuNP system and integration into an electrolyte-gated field-effect transistor. The biosensor, operating in 1X PBS buffer, provided excellent response to cortisol in the range of 1 – 1000 nM, overlapping with the sweat-cortisol physiological range.

SUN 37

Exciton transport in lateral TMD heterostructures

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Lateral heterostructures built of monolayers of transition metal dichalcogenides are characterized by a thin 1D interface exhibiting a large energy offset. Recently, the formation of spatially separated charge-transfer (CT) excitons at the interface has been demonstrated. The impact of these CT excitons on the exciton propagation across the interface has remained undiscovered yet. In this work, we microscopically investigate the spatio-temporal exciton dynamics in hBN-encapsulated lateral MoSe₂-WSe₂ heterostructures and reveal a counterintuitive thermal control of the unidirectional exciton propagation across the interface. We observe that exciton propagation becomes less efficient when the temperature is decreased from 300 K to 150 K, which is the opposite compared to the typical mobility dependence on temperature in conventional semiconductors. We trace this back to the efficient capture into CT excitons, also resulting in high densities at the interface. We demonstrate clear signatures accessible in far- and near-field photoluminescence experiments. Our microscopic results provide crucial understanding of the unidirectional exciton transport in lateral heterostructures.

SUN 38

Roll-to-Roll Polymer Membranes with 2D Upright and Size-Tunable Subnano channels for Ultrahigh Permeance and Selectivity Sieving

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Subnanochannel membranes enable an energy-efficient way for ion separation,

serving as the “heart” in many ion-separation apparatus. However, a permeability-selectivity trade-off effect sets an upper bound on ion-separation performance. Here, we demonstrate a shear-controllable self-assembly strategy for scalable production of membranes which breaks the permeability-selectivity trade-off. Continuous photopolymerization allows the membrane preparation in a meter scale. Controllable self-assembly enables the size tunability of membrane channels in the range of 0.4 - 1.0 nm, which covers most of ionic hydration diameters and ensures high ionic selectivity. The membranes have self-contained water content, straight paths, two-dimensional morphology and cross-membrane orientation. Breaking the permeability-selectivity trade-off brings the ion-separation efficiency of the membranes to a record level, as demonstrated by 10 times increase in the permeance/permeability without sacrificing high ionic sieving/rejection ratio, for applications of reverse-osmosis based salt-lake lithium extraction and forward-osmosis based seawater desalination.

SUN 39

Fabrication of electronic structures based on WS₂ films

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Tungsten disulfide (WS₂) is a prominent member of the family of Transition Metal Dichalcogenides (TMDs). WS₂ layers have great potential in various applications, such as electronic devices, and sensors. We prepared electronic structures based on few-layers WS₂. Tungsten films were patterned by the photolithography and lift off process and subsequently annealed in one-zone reactor with sulfur powder. Different thicknesses, substrates, and growth parameters were studied in order to prepare the films with different orientations (horizontally aligned, vertically aligned, polycrystalline). The WS₂ layers were characterized by various methods, such as Raman Spectroscopy, X-Ray Diffraction, Grazing Incidence Wide Angle X-Ray Scattering, or Atomic Force Microscopy. The prepared devices were evaluated in relation to the thickness and orientation of the WS₂ layers.

SUN 40

Temperature-Induced Synchronization of Vibrational Modes in alpha-Glycine Single Crystals

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Synchronization is a phenomenon where two or more incoherent oscillators couple and align their frequencies and phases. Despite its abundance in nature, such as in the unified flashing of fireflies and synchronous neuron pulses in the brain, it has not been observed in vibrations in materials. In this work, by employing temperature-dependent Raman spectroscopy, we study the unconventional evolution of two specific vibrational modes of α -glycine. Instead of broadening or merging due to a structural phase transition, the peaks asymmetrically shift and eventually coalesce into a single feature. To explain this phenomenon, we developed a Green's function-based model incorporating explicit coupling between the two modes through a dissipative mechanism. With increasing temperature, enhanced coupling between the modes drives them to oscillate in phase and match their frequencies, resulting in their eventual synchronization. This coupling-driven coherence challenges the conventional expectation that higher temperatures increase vibrational disorder, demonstrating instead that thermal effects can enhance vibrational coherence.

SUN 41

Rational Ambipolar Doping of Single-Walled Carbon Nanotubes via Covalent Charge-Transfer Engineering

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Precisely controlling the doping level of single-walled carbon nanotubes at the individual particle scale unlocks new opportunities for their application. While electrochemical gating enables fine-tuned modulation of the Fermi level, it is typically applied to ensembles of nanotubes rather than individual ones. Conversely, the introduction of charge transfer molecules within the nanotubes allows doping at the single-nanotube level but lacks precise regulation of the transferred charge. In this study, we present an alternative approach based on covalently attached, custom-synthesized charge-transfer compounds. This strategy preserves the π -conjugation of the carbon framework, thereby maintaining the nanotubes' optoelectronic properties. By precisely controlling the number of functional groups attached to the tubes, we can regulate charge transfer in a systematic manner, enabling a seamless transition from p-doping to n-doping. Furthermore, our approach employs a rational ambipolar design that exploits the same molecular building blocks -methoxy groups attached to aniline rings- while achieving either electron donation or withdrawal, depending on the assembly configuration.

SUN 42**Enhancing Metal-Graphene Nanoribbon Contacts via Electrode Engineering and Post-Processing**

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Bottom-up synthesized graphene nanoribbons (GNRs) are gaining increasing attention due to their ability to precisely define structural features, such as width and edge functionalities. This level of structural control opens up the possibility of replacing traditional electronic components, such as field-effect transistors, with GNR-based devices. However, the poor contact quality between GNRs and metal electrodes significantly hinders the performance of these devices, as the voltage drop predominantly occurs at the contact interface. In this work, we investigate strategies to improve the contact quality by employing different electrode materials and incorporating post-processing procedures. Specifically, we fabricated electrodes with nanogaps (≈ 20 nm) using high work function metals such as palladium, platinum, and gold. After establishing contact with the GNRs, we applied gentle annealing treatments. Our results demonstrate that annealing significantly enhances the contact quality between noble GNRs and noble metals.

SUN 43**Resonators for reading out topological Qbits**

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Our goal is to optimize the geometry, material parameters and lithographic processing of superconducting co-planar waveguide resonators. The quality factor of these resonators is of particular importance for two-tone microwave spectroscopy measurements and transmon qubit experiments. In conjunction with the resonator is a topological insulator Josephson junction. The lithographically fabricated junction is based on an epitaxial mercury cadmium telluride heterostructure and is embedded into a rf squid loop. Resonator and rf squid chips are coupled inductively using a flip chip method. This approach allows for example the observation of Andreev bound states by two-tone spectroscopy measurements. Our preliminary experiments already demonstrate the presence of Andreev bound states. The scientific goal is now to identify Andreev levels with topological properties that originate from Majorana

ranas, i.e., midgap or Majorana bound states. To this end, we are pursuing several approaches to improve the quality of the signal.

SUN 44

Implementing spiking neurons with filamentary memristors for signal processing in neuromorphic computing

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Spike-based neuromorphic computing emerges as an efficient computing solution with sparse, asynchronous spatiotemporal spike-based information representation. The key for the realization lies in spiking neuron implementation. Though thus far multiple neuron models have been developed, spiking neuron implementation with silicon electronics can suffer from large and complex circuitry and high-power consumption. Emergent threshold switching memristors (TSMs) with distinct self-rest threshold switching are promising for enabling compact spiking neurons designs. Herein, we model the switching behavior of TSMs in standardized Verilog-A and design a TSM-based spiking neuron on Cadence Virtuoso. The neuron has a compact circuit, and can process both digital and analog signals for neuromorphic computing. Particularly, to realize signal processing with high data throughput in parallel, the neuron is designed to simultaneously process multi-channel signals. To verify the feasibility of practical implementation of our neurons, we fabricate TSMs from solution-processed hexagonal boron nitride, and implement spiking neurons capable of performing spike-based digital and analog signal processing.

SUN 45

Probing the electronic band structure of the 2D magnetic materials MPS_3 (M=Fe,Ni) across magnetic phase transitions

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We investigate the band structure of the van der Waals materials FePS_3 [1] and NiPS_3 , both 2D antiferromagnetic insulators, using μm scale Angular Resolved Photoelectron Spectroscopy (ARPES), above and below their Néel temperatures (T_N). The data is compared with DFT+U calculations in combination with simplified selection rules to deduce the orbital character of changing bands. In FePS_3 , we ob-

serve three distinct band structure changes across T_N , involving bands with Fe 3d, S 3p, and pure P 3p orbital character, reflecting the intricate competition of direct exchange between the Fe atoms and superexchange via S and P atoms, partially involving third nearest neighbors. In NiPS₃, we identify one characteristic band shift near Γ across T_N , containing a band of mixed Ni and S character. In that case, pronounced deviations from the DFT+U calculations point to a strong influence of more complex electronic correlations. In addition, we refine the photoelectron selection rules using μ -ARPES data from CrPS₄.

[1] B. Pestka et al., ACS Nano 2024, <https://doi.org/10.1021/acsnano.4c12520>

SUN 46

The resonant Raman response of confined carbyne is solely driven by anharmonic interactions

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The resonant Raman response is due to electronic and vibrational excitations. Interestingly, the resonant Raman fingerprint of confined carbyne is highly unconventional and comes concomitant to several new features which can neither be assigned to the hosting tube, nor to the linear carbon chain a.k.a carbyne. This identifies the tube-chain system as a true hybrid structure in which the spectrum is usually driven by strong modifications in the electronic excitations via charge transfer. Surprisingly, we show that the electronic structure results from those of the two isolated systems and the large spectral modifications are solely due to the strong anharmonic interactions between the tube and the chain. Our work establishes confined carbyne as the ideal test system to probe strong anharmonicity in one dimension and its huge implications on the resonant Raman response.

Preprint: <https://doi.org/10.21203/rs.3.rs-5247129/v1>

SUN 47

Moire engineering of square lattice Hubbard models in 90 degrees twisted rectangular lattices

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Moiré superlattices of twisted van der Waals materials have recently attracted tremendous attention and emerge as novel platforms to simulate correlated Hubbard model physics in 2D prototype lattices. However, few studies have explored the possibility of using twisted van der Waals materials to realize and simulate correlated physics in square lattices, which is one of most important type of model lattices that are directly related to the description of the correlated physics in high-T_c cuprates and their unconventional superconductivity. Here we propose a new type of strategy to construct moiré square lattices using 90° twisted 2D rectangular lattices in this work. Using large-scale first principle calculations, we demonstrate the validity of this strategy on a series of twisted bilayer and multilayer Ge/SnX(X=S,Se) systems. We show that the low-energy moiré flat bands appearing at the conduction band edges in these systems can be well described by a simple square lattice model with up to second nearest neighbor hopping. The material platform we establish thus can be used to simulate square lattice Hubbard model physics with frustration.

SUN 48

MoS₂ growth on molten glass substrates and its device integration

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MoS₂ is a 2D semiconductor of paramount importance for More-Moore and More-than-Moore applications. This work specifically focuses on developing efficient and reliable MoS₂ Field Effect Transistors to be monolithically integrated with multiplexed graphene sensors on flexible probes for biomedical applications. To achieve this, advancements in MoS₂ growth and its integration into devices are crucial for industrial manufacturing readiness.

Metal-Organic Chemical Vapor Deposition (MOCVD) is a promising technique to prepare large-area, uniform, and coalesced mono- to few-layers of MoS₂. This study investigates the MOCVD MoS₂ growth on molten glass substrates containing alkali compounds, demonstrating its potential as an inexpensive substrate with alkali catalytic effect, which is known to enhance MoS₂ crystal grain size. Moreover, the issue of carbon contamination is also investigated, which is one of the important limitations of the MOCVD technique, due to the use of precursors with organic ligands. Additionally, the work addresses the nanofabrication challenges involved in the MoS₂ integration into devices, focusing particularly on the high-k dielectrics.

SUN 49**Electroluminescence From Carbon Nanotubes With Quantum Defects**Ralph Krupke^{1,2,3}¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe²Institute of Quantum Materials and Technologies, Karlsruhe Institute of Technology³Institute of Materials Science, Technical University Darmstadt

We present electroluminescence spectroscopy data from single-tube devices based on (7,5) carbon nanotubes functionalized with dichlorobenzene molecules and connected to graphene electrodes. We observe electrically generated, defect-induced emissions that are controllable by electrostatic gating and are strongly red-shifted compared to emissions from pristine nanotubes. These defect-induced emissions are attributed to excitonic and trionic recombination processes, as determined by correlating electroluminescence excitation maps with electrical transport and photoluminescence data. Under cryogenic conditions, additional gate-dependent emission lines are identified as phonon-assisted hot-exciton electroluminescence from quasi-levels. Furthermore, we report single-photon defect-state emission observed via second-order correlation function measurements in a Hanbury Brown and Twiss experiment. Additionally, we demonstrate the integration of electroluminescent semi-conducting carbon nanotubes into hybrid 2D-3D photonic circuits and outline our initial steps towards picosecond pulsed excitation.

Li et al., ACS Nano 2022

Li et al., ACS Nano 2024

Ovvyan et al., Nat. Commun. 2023

SUN 50**Electron Energy-loss spectroscopy of low-D materials combining high energy and momentum resolution**Thomas Pichler¹¹faculty of physics, university of vienna, vienna

Our new MORE-TEM EELS nanospectrometer with a combined high energy & q-resolution is a perfect tool to determine the energy vs. momentum (q) dispersion and lifetime of fundamental excitations of materials. This opens the so-far unexplored possibility to investigate dispersion and lifetime of phonons, plasmons & excitons in nanomaterials including molecules, 1D & 2D materials and heterostructures with few nm of lateral resolution on samples as thin as an atomic monolayer. I give an overview on our recent progress in analysing fundamental excitations such as phonons, excitons, and plasmons in 2D materials such as graphene, h-BN and transition metal dichalcogenides (TMDC). For graphene we also show new results on the plasmon dispersion including the gap opening close to the optical limit unravelling the Dirac cone in the excitation spectrum [1] concomitant to the direct observation of a vanishing EELS cross section approaching the optical limit [2].

[1] A. Guandalini, et al., *Nanoletters* 23, 11835 (2023).

[2] A. Guandalini, et al. <https://arxiv.org/abs/2406>, (2024).

SUN 51

The Electronic Structure of 1D Pd@Ni Nanospikes and Their Electrochemical Properties

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The world's sustained high demand for electricity requires the development of ever more efficient, cost-conscious catalysts for its production. Among the many catalysts based on Pd, combination of PdNi electrocatalyst has gained the great attention. Due to the nano-structural architecture plays a crucial role in the catalytic activity, we synthesized novel PdNi unsupported with carbon black catalyst in form of one-dimensional nickel nanospikes decorated by small nanometer palladium nanoparticles (Pd NPs). In this work, the impact of the changing in electronic structure of Pd@Ni catalysts on their catalytic properties was studied (XANES, EXAFS, XPS, TEM). For very small Pd crystals surrounded by a large dispersion of Ni substrate atoms, can refer to an increased metal-substrate interaction, which is associated with an increase in d-state vacancies in the Pd@Ni catalyst. This may imply a greater susceptibility to chemisorption of unsaturated hydrocarbons (acetylene, ethylene), which may be electron donors. The higher number of d-state vacancies in catalyst may indicate greater susceptibility to chemisorption of ethanol molecules, which further improves its catalytic activity.

SUN 52

Neural network pre-training for calculating vibrational and optical properties of defects in 2D materials

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Accurate defect modeling in semiconductors remains computationally challenging due to the need for large supercells to simulate their effects on electronic structure and phonons of materials of interest. We propose a novel approach combining machine learning (ML) with semi-empirical methods. This methodology aims to enable large-scale defect simulations while maintaining quantum-mechanical accuracy and description.

We develop ML-enhanced techniques (neural network-based pre-training) to model both electronic structure and lattice dynamics in semiconductor materials, with particular emphasis on layered BN and transition-metal dichalcogenides (TMDs). For the electronic properties, we extend existing ML-based tight-binding parameterization methods to handle more complex orbital configurations, including d orbitals. For vibrational properties, we use ML approaches to parameterize force-constant models for phonon dispersions and localized defect modes. This combined approach promises to overcome current computational limitations in the description of Raman and luminescence spectroscopy in the presence of defects.

SUN 53

Spatial imaging of tunable electronic properties in Bernal bilayer graphene via WSe₂ sensor layer

David Tebbe¹, Sophia Lackhoff¹, Jonas Blum¹, Takashi Taniguchi², Kenji Watanabe², Bernd Beschoten^{1,3}, Christoph Stampfer^{1,4}, Lutz Waldecker¹

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⁴Peter Grünberg Institute (PGI-9) Forschungszentrum Jülich, Jülich, Germany

In Bernal bilayer graphene the charge carrier density as well as the band gap can be tuned, making it interesting as a 2D semiconductor for quantum technological applications. Bilayer graphene has been extensively studied using electrical transport and capacitance measurement techniques. However, due to their nature, these measurements have never been able to spatially resolve the electronic properties. To achieve spatial resolution, we have placed a WSe₂ sensor layer beneath the bilayer graphene, in a double-gated device structure. The WSe₂ hosts Rydberg excitons, which are sensitive to the surrounding dielectric environment and thus sense small changes in carrier density within the bilayer graphene. These excitonic states can be resolved using white light reflection spectroscopy, which allowed us to spatially map the potential landscape in the bilayer graphene. Furthermore, we were able to image the injection of carriers on one side of the sample under an applied bias, resulting in transport through the bilayer graphene.

SUN 54**Topologically constrained atomic limits in 1D crystals**Ivanka Milosevic¹, Milan Damjanovic²¹Faculty of Physics, University of Belgrade, Belgrade, Serbia²Serbian Academy of Sciences and Arts, Belgrade, Serbia

Using line group symmetry, various manifestations of obstructed atomic limits in quasi-one-dimensional systems are explored. The analysis revisits conventional theory, emphasizing its group-theoretical aspects, and ultimately yields a theorem that effectively identifies possible scenarios. This theoretical framework is then applied to different categories of quasi-one-dimensional systems, with the obstructed atomic limit serving as the key topological indicator. The results are illustrated on specific examples using density-functional tight-binding calculations.

SUN 55**Direct Imaging of the Energy Bands of Magic Angle Twisted Bilayer Graphene with the Quantum Twisting Microscope**Jiewen Xiao¹, Alon Inbar¹, John Birkbeck¹, Shahal Ilani¹¹Condensed Matter Physics, Weizmann Institute of Science, Rehovot

One of the core mysteries of magic-angle twisted bilayer graphene (MATBG) lies in understanding the nature of its strongly interacting energy bands. While MATBG has shown topological phenomena, explained by topological Chern bands in momentum space, its electronic behavior also displayed localized moment characteristics, hinting at a real-space picture. This dichotomy has led to various theoretical models, including the topological heavy fermion model and the Mott semimetal framework, each attempting to reconcile how these contrasting features emerge within the flat bands of MATBG. Until now, no tool has been capable of imaging these energy bands at low temperatures and with high enough energy and momentum resolution to resolve these puzzles. Recently, we developed the Quantum Twisting Microscope (QTM), which utilizes momentum-resolved tunneling at a twisting van der Waals interface to directly map the energy bands of interacting quantum materials. Here I will present the first cryogenic measurements of the strongly interacting MATBG bands in momentum space.

SUN 56**Single-layer boron phosphide on metallic surfaces: screening of promising substrates by first-principles**Walter Zuccolin¹, Maria Peressi¹¹Department of Physics, Università degli Studi di Trieste, Trieste (Italy)

Single-layer hexagonal boron phosphide (h-BP) is a predicted graphene-structured semiconductor with interesting properties for photovoltaics[1].

We investigate by ab-initio calculations the ground-state properties of h-BP on (111) surfaces of different d-shell metals of groups X, XI and XII, with the aim of identifying

suitable substrates for its synthesis. Due to the lattice parameter mismatch with the substrates, the h-BP overlayer generates Moiré patterns that we describe using minimal simulation cells with a tolerance of about 3% for tensile or compressive strain applied to the overlayer.

Adhesion energy, separation, and charge transfer between substrate and overlayer, projected density of states indicate that the least interacting substrate is Ag, closely followed by Au. The epitaxial h-BP monolayer assumes a buckled structure, with a buckling which is minimum on Ag and maximum on Au.

We complete the investigation of h-BP on Ag(111) by considering also the formation of flakes of finite, small size, that are typically more strongly anchored to the substrate through their edges, zig-zag or Klein type.

[1] Suzuki T., Applied Surface Science 598 (2022) 153844

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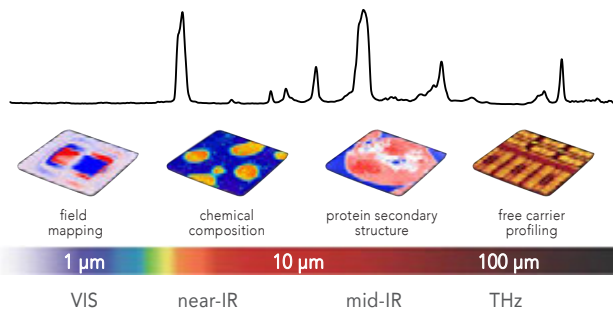
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Monday, March 10th

- 08:30 – 09:00 **M. Rossi, Hamburg**
The Quantum Properties of Hybrid Molecular Interfaces
- 09:00 – 09:30 **S. Jürgensen, Berlin**
Collective Optical States in One- and Two-Dimensional Molecular Lattices
- 09:30 – 10:00 **S. Louie, Berkeley**
Excitons in 2D Materials: Field-Driven Time-Dependent Phenomena, Nonlinear Optical Responses, and Correlated Ground State
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **A. Raja, Berkeley**
Painting Potential Landscapes on an Atomically Thin Canvas
- 11:00 – 11:30 **O. Frank, Prague**
Intricate Relations Between 2D Materials and Metals
- 11:30 – 12:00 **S. Ryu, Pohang**
Interferometric Second-Harmonic Generation Spectroscopy of Two-Dimensional Materials
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **A. Chernikov, Dresden**
Mobile, tunable Excitons in Two-Dimensional Semiconductors and Antiferromagnets
- 19:00 – 19:30 **I. Barcelos, Campinas**
Phyllosilicates as Earth-Abundant Layered Materials for Electronics and Optoelectronics: Prospects and Challenges in their Ultrathin Limit
- 19:30 – 20:00 **C. Barbec, Erlangen**
A Hybrid Workflow to Discover Tailored Functional Materials
- 20:00 **Poster II**

Monday, March 10th

08:30

The quantum properties of hybrid molecular interfaces

Mariana Rossi¹

¹MPI for Structure and Dynamics of Matter, Hamburg

Weakly bonded interfaces, commonly encountered in hybrid organic-inorganic architectures, give rise to a rich variety of nuclear motion and tunable nuclear structure that is tightly connected to diverse electronic properties in these systems. In this contribution, I will discuss how we push the limits of density-functional theory and different ab initio techniques that capture nuclear motion to unravel the properties of realistic interfaces [1].

I will discuss how they can be connected to first-principles electronic structure and machine-learning approaches [2,3]. Applications where the quantum nature of the nuclei become indispensable to assess structural and electronic properties of 2D materials and interfaces will be shown and discussed [4], as well as how these can be characterised by the simulation of experimentally observable quantities like tunneling rate constants and advanced vibrational spectroscopy [5,6].

[1] J. Chem. Phys. 154, 170902 (2021); [2] J. Chem. Theory Comput. 17, 7203-7214 (2021); [3] J. Chem. Phys. 159, 014103 (2023); [4] SciPost Phys. 16, 046 (2024) [5] J. Chem. Phys. 156, 194106 (2022); [6] J. Phys. Chem. Lett. 14, 6850 (2023)

09:00

Collective optical states in one- and two-dimensional molecular lattices

Sabrina Juergensen¹, Chantal Mueller¹, Jean-Baptiste Merceau², Eduardo B. Barros^{3,4}, Patryk Kusch¹, Antonio Setaro^{1,5}, Etienne Gaufrès², Stephanie Reich¹

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⁴Department of Physics, Technische Universität Berlin, Berlin, Germany

⁵Engineering Department, Pegaso University, Naples, Italy

Two-dimensional layers and one-dimensional nanotubes can act as templates and containers for molecules and nanomaterials. We examine the formation of well-ordered molecular lattices inside nanotubes and on atomically flat two-dimensional substrates. Using α -sexithiophene and MePTCDI (perylene derivate) molecules, we show how in such molecular lattices the optical excitations couple into collective and delocalized excitons. The coupling changes the energetics and dynamics of the molecules giving rise to characteristic optical properties like strong and narrow emission, shifted emission/absorption, and a vanishing Stokes shift. We study how the interaction with the one- and two-dimensional hosts and substrates induce hybridized states with focus on changes in the molecule-related response.

Monday, March 10th

09:30

Excitons in 2D materials: Field-driven time-dependent phenomena, nonlinear optical responses, and correlated ground state

Steven G. Louie¹

¹University of California at Berkeley and Lawrence Berkeley National Lab

Two-dimensional van der Waals materials exhibit novel photo-excited states, intriguing pump-probe responses, as well as exotic ground states. Here, we present some recent theoretical studies in their understanding and predictions. We showed that there is a rich diversity of excitons in transition metal dichalcogenide (TMD) moiré superlattices, including unforeseen intralayer charge-transfer moiré excitons. We discovered a self-driven exciton-Floquet effect in time-resolved ARPES of 2D materials, wherein prominent satellite bands and renormalization of the bands are induced by excitons, analogously to the optical Floquet effect driven by photons. We further showed that strong excitonic physics in 2D materials can greatly enhance their nonlinear optical responses (e.g., shift currents and second harmonic generation). This led to the discovery of the formation of light-induced shift current vortex crystals in TMD moiré systems. Finally, for some TMD systems, it is predicted that spontaneous excitons condense to an excitonic insulator ground state with telltale spectroscopic signatures.

Work supported by the Department of Energy and National Science Foundation.

10:30

Painting potential landscapes on an atomically thin canvas

Archana Raja^{1,2}

¹Lawrence Berkeley National Laboratory, Berkeley

²Kavli Energy Nanoscience Institute, Berkeley

In this talk, I will discuss two stories from our joint experimental and theoretical work focusing on the prototypical 2D semiconductor interface of monolayer WS_2 and monolayer WSe_2 . In part one, we use ultrafast electron diffraction to uncover the role of layer-hybridized electronic states as a powerful route to control energy and charge transport across atomic junctions [1]. In part two, we use electron energy loss spectroscopy to directly visualize the nanoscale real space localization of excitonic states within the moiré unit cell of WS_2 and WSe_2 , opening the possibility for on-demand engineering of excitonic superlattices with nanometer precision [2]. The theoretical part of these works utilized BerkeleyGW and are a result of fruitful collaborations with colleagues at various institutions including UC Berkeley, SLAC National Laboratory, Stanford, Molecular Foundry, Purdue University and NIMS Tsukuba.

[1] Sood*, Haber* et al. Nature Nanotechnology 18 (1), 29-35 (2023)

[2] Susarla*, Naik* et al. Science 378 (6625), 1235-1239 (2022)

Monday, March 10th

11:00

Intricate relations between 2D materials and metals

Matěj Velický¹, Luka Pirker¹, Michaela Hanušová^{1,3}, Martin Vondráček², Jan Honolka², Otakar Frank¹

¹J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic

²Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

³Faculty of Chemical Engineering, University of Chemistry and Technology, Prague, Czech Republic

The integration of metals in the exfoliation of 2D materials has recently opened up new avenues, uncovering various interactions ranging from dispersive forces to covalent bonding. The resulting modifications in 2D materials, particularly TMDCs, offer many puzzles [1]. Despite the recent surge of interest and extensive studies, critical gaps remain in our understanding of these intricate interfaces. Some of the controversies include the changes in Raman or photoemission signatures of the TMDCs, which depend on the particular metal and the state of its surface [2-4]. The interplay between charge redistribution, substrate-induced lattice deformation, and interface charge transfer processes are examined, including the spatial homogeneity of these effects, by means of tip-enhanced spectroscopies [2,5].

[1] Pirker et al. 2D Mater. 11, 022003 (2024); [2] Velický et al. J. Phys. Chem. Lett. 11, 6112 (2020); [3] Velický et al. Adv. Mater. Interfaces 7, 2001324 (2020); [4] Rodriguez et al. Phys. Rev. B 105, 195413 (2022); [5] Rodriguez et al. J. Phys. Chem. Lett. 13, 5854 (2022)

11:30

Interferometric Second-Harmonic Generation Spectroscopy of Two-Dimensional Materials

Sunmin Ryu¹

¹Department of Chemistry, POSTECH, Pohang

Optical second-harmonic generation (SHG) spectroscopy has been established as a powerful tool for probing the structure and electronic properties of 2D materials. Incorporating phase information alongside SH field amplitudes enhances the power of the method. In this talk, I will introduce interferometric SHG spectroscopy, covering its principles and applications. Using spectral phase interferometry (SPI), we characterized elliptically polarized SH fields and photoinduced charge-transfer interactions in TMD heterobilayers. Differential phase SPI enabled the determination of material-specific SHG phases, imparting chemical sensitivity to SHG spectroscopy. Additionally, polarization-resolved SPI disentangled two interfering SH fields in heterobilayers, facilitating one-shot stack angle measurements. I will also demonstrate how SHG polarimetry serves as an efficient structural probe for domain imaging and assessing the crystallinity of hexagonal BN. These studies, demonstrating the SH analog of Young's interference, highlight the potential of interferometric parametric generation through atomically thin nonlinear optical materials.

Monday, March 10th

18:30

Mobile, tunable excitons in two-dimensional semiconductors and antiferromagnets

Alexey Chernikov¹

¹Faculty of Physics, TUD Dresden University of Technology, Dresden

Two-dimensional materials offer an excellent platform to study non-linear dynamics of tightly-bound exciton quasiparticles. Excitons are both tunable in external fields and recently demonstrated to dominate optical properties of 2D antiferromagnets, opening up perspectives to couple exciton transport to magnetic excitations. The first part of the talk will be focused on intense THz pulses transiently modifying light-emission of exciton-electron ensembles in a monolayer semiconductor. We demonstrate a near complete, THz-induced trion-to-exciton conversion by monitoring time resolved photoluminescence after optical excitation on picosecond timescales. In the second part, exciton propagation in 2D antiferromagnet CrSBr will be discussed. Among key results is the enhancement of exciton transport at the Néel temperature, non-linear, density induced propagation, as well as superdiffusive behavior in ultrathin layers. I will show how conventional mechanisms fail to account for the experimental findings, strongly indicating the central role of the exciton coupling to propagating magnons or spin fluctuations.

19:00

Phyllosilicates as earth-abundant layered materials for electronics and optoelectronics: Prospects and challenges in their ultrathin limit

Ingrid David Barcelos¹

¹Brazilian Synchrotron Light Laboratory, Brazilian Cent of Research in Energy and Materials, Campinas

Phyllosilicate minerals are an emerging class of naturally abundant two-dimensional (2D) layered insulators with large bandgap energy, representing an exciting frontier in the study of novel materials [1]. Despite being underexplored, these materials exhibit unique mechanical, optical, and electronic properties critical for advancing next-generation devices. Their potential spans from graphene-based systems to 2D heterostructures [2], where they complement and enhance the properties of transition metal dichalcogenides [3] and other materials. In this presentation, we will explore the electronic and optical properties of phyllosilicates using advanced nanoprobe techniques to investigate their local chemistry and nanoscale behavior[4]. These results position phyllosilicates as promising, low-cost candidates for applications in optoelectronics, nanophotonics, and other technologies requiring innovative electronic materials[5].

Refs: 1-Oliveira, R. et al. *Nanotech* 35,505703(2024) 2-Barcelos, I. D. et al. *ACS Photonics* 5,2662(2018) 3-Prando, G. A. et al. *Phys Rev Appl* 16,064055(2021) 4-Longuinhos, R. et al. *JPCC* 127, 5876(2023) 5-Barcelos, I. D. et al. *J. Appl.* 134, 090902(2023)

Monday, March 10th

19:30

A hybrid workflow to discover tailored functional materials

Christoph J. Brabec^{1,2}

¹Institute of Materials for Electronics and Energy Technology, Department of Materials Science and Engineering, FAU, Erlangen, Germany

²Helmholtz-Institute Erlangen-Nürnberg, Forschungszentrum Jülich, Erlangen, Germany

The inverse design of tailored organic molecules for specific optoelectronic devices of high complexity holds an enormous potential but has not yet been realized. Current models rely on large data sets that generally do not exist for specialized research fields. We demonstrate a closed-loop workflow that combines high-throughput synthesis of organic semiconductors to create large data sets and Bayesian optimization to discover new hole-transporting materials with tailored properties for solar cell applications. The predictive models were based on molecular descriptors that allowed us to link the structure of these materials to their performance. A series of high-performance molecules were identified from minimal suggestions and achieved up to 26.2% (certified 25.9%) power conversion efficiency in perovskite solar cells.

That milestone underlines the feasibility of developing autonomous research strategies that discover materials tailored for specific applications. That requires a highly interconnected workflow including synthesis, purification, characterization and device optimization. Such lines could specifically develop optimized interface materials for perovskite cells with various bandgaps, but also discover optimized interfaces for LEDs, photodetectors or X-Ray detectors. The outlook will summarize the advantages but also the limitations of data driven methods and will give further examples of such campaigns searching to find optimized materials for very different applications



POSTER II

MON 1**Polarized optical contrast spectroscopy of in-plane anisotropic van-der-Waals heterostructures**

Ernst Knöckl^{1,2}, Alexandre Bernard^{1,2}, Alexander Holleitner^{1,2}, Christoph Kastl^{1,2}

¹Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany

²Munich Center For Quantum Science and Technology (MCQST), München, Germany

We discuss polarized optical contrast spectroscopy as a simple and non-destructive approach to characterize the crystalline anisotropy and orientation of two-dimensional materials in van der Waals heterostructures. We developed a 3D-printed motorized polarization module which is compatible with typical microscope platforms and enables to perform broadband polarization-resolved reflectance spectroscopy. As proof of principle, we present the in-plane birefringence of exfoliated MoO₃ thin films and few-layer WTe₂ crystals and compare the measured spectra to a model based on a transfer matrix formalism. Compared to other polarization-sensitive approaches, such as Raman and second harmonic generation spectroscopy, optical contrast measurements require orders of magnitude less excitation densities. This is particularly advantageous to avoid the degradation of delicate van der Waals layers. Furthermore, the presented method allows quick and simple polarization-sensitive absorbance measurements to resolve anisotropic excitonic properties in symmetry-breaking heterostructures or anisotropic semiconductors, such as CrSBr.

MON 2**Ferroelectric switching in polar hBN islands**

Flavia Cimpean¹, Roman Gorbachev¹

¹Physics and Astronomy, The University of Manchester, Manchester

Properties of novel van der Waals materials, including their conductivity and optical response, are dependent on the stacking order of their constituent layers. Therefore, control of the layer stacking order enables modulation of their intrinsic properties. One system that demonstrates this is the sliding of hBN layers with respect to one another, which gives rise to structures of alternating ferroelectric polarization polytypes AB or BA. These polytypes are mirror-symmetric and Yeo et al. (arXiv:2409.07225) demonstrated that the system switches between them when external electric field is applied.

In this work, hBN spacers (2-5nm thick) with an array of etched cavities are encapsulated by parallel hBN crystals and their sliding ferroelectric switching response is investigated. These hBN crystals sag into the spacer cavities, creating contact islands of different polytype domains. The ferroelectric switching at these contact interfaces is investigated using EFM/KPFM. Utilising hBN spacers, rather than the graphene spacers used in previous works, removes interference from screening effects improving the observation of polarization switching.

MON 3**Vibrational spectroscopy and optomechanical interactions inside tip-controlled nanocavities**

Philippe Roelli¹, Isabel Pascual^{1,3}, Iris Niehues⁴, Javier Aizpurua², Rainer Hillenbrand¹

¹CIC nanoGUNE, San Sebastian

²Donostia International Physics Center, San Sebastian

³Materials Physics Center, CSIC-UPV/EHU, San Sebastian

⁴Institute of Physics, University of Münster, Münster

Subwavelength nanocavities have been an essential tool in interrogating matter at the nanoscale and investigating fundamental processes that govern light-matter interactions. Particularly, in the field of spectroscopy, nanocavities have enabled access to the optoelectronic properties of single molecules through various optical processes including Raman, PL, CARS and 2PA. However, several issues like (i) coupling efficiently the incoming light to the nanocavities, and (ii) tuning in-situ the interaction between the molecules and nanocavities remain open. In our work, we demonstrate control of the field enhancements inside nanocavities across VIS and IR regions of the electromagnetic spectrum via the scanning metallic tip of a s-SNOM microscope. Specifically, we validate the concept of tip-controlled nanocavity with continuous wave (CW) SFG of a single layer of molecules localized in the gap of a nanoparticle on mirror (NPoM) nanocavity. Our proof-of-principle study opens the path for a novel near-field microscopy modality where the hyperpolarizability of thin molecular films and 2D materials could be probed at the nanoscale.

MON 4**Modelling wave packet hopping in multilayer graphene grain boundaries**

Géza I. Márk¹, Péter Vancsó¹, Márton Szendrő¹, Alexandre Mayer²

¹Hungarian Research Network, Centre for Energy Research, Institute of Technical Physics and Materials Science, Budapest, Hungary

² Department of Physics, University of Namur, Namur, Belgium

We created a one-electron local pseudopotential [1] for van der Waals stacks of carbon sheets. It correctly describes single-layer, AA, AB bi-layer graphene, ABC tri-layer graphene, as well as AA, AB, and ABC graphite. Then we calculated the time development of quasiparticle wave packets and studied the hopping dynamics between the graphene sheets in multilayer systems. The hopping dynamics is governed by the band splitting, caused by the interlayer coupling. For the ABC graphene, the time dependence of the wave packet probability density is an aperiodic function for the outer layers, but a quasi-periodic function for the inner layer. This behavior was explained by treating the electronic states of the adjacent graphene sheets as weakly coupled linear oscillators. Then we applied our method to molecular dynamics calculated 3- and 6-layer ABC-ABA graphene grain boundaries in order to identify features seen on Scanning Tunneling Microscopy images

measured in our group.

[1] G. I. Márk, P. Vancsó, and A. Mayer: New local pseudopotential for multilayer carbon materials and its application in wave packet dynamics; Carbon Trends 13 (2023)

MON 5

Modular Chemical Patterning of Graphene by Direct Laser Writing Using Trivalent Iodanes

Kevin Gerein¹, Tao Wei¹, Frank Hauke¹, Andreas Hirsch¹

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Covalently binding addends on graphene represents a viable option to address the challenge of the material's lacking band gap and simultaneously allows for fine-tuning its chemical properties by introducing functional moieties. Precise and local control over the entire process, extends the flexibility of the material and allows for the development of surfaces and devices tailored for specific demands. The emerging laser writing represents an efficient and promising strategy for covalent 2D patterning of graphene, yet the bottleneck of this elegant procedure lies in the lack of applicable reagents and in the generation of suitable reagent coatings. Here, we present a versatile approach for the covalent laser patterning of graphene using trivalent organic iodine compounds, allowing for the engraving of various functionalities onto the graphene surface. This laser writing procedure can be achieved iteratively in liquid-phase simulating a flow-cell-like process. The tailor-made attachment of distinct functional moieties with varying electrical properties as well as their thermally reversibility, enables programming the surface properties of graphene.

MON 6

Modulated elemental reactants growth of MoS₂ thin films for Hydrogen Evolution Reaction

Eunseo Jeon¹, Vincent Masika Peheliwa^{2,3}, Marie H. Kratochvílová², Tim Verhagen², Yong-Kul Lee^{1,2}

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²Department of Dielectrics, Institute of Physics of the Czech Academy of Sciences, Praha

³Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Molybdenum disulfide (MoS₂) has garnered significant attention as promising catalyst for hydrogen evolution reaction (HER) due to its unique electronic properties, high surface area, and favorable catalytic activity. MoS₂ exhibit a layered structure that facilitate charge transfer and enhances catalytic performance. Recent studies have demonstrated that both bulk and nanoscale MoS₂ can efficiently promote HER, exhibiting comparable activity to traditional platinum-based catalysts. We grew vari-

ous films of layered MoS₂ on silicon substrates using modulated elemental reactants (MER) growth by molecular beam epitaxy. The grown MoS₂ was characterized in-situ using reflection high-energy electron diffraction and ex-situ using Raman spectroscopy, X-ray Diffraction and X-ray Florescence spectroscopy. MER grown MoS₂ samples exhibited an overpotential of -0.4V (vs RHE) at -10 mA/cm² in the alkaline HER exceeding the activity of chemically synthesized MoS₂ catalysts, which have an overpotential of -0.7V. The findings show the potential of layered MoS₂ as a viable alternative to precious metal catalysts and a platform for further innovations in sustainable hydrogen production technologies

MON 7

Mem-Emitters in MoSe₂/Clinochlore Heterostructures: Unveiling Memory-Driven Optoelectronic Dynamics for Advanced Computing

Alisson R Cadore¹, Alessandra Ames², Frederico Sousa², Raphaela de Oliveira³, Ingrid D Barcelos³, Victor Lopez-Richard², Marcio D Teodoro²

¹LNNano, CNPEM, Sao Paulo

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Van der Waals heterostructures (vdWHs), particularly those using TMD monolayers (MLs), have shown significant potential in developing optoelectronic devices with unique memory functionalities. Recently, we introduced Mem-emitters[1], memory-driven optical devices that utilize the intrinsic properties of semiconducting MLs on dielectric substrates. By exploiting these materials' atomic-scale thickness, tunable electronic properties, and strong light-matter interactions, Mem-emitters offer a novel approach to advanced computing, with potential for enhanced speed, efficiency, and optoelectronic switches. This work demonstrates a pronounced memory effect in ML-MoSe₂/clinochlore heterostructures, where electric hysteresis modulates emission intensity and energy, revealing both population-driven and transition rate-driven dynamics[2]. Our theoretical model links these effects to the substrate's internal states, underscoring clinochlore's role in delivering a robust memory response. These findings highlight Mem-emitters' promise in advanced communication and computation systems, emphasizing alternative insulators' role in vdWHs. [1]arXiv:2407.18164,2024 [2]arXiv:2410.07042,2024

MON 8

Polymer-free stacking and Micro-ARPES of multiferroic CuCrP₂S₆

Niklas Leuth¹, Tim Jacobs¹, Wendong Wang², Jeff Strasdass¹, Vitaly Feyer³, Benjamin Pestka¹, Marcus Liebmann¹, Elena Voloshina⁴, Yuriy Dedkov⁴, Roman Gorbachev², Markus Morgenstern¹

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Transition-metal (Tm) phosphorus trisulfides are antiferromagnetic van-der-Waals materials with various magnetic orders, providing a platform for detailed studying and tuning of 2D magnetism [1,2]. The binary Tm compound CuCrP_2S_6 exhibits additional ferro-/ antiferroelectricity and magnetoelectric coupling enabling gate induced magnetic orders [2]. We present results on stacking of this material by a fully inorganic transfer process in a glovebox developed by the University of Manchester, leading to polymer-free inter- and surfaces [3]. These stacks are analysed by atomic force microscopy and x-ray photoelectron spectroscopy. After transfer in ultra-high vacuum, they are suitable for surface-sensitive angular-resolved photoelectron spectroscopy (ARPES) with micrometre focus. We tracked the band structure from 300 K to 40 K covering several known phase transitions and discuss changes of the band structure in comparison with density functional theory calculations and analyse the relevant photoelectron matrix elements.

[1] Samal et al., J. Mater. Chem. A 9, 2560-2591 (2021) [2] Hu et al., Nat. Commun. 15, 3029 (2024) [3] Wang et al., Nat. Electron. 6, 981–990 (2023)

MON 9

Towards using coupled graphene quantum dots for achieving super(sub)radiant emission

Sébastien Quistrebert¹, Huynh Thanh¹, Suman Sarkar¹, Hugo Levy-Falk¹, Stéphane Campidelli², Fabien Bretenaker¹, Nikos Fayard¹, Jean-Sébastien Lauret¹

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Solid-state quantum emitters are a promising platform in the search for novel photon sources. In particular, graphene quantum dots (GQDs) have been proven to be efficient single-photon sources [1]. Their bottom-up chemical synthesis provides excellent control on the size and shape of the structure, which enables tailoring the optical properties of the GQDs [2, 3].

We designed a new family of elongated GQDs with transition dipoles up to 16 Debye, which may be well suited to achieve super(sub)radiant emission through dipole-dipole coupling. In the literature, control of the entanglement degree of pairs of molecules coupled by dipole-dipole interaction has been demonstrated by tuning the emission energies through Stark effect [4]. Here, we present simulations showing how the GQDs' large transition dipole reduces the constrain on the detuning. Finally, we report our latest experimental advancements towards achieving lifetime-limited emission from GQDs and the possibility of coupling pairs of GQDs embedded in nanocrystals.

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2- M.G.Debije, J. Am. Chem. Soc. 2004

3- D.Medina-Lopez, Nat. Commun. 2023

4- J.-B.Trebbia et al., Nat. Commun. 2022

MON 10

Strain-driven hybridization of excitons as the main mechanism for single photon emission in WSe₂

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Two dimensional materials host single photon emitters (SPEs), a crucial component for quantum communication technology. SPEs in monolayer WSe₂ emitting in the 850 nm telecom window, have been extensively reported in different strain-engineered devices, coupled with optical cavities and used to implement quantum key distribution protocols. However, the origin of SPEs in WSe₂ remains debated. Here, we study SPEs in 1L-WSe₂ nanobubbles to establish strain-driven hybridization of free and localized defect excitons as the main mechanism behind single photon emission. We compare tip-enhanced photoluminescence (TEPL) on WSe₂ nanobubbles with controlled strain-engineering experiments to map the strain distribution at nanoscale resolution. We analyse bubbles with different strain distributions and find spectral signatures of the previously reported and theoretically described hybridization between dark and localized states. We characterize SPEs at cryogenic temperatures and study their thermal onset with temperature-dependent photoluminescence. Nanobubbles offer a simple system to understand hybridization and SPEs in WSe₂, paving the way towards highly tailored quantum sources

MON 11

Highly Controlled 2D-Engineering of Graphene

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Covalent functionalization of graphene is a powerful tool to tune the materials unique properties. The development of various methods to achieve locally controlled, chemical modifications is a tremendous step towards tailor-made graphene-based materials. Herein, we present a fundamental study regarding the laser-activated spatially resolved functionalization of graphene using acyl peroxides as model compounds with an unprecedented level of control. The high precision offered by this method paves the way to use covalent functionalization of graphene for adjustable doping in electronic applications.

MON 12**Towards Patterned Functionalization of Graphene and Black Phosphorus Heterostructures**Jasmin Eisenkolb¹, Mhamed Assebban¹, Frank Hauke¹, Andreas Hirsch¹¹Lehrstuhl für Organische Chemie II, Friedrich-Alexander-Universität Erlangen, Fürth

Since the first isolation of graphene, the field of 2D materials has readily evolved. Graphene is a promising candidate for electronic applications, however, its lack of an intrinsic bandgap severely limits its potential. Other 2D materials like black phosphorus (BP), an allotrope of the element phosphorus, have their own unique properties and show varying bandgaps depending on the material. Combining specific characteristics of selected materials in an adaptable way would be ideal as it allows for the fabrication of specialized platforms. Hybrid materials are a promising approach towards this goal as they have the potential to combine certain properties of several materials into one. Hence, we investigate the formation of graphene and black phosphorus heterostructures and their covalent, laser-induced functionalization. Direct laser writing has emerged as an excellent tool to alter the surface properties of graphene in a straightforward and facile manner and this rationale will be adapted to the formed G-BP heterostructures, paving the way for the fabrication of sophisticated materials and enabling the alteration of their properties in a tailor-made fashion.

MON 13**Acousto-Optoelectric Spectroscopy on Transition Metal Dichalcogenides with Surface Acoustic Waves**Emeline Denise Sophie Nysten¹, Matthias Weiss¹, Benjamin Mayer¹, Felix Ehring¹, Tobias Petzak², Ursula Wurstbauer¹, Hubert Krenner¹¹Physikalisches Institut, Universität Münster, Münster²Lehrstuhl für Experimentalphysik 1, Universität Augsburg, Augsburg

Surface acoustic waves (SAWs) have proven to be a multifaceted and efficient tool for the manipulation, control and probing of the charge carrier dynamics inside semiconductor nanostructures [1,2,3]. By integrating 2D semiconducting transition metal dichalcogenides (TMDCs) onto SAW-devices, we can investigate their interesting optoelectronic properties. Firstly, by systematically studying the impact of SAWs on the photoluminescence of a WSe₂ monolayer in the time domain, we could unearth unavoidable inhomogeneities present in 2D TMDCs in experiments, which were not detectable through static photoluminescence measurements. Secondly, the study of the photogated SAW-induced acousto-electric current in exfoliated few-layer WSe₂ enabled us to have insight into the charge carrier dynamics and the quality of the contact between electrode and 2D semiconductor. These results show the power and versatility of SAWs as a contactless investigation method.

[1] Preciado et al., Nature Communications 6(1):8593 (2015) [2] Kinzel et al., ACS Nano 10(5):4942 (2016) [3] Sonner et al., Science Advances 7(31):eabf7414 (2021)

MON 14

Inorganic perovskites confined into nanotubes

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Boron nitride nanotubes (BNNTs) are ideal candidates to be used as nanocontainers for luminescent materials due their optical transparency in the visible range, inertness, and high structural stability. Here we report synthesis of an inorganic perovskite, CsPbBr₃ inside boron nitride nanotubes by melt insertion. Inorganic perovskite fluorophores generated significant research interest due to their high photoluminescence quantum yield and easily tunable emission wavelength, but to prevent their degradation it is necessary to encapsulate them. Unlike other nanoporous matrices that have been explored as protective packaging for perovskite quantum dots, BNNTs have the advantage of containing only one single unit of perovskite nanocrystal, that can be manipulated according to the needs of the application. In this work we investigate the luminescent properties and the environmental stability of CsPbBr₃@BNNT.

MON 15

2D semiconductors: Nanomechanics to defects and excitons

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We used nanomechanical resonators to detect excitonic states in two-dimensional (2D) materials. Very recently, it was demonstrated that the mechanical resonance frequency of a 2D mechanical resonator is very sensitive to its ground state properties. For example, an electronic phase transition can be detected from the shift in the resonance frequency. Here, we take this approach further and probe dark interlayer excitons (IXs) in 2D Transition Metal Dichalcogenides (TMDs). Such bound electron/hole complexes appear in 2D Transition Metal Dichalcogenides (TMDs) or their heterostructures. They are “dark” (no direct coupling to light) but affect the transport and dynamical properties of these materials. The presence of photogenerated excitons is detected from the shift of the mechanical resonance frequency of a suspended hetero-bilayer TMD. Furthermore, this approach can be used in probing for

the exciton insulator state – condensed excitons in the ground state – in certain types of heterostructures.

MON 16

Nanoscale He-ion beam patterning of topological insulator thin films

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The helium ion microscope is a versatile tool for both nanoanalytics and nanoscale fabrication with a resolution below 10 nm [1]. We discuss the application of He-ion beam milling in topological insulator thin films with the goal of creating nanoscale patterned superlattices with lattice constants on the order of 10 nm. Such superlattices are predicted to renormalize the Dirac velocity of the surface states and correspondingly enhance electronic interactions, which may ultimately result in the emergence of correlated states, such as topological superconductivity [2]. Furthermore, we extend optoelectronic measurements from near-infrared (from 0.8 μm) to mid-infrared wavelengths (up to 20 μm). The latter may allow a selective excitation and read-out of the (nanopatterned) surface state and its quantum geometric properties [3] without contribution from bulk bands.

[1] E. Mitterreiter et al., Nano Lett. 2020, 20, 4437–4444.

[2] J. Cano et al., Phys. Rev. B 2021, 103, 155157.

[3] G. Topp et al., Phys. Rev. B. 2021, 104, 064306.

MON 17

Strong coupling of metal nanoparticles and atomically thin semiconductors: Physics behind a minimal model

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Monolayers of transition metal dichalcogenides (TMDCs) exhibit strong light-matter interaction, dominated by tightly bound, 2d-delocalized excitons. In contrast, metal structures support localized plasmons that enable nanoscale electric field control. TMDC-metal nanoparticle hybrids combine excitons and plasmons, reaching strong coupling in numerous experiments. Such experimental results are typically fitted using the coupled oscillator model (COM) employing a phenomenological coupling constant. Here, we develop an analytical theory based on Maxwell's equations and a microscopic perspective of the material dynamics [1]. The emergent minimal model can be easily applied to fit experimental results, provides a clear physical interpretation and highlights the importance of the spatial dispersion of 2d excitons. We explicitly derive all coupling and dephasing constants in a COM combining three

oscillators: plasmons, bright and momentum-dark excitons. Strong coupling (peak splitting) is observed for momentum-dark excitons, while the weakly coupled bright exciton appears as a distinct third peak in the spectrum.

[1] Greten, Salzwedel, Göde, Greten, Reich et al., ACS photonics 11.4 (2024)

MON 18

Electron localization in amorphous graphene

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Two-dimensional (2D) amorphous graphene is a non-crystalline carbon layer with a disordered atomic structure, where small islands of sp^2 -bonded carbon are dispersed throughout the amorphous matrix, providing a template for electron confinement. These nanoscale carbon clusters effectively behave as quantum dots with size-dependent band gaps and vibrational modes. We study their properties with resonant Raman spectroscopy that selectively excites different carbon quantum dots within the ensemble. We observe the D mode dispersion of ~ 44 cm⁻¹/eV comparable to graphene, although arising from a different mechanism where smaller quantum dots resonate with UV photons while larger dots resonate with photons in the IR range. Amorphous graphene exhibits intense Raman G mode visible excitation, reaching intensities up to 70 times higher than in crystalline graphene due to the quantum dot resonances. Finally, we show that amorphous graphene can serve as an efficient and uniform light absorber ($\sim 20\%$) across the visible spectrum due to quantum dots with varying band gaps. These findings establish amorphous 2D carbon as a promising system for exploring order-disorder transitions and enhanced light-matter interaction.

MON 19

Characterization of in-plane propagating luminescence in TMDs using laser-written waveguide circuits

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Photoluminescence (PL) spectroscopy is a well-established technique for studying the excitonic properties of two-dimensional crystals. Yet, the typical approach of exciting these materials in vertical incidence means that the measurements are performed with light polarized in the plane of the sample layer. This neglects the components of the emitted signal polarized perpendicular to the sample that propagate

along the layer and require side-on detection for characterization.

Here, a side-on detection is established by means of fused silica glass substrates containing femtosecond laser direct written waveguides [1]. By defining waveguides directly under the surface of the glass, interactions of the sample and the waveguide's evanescent field are enabled. This allows the sample to be excited due to its proximity to the waveguide, but also allows the excitonic emission to be collected by the waveguide for subsequent detection.

This work analyzes the in-plane propagating luminescence in TMDs with an emphasis on determining influences on the signal that arise from combining TMDs and surface waveguides.

[1] A. Szameit et al., *J. Phys. B: At. Mol. Opt. Phys.*, 43 163001 (2010)

MON 20

Comparative Study of TERS Performance: High NA Oil vs. Low NA Air Objectives with Radially Polarized Transmission Illumination

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TERS enables nanoscale optical analysis using a metallic tip coupled with a light collection apparatus, such as an objective lens. In coaxial backscattering, where excitation and collection align with the probe, challenges arise in effectively exciting the probe and collecting the scattered signal. This is typically modeled as a dipole perpendicular to the sample plane. However, experimental results have shown that the Plasmonic Tunable Tip Pyramid (PTTP), featuring a nanometric pyramid mounted on a plateau, significantly enhances localized fields even with low numerical aperture objective lenses. These findings suggest that the standard dipole model may not fully capture the plasmonic behavior of the PTTP and its influence on TERS performance, motivating further investigation into its plasmonic resonance properties. In this study, we conduct a multiparameter optimization of the PTTP's plasmonic resonance, using both numerical simulations and experimental validation. We evaluate how different configuration parameters such as tip geometry, excitation wavelength, and objective lens NA affect plasmonic field enhancements, aiming to improve TERS sensitivity and resolution.

MON 21

Proximity-induced exchange interaction and dynamic charge transfer in MoSe₂/CrSBr van-der-Waals Heterostructure with orthogonal spin texture

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Van der Waals (vdW) heterostructures composed of 2D transition metal dichalcogenides and vdW magnetic materials offer an intriguing platform to functionalize valley and excitonic properties in non-magnetic TMDCs. Here, we report a comprehensive optical study of a monolayer MoSe₂ on the layered A-type antiferromagnetic semiconductor CrSBr.

We adopt the type-III band alignment picture, found in a previous magneto-PL study. By performing co-circular polarized PL and reflection contrast, we observe that the atomic proximity of the materials leads to an unexpected breaking of time-reversal symmetry, despite the originally perpendicular spin texture in both materials, which is further supported by first-principles calculations.

Moreover, time-resolved PL and time-resolved reflectivity measurements identify a very long-lived dynamic charge-transfer process in the heterostructure, consistent with a type-III band alignment. Additionally, time- and polarization-resolved experiments suggest that the excited charge carriers exhibit behavior resembling band bending, alongside evidence of efficient Förster resonance energy transfer (FRET) within the heterostructure.

MON 22

Theoretical characterization of tip-enhanced nanocavities for active control of vibrational sum-frequency generation

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Sum-frequency generation (SFG) in dual nanoantennas, combining IR- and VIS-resonant plasmonic nanostructures, enables coherent upconversion of infrared (IR) photons into visible (VIS) light via molecular vibrations acting as optomechanical transducers. While some dual-nanoantenna designs address this, they often lack flexibility for targeting specific molecular vibrations. We propose a novel approach using scattering-type Scanning Near-field Optical Microscopy (s-SNOM) with a nano-

particle-on-mirror (NPoM) structure. By scanning a VIS-resonant NPoM with an IR-resonant s-SNOM tip, the tip-enhanced nanocavity acts as a cascaded nanolens. Here, we perform numerical simulations revealing the s-SNOM tip's role in activating and modulating NPoM plasmonic resonances critical for upconversion. We examine how the tip's positioning relative to the NPoM influences responses across VIS and IR wavelengths. Simulations show significant enhancement of linear (SERS) and nonlinear (SFG, DFG) optical signals, outperforming bare NPoM enhancements. Experimental data confirm tip-induced control of SERS, SFG, and DFG signals from molecules under ambient conditions with continuous wave illumination.

MON 23

Magnetic anisotropy of 2D magnetic semiconductor revealed by collective excitations

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The van der Waals material CrSBr is an optical active, air stable magnetic semiconductor. The A-type ferromagnetism (AFM) is caused by ferromagnetic order (FM) within each layer and AFM coupling between adjacent layers. Its highly anisotropic electronic band structure gives it quasi-1D properties, which influence its excitonic behavior [1] that is sensitive to the spin order [2,3]. We study the spin dependence collective excitations and coupled degrees of freedom by magnetic field-dependent PL and resonant Raman scattering (RRS) experiments at low temperatures. RRS reveals two additional modes sensitive to the magnetization direction. These modes show a similar magnetic field dependence as PL signatures following the triaxial magnetic anisotropy. Comparison with literature [2,3] allows an initial interpretation as low-momentum high energy magnon and an assignment of those modes as magnon of the AFM multilayer system strongly coupled to the bulk exciton, and as magnon mode within the FM ordered surface layer showing strong coupling to an exciton interpreted as surface exciton.

[1] J. Klein et al ACS Nano Lett.(2023) [2] Y. Bae et al. Nature (2022) [3] D. Esteras et al. nano Lett.(2022)

MON 24

Synthesis and characterization of novel amorphous carbon-diamond composites

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Recent reports on synthesis of disordered carbon materials exhibiting combination of extraordinary mechanical and electronic properties triggered extensive research on these novel forms of carbon^{1,2}. We have synthesized amorphous carbon-nanocrystalline diamond composite materials from fullerene C₆₀ precursor at p=25 GPa, T= 1250-1300C. The materials' structure and vibrational properties were probed by HRTEM, synchrotron XRD and Raman spectroscopy, respectively. Hardness of the samples was characterized by several methods yielding consistent results. The composites possess exceptional mechanical properties with hardness exceeding that of single crystalline diamond. Raman mapping revealed inhomogeneities in nanocrystalline diamond distribution in the amorphous matrix that are accompanied by variation in the mechanical properties. We discuss mechanism of the composites formation and origin of the superior mechanical properties they exhibit along with optimization of the composites synthesis protocol.

1. Zhang, S. et al. National Science Review 9, nwab140 (2021).
2. Shang, Y. et al. Nature 599, 599-604 (2021).

MON 25

Charge confinement in twisted bilayer graphene

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Twisted bilayer graphene (tBLG) near the magic angle is a unique platform where the combination of topology and strong correlations gives rise to exotic electronic phases. These phases are gate-tunable and related to the presence of flat electronic bands, isolated by single-particle band gaps. This enables charge confinement and allows to explore the interplay of confinement, electron interactions, band renormalisation and the moire superlattice, potentially revealing key paradigms of strong correlations. Here, we will present two experiments where we study charge confinement in tBLG. First, we report on the observation of negative electronic compressibility in tBLG for Fermi energies close to insulating states. To observe this

negative compressibility, we take advantage of naturally occurring twist-angle domains that emerge during the fabrication of the samples, leading to the formation of charge islands. We accurately measure their capacitance using Coulomb oscillations, from which we infer the compressibility of the electron gas. Second, we present gate-defined single-electron transistors (SETs) in near-magic-angle tBLG with well-tunable Coulomb blockade resonances.

MON 26

Investigation of the interlayer coupling of twisted bilayer CVD-grown MoS₂ via Raman spectroscopy

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Stacking two monolayers of TMDCs on top of each other introduces several novel phenomena as, e.g., the formation of moiré phonons and might change the band structure. In addition, the fabrication process and the twist angle both influence the coupling between the two layers. Here, this interlayer coupling shall be investigated via Raman spectroscopy. By exciting the C exciton resonance, interlayer Raman modes are activated that are not visible in a single layer but become active in bilayers. This is because the C exciton - in contrast to A and B excitons - expands over both layers and, therefore, couples the layers electronically. This is how taking Raman spectra of twisted bilayer TMDCs shows whether the two layers are in good contact. Taking well-coupled twisted bilayer samples as a starting point we investigate the influence of the twist angle on the C exciton resonance by taking Raman spectra of several samples with different twist angles at different laser excitation energies. So far, this has been done using twisted bilayer MoS₂. In the

MON 27

Gate-tunable Josephson diodes in magic-angle twisted bilayer graphene

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We report on low-temperature measurements of gate-tunable Josephson junctions (JJs) in magic-angle twisted bilayer graphene (MATBG), where the weak link between the superconducting leads is defined by the correlated insulating state at half-filling of the hole band ($\nu = -2$). Magnetotransport measurements reveal a complex evolution of disordered Fraunhofer-like patterns showing characteristics of multipath interference, highlighting a non-uniform current distribution across the JJs. The particularly large kinetic inductance of the superconducting phase in MATBG results in a Josephson diode effect originating from this non-uniform current distribution. We observe a strong gate-tunability of this non-reciprocal behavior which we attribute to changes in the supercurrent density. Thus, our work highlights the importance of disorder and the kinetic inductance for the observation of non-reciprocal effects in MATBG JJs.

MON 28

Infrared correlation nanoscopy for organic and inorganic material analysis at the nanoscale

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Nanoscale resolved imaging and spectroscopy using tip-enhanced microscopy enables bypassing the diffraction limit of light and to achieve a wavelength-independent spatial resolution of < 20 nm in the visible, infrared (IR) and terahertz (THz) frequency range [1]. Correlation of scattering-type Scanning Near-field Optical Microscopy (s-SNOM), tapping AFM-IR (local detection of photothermal expansion) or measurement of inelastic lightscattering can provide complementary information for chemical analysis of specimens enabling more comprehensive characterization of functional nanostructures or fundamental properties of materials [2,3,4]. In this work we demonstrate the implementation of different measurement techniques into a single neaSCOPE instrument enabling analysis of e.g. a thin polymer film by s-SNOM and tapping AFM-IR imaging. The poster illustrates the capabilities of correlating tip-enhanced imaging methodologies in the infrared spectral range for characterization of phase separation in a thin PS-PVAC sample. Clearly, infrared absorption imaging can provide material-specific information about the specimens heterogeneity. However, measuring the IR tipscattered light provides also information about the sample's reflectivity at the selected wavelength, thus providing additional complementary information with higher reflectivity for the PVAC islands compared to the PS matrix. Analysing spectroscopic signatures obtained by s-SNOM and AFM-IR spectroscopy can provide further insights into vertical sample heterogeneity as well as potential molecular orientation effects by considering the polarization of the incident light. Further, we present results that correlate the near-field optical response of semiconducting nanostructures in different frequency ranges (mid-IR & THz) to Kelvin Probe Force Microscopy (KPFM) mapping, providing novel spatial information about doping gradients and material interfaces. Finally, nanoscale re-

solved measurements of elastic light scattering by s-SNOM in the infrared spectral range will be compared with inelastic light scattering (that is Photoluminescence or Raman) for the very same sample location, providing complementary analysis of complex specimens. Thus, integrating different optical imaging and spectroscopy methodologies into a single instrument enables novel characterization capabilities of functional nanostructures or interfaces as well as fundamental properties of material systems.

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[4] T. Deckert-Gaudig, A. Taguchi, S. Kawata, and V. Deckert, *Chem. Soc. Rev.*, 46, 4077 (2017).

MON 29

Ultrafast All-Optical Probe of Broken Time-Reversal Symmetry in Monolayer WSe₂

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The combination of broken space inversion and preserved time-reversal symmetry (TRS) underlies the spin-valley degree of freedom in monolayer transition metal dichalcogenides (TMDs). Introduction of an imbalance between the energy degenerate, but non-equivalent valleys (local extrema of the bandstructure) at the $\pm K$ points of the Brillouin zone breaks TRS. We probe broken TRS and a valley im-

balance on ultrashort time scales by comparing the second harmonic (SH) intensity for a circularly vs. linearly polarized fundamental beam (FB). By numerically and analytically solving the semiconductor Bloch equations, we show that a two-photon resonant right/left circularly polarized FB interacts exclusively with the $\pm K$ valley. Thus, a circularly polarized FB probes the C_{3h} wave vector group of the $\pm K$ valleys, in contrast to a linearly polarized FB probing the D_{3h} group of the Γ point. This difference between wave vector groups at K and Γ fully captures and explains the experimentally measured deviation from the otherwise expected ratio of 2 in the circular vs. linear SH intensities.

MON 30

Graphene nanoribbons as a quantum platform

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Graphene nanoribbons (GNRs) are quasi-one-dimensional strips of graphene that exhibit unique electronic properties arising from quantum confinement, enabling tunable band gaps. The ability to adjust GNRs' electronic and magnetic characteristics at the atomic level positions them as a promising platform for probing quantum phenomena and developing quantum devices (1).

In this poster, I provide an overview of our approach to investigating quantum properties using GNRs and their potential applications in future quantum technologies. I will discuss the on-surface synthesis methods employed to fabricate GNRs with tailored structures that reveal diverse quantum behaviors, such as topological and localized spin states (2, 3). Additionally, I will present our recent advancements in optimizing 17-armchair GNR growth and the exploration of a new synthetic motif to tune GNR properties toward their device integration. This research opens avenues for scalable GNR-based quantum devices, showcasing the critical role of tailored GNR structures in future quantum applications.

1. Nat Rev Phys. 3, 791–802 (2021).

2. Nature. 560, 209–213 (2018).

3. Adv. Materials. 35, 2306311 (2023).

MON 31**Heteroatomic doping of MoS₂ to turn the selectivity of the gas-sensing element**

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MoS₂-based nanomaterials were synthesized by the rapid decomposition of (NH₄)₂MoS₄ at 600 °C in argon. A study of the chemiresistive properties MoS₂ showed a quick and reproducible response to trace amounts of NO₂. To change the conductivity of nanomaterials and to create specific adsorption sites, we doped MoS₂ with nitrogen and nickel. To introduce heteroatoms, thermolysis of the (NH₄)₂MoS₄ aerogel was carried out in an NH₃ atmosphere or in argon with the addition of nickel acetate to the aerogel. The composition of the synthesis products and the chemical state of the elements were determined based on the analysis of X-ray photoelectron spectroscopy data. The N-MoS₂ sample was able to detect 25 ppb NO₂ at room temperature, which is two times less than in the case of undoped MoS₂. Moreover, the conductivity of the N-MoS₂ sensor did not change upon NH₃ adsorption. In contrast to this result, the Ni-MoS₂ sample had high selectivity to NH₃ and sensed this molecule down to 5 ppm in dry air.

MON 32**Flat bands in magic-angle twisted bilayer graphene by chemical vapor deposition**

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We present nano angle-resolved photoemission spectroscopy (nARPES) and Raman data from a near- magic-angle twisted bilayer graphene (MATBG) sample realized by stacking graphene grown by chemical vapor deposition (CVD).

MATBG by exfoliation and stacking was the first moiré system to exhibit flat dispersion and strong correlations in the lowest-energy hole and electron minibands.

Here, we report on flat bands very close to the Fermi level and thus experimentally accessible.

CVD is a versatile and scalable 2D-materials deposition technique that holds the potential to bridge the gap between research and industrial applications. ARPES, conversely, is able to directly image the dispersion of a crystal band structure by photoelectric effect. Being surface sensitive, it is particularly suited for 2D materials. The use of nARPES with sub micrometric lateral resolution allows us to prove the presence of flat bands extended over such surface area, while simultaneously providing knowledge on how the stacking relaxation affects the band structure.

MON 33

Energy transfer excitation of excitons by tunneling electrons

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The gap between state-of-the-art electronic devices and light-based communication technology poses a major challenge for integrated optoelectronic circuits. Two-dimensional materials are one of the most promising platforms to bridge that gap by unifying strong light-matter interaction with silicon compatibility. One of the biggest challenges remains the electrical excitation on the nanoscale. Here, tunneling structures have proven to be an efficient pathway. However, conventional tunneling junctions place the active material between two electrodes, leading to faster degradation and limiting the thickness.

Here, we present a novel electrical excitation scheme beyond carrier injection based on the energy transfer from tunneling electrons to excitons. By placing the 2D material close to a graphene-based tunnel junction, the dipole of the tunneling electron can couple optically to excitons. This open electrode design enables the use of different 2D materials with variable thicknesses. Finally, we demonstrate the stable electrical excitation of self-hybridized polaritons in two-dimensional perovskites and layered magnetic materials.

MON 34

Making nanomaterial inks from insoluble rocks

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Liquid exfoliation of layered materials has become an important production technique to give access to large quantities of two-dimensional nanosheets in colloidal dispersion. Importantly, this is a highly versatile technique that can be applied to nu-

merous layered materials beyond graphene. While this was clear already 10 years ago, some major obstacles on the fundamental level of exfoliation, size selection and characterisation had to be overcome. In this poster, I will summarise the most important steps that allowed us to arrive at a point, where it is possible to produce samples suitable for (device) applications. This includes aspects of deposition as individual nanosheets or in tiled networks, microscopic and spectroscopic characterisation and is illustrated through material comparisons with regard to exfoliation efficiency based on AFM statistics, centrifugation-based size selection, identification of size-dependent optical properties and the quantitative assessment of degradation in the presence of water and oxygen across a range of layered materials and their nanosheets.

MON 35

Cavity optomechanics with a carbon nanotube nanomechanical resonator

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Carbon nanotubes (CNTs) are the smallest and lightest nanomechanical resonators. Suspended between electrodes and gated, they can act simultaneously as beam resonators with large Q and as quantum dots.

We have realized optomechanical coupling of a CNT nanomechanical resonator to a microwave cavity and quantified it through optomechanically induced transparency measurements [1,2]. The nonlinearity of Coulomb blockade in the CNT was exploited to significantly enhance the coupling strength, reaching $g_0 \sim 100$ Hz [1,2]; also back-action of the CNT on the microwave cavity has been demonstrated [1,2]. Ongoing work is directed towards strong coupling and ground state cooling of the nanomechanical resonator. This requires improvements of the microwave cavity [3] and the transfer assembly procedure. Suspended CNTs have been proposed as long-lived nano-electromechanical qubits [4], a topic of high current research interest [5].

[1] S. Blien et al., Nat. Commun. 11, 1636 (2020). [2] N. Hüttner et al., PR Appl. 20, 064019 (2023). [3] N. Kellner et al., PSSB 260, 2300187 (2023). [4] F. Pistoiesi et al., PRX 11, 031027 (2021). [5] Y. Yang et al., Science 386, 783 (2024).

MON 36

Imaging Propagating Polaritons in Ångstrom Thick WS₂ in Real Space

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Transition metal dichalcogenide (TMDC) monolayers support excitonic states in the visible at room temperature with strong binding energies, which makes them interesting for polariton based devices. Polariton propagation in thin slabs of TMDCs have been shown, however, they have never been imaged in ångstrom thick samples in real space, due to the requirements on the refractive indices of the cladding media to support propagating modes. Here we study exciton-polariton waveguiding in a freestanding WS₂ monolayer by imaging their propagation in real space using scattering-type scanning near-field optical microscopy (s-SNOM). Combined with a fully tunable laser in the visible for excitation we obtain the dispersion relation, which exhibits the coupling between exciton and guided light leading to the formation of polaritons. The results indicate the excitation of surface exciton-polaritons that have been predicted but not yet demonstrated experimentally. As a consequence the dielectric function takes on negative values.

MON 37

Large-Scale Modeling of Multilayer Graphene Using a Versatile, *ab-initio* Based Tight-Binding Model

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Graphene's electronic properties are strongly influenced by its structural features and external environment. Using a combination of an *ab-initio* based tight-binding (TB) model, capable of describing arbitrary geometrical arrangements and density functional theory (DFT), we perform large-scale simulations to investigate the impact of substrates, grain boundaries, and stacking configurations on graphene. Substrates are found to modify the electronic structure, inducing bandgaps and charge redistribution effects. Grain boundaries alter the local density of states, introducing localized electronic states and affecting overall material behavior. Additionally, we examine stacking arrangements such as rhombohedral (ABC) and hexagonal (ABA), revealing distinct interlayer coupling phenomena, including the emergence of flat bands in ABC stacking. These findings provide critical insights into optimizing graphene's properties for advanced device applications, emphasizing the importance of substrate selection, grain boundary engineering, and stacking control.

MON 38

Moiré lattice of twisted bilayer graphene as template for non-covalent functionalization

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We present an innovative approach to achieve spatial variations in the degree of non-covalent functionalization of twisted bilayer graphene (tBLG). The tBLG with local twist angle variations between $\sim 5^\circ$ and 7° was non-covalently functionalized with 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) molecules. We observe a correlation between the twist angle of tBLG and the degree of functionalization, determined through Raman spectroscopy. We propose that the adsorption of HATCN molecules follows the moiré pattern of twisted bilayer graphene, preferentially avoiding AA-stacked regions and primarily attaching to regions with local AB-stacking order, resulting in an overall ABA-stacking arrangement. This hypothesis, is further supported by density functional theory (DFT) calculations [1].

[1] Dierke et al., *Angew. Chemie Int. Ed.*, accepted (2024),

DOI: 10.1002/anie.202414593

MON 39

Modulated Elemental Reactants Growth of two-dimensional MnS_2 - SnS sandwiches

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The general interest of research on multiferroic materials is that these materials exhibit more than one ferroic order, making them highly attractive for advanced technological applications. But, even despite exhaustive material exploration, only a handful of single-phase multiferroics, such as BiFeO_3 , have been found that operate at room temperature (RT). One of the appealing options to create RT multiferroic materials is via the creation of two-dimensional (2D) heterostructures. Here, such 2D sandwiches are created using layer-by-layer growth of layered materials using the modulated elemental reagents method within an MBE system. This method is expected to eliminate the main difficulties in the growth of 2D multiferroics, which consists of the difficulty of growing layered, 2D heterostructures having a strong coupling between the layers.

In this work, we combine the magnetic MnS_2 and SnS , which is ferroelectric due to its non-centrosymmetric nature. The characterization of the individual layers and 2D sandwiches of these materials was done by in-situ reflection high energy electron diffraction, X-ray fluorescence, Raman, X-ray diffraction, and atomic force microscopy.

MON 40**SET measurements of the Schwinger effect in graphene**Atri Dutta¹, Yael Rich¹¹Weizmann Institute of Science, Rehovot

Monolayer graphene aligned to hexagonal boron nitride forms a moiré superlattice, significantly modifying the graphene band structure and giving rise to secondary Dirac points (2DPs). Recent investigations of high-bias transport near the hole-side 2DP have revealed signatures of the "Schwinger effect," wherein strong electric fields are proposed to induce the generation of electron-hole pairs directly from the Fermi sea. This phenomenon manifests as a characteristic peak in the differential resistance measured via four-probe techniques. In this study, we employ a nanotube single electron transistor to spatially image electronic flow within a Hall bar geometry, enabling us to resolve additional features in the current-carrier density space near the 2DP. Specifically, we observe that the 2DP position as a function of gate voltage shifts monotonically along the length of the device, identifying it as distinct from the resistance peak usually associated with the Schwinger effect. Furthermore, our findings underscore the critical role of self-gating effects in shaping the transport behavior of graphene under high-bias conditions.

MON 41**Sorting and Assembling of Single-Walled Carbon Nanotubes**Yan Li¹¹Peking University, Beijing

Single-walled carbon nanotubes (SWCNTs) present chirality-dependent electron and band structures and unique physical properties. Therefore, the conductivity- and chirality-based sorting and the well-organized assembling of SWCNTs is of both important scientific significance and application value. Among the solution-based techniques for SWCNT sorting, the two-phase aqueous extraction separation has the advantages of high precision, large concentration and easiness in scaling up. We developed a simpler PEG/ salt two-phase system for the separation of DNA dispersed SWCNTs. We found that the cation type has an important effect on the distribution of nanotubes in the two phases. By selecting suitable salt type and concentration, the separation of SWCNTs with single chirality was realized. More importantly, various enantiomers of high purity were obtained. We also developed a Marangoni flow-based method to prepare well-aligned SWCNT arrays with the density of 100-300 tubes/microns. The arrays of chirality and enantiomer pure SWCNTs exhibit unique properties.

MON 42**MoS₂ mechanical resonators, a promising platform for defect-based optomechanics**

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The development of performant single photon sources is important in the context of quantum technologies, including quantum communications and sensing.¹ Particularly, transition metal dichalcogenides are of great interest, as they can host precisely positioned and scalable single photon emitters.² Recently, the focus has been placed on dynamically manipulating the emission of single photons, leading to the development of mechanical devices that can be coupled to quantum systems.³ In particular, the mechanical motion of suspended membranes can be coupled to single photon sources implanted inside them.

We present a study of suspended monolayers MoS₂ membranes, having mechanical resonances in the tens of MHz range with Q-factors around 1000. We extract the elastic properties of the membranes from atomic force microscopy measurements. Furthermore, the mapping of the photoluminescence shows indications of a strain-induced exciton trap. Understanding of the properties of suspended MoS₂ membranes will enable us to next explore defect-based optomechanics.

1. Nat. Nanotechnol. 16, 367 (2021)

2. Appl. Phys. Lett. 117, 070501 (2020)

3. Nat. Phys. 18, 15 (2022)

MON 43**IMAGING THE CRITICAL ROLE OF STATIONARY ATOMS DURING SOLIDIFICATION OF PT-NANOCLUSTERS**

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Solidification of liquids is a complex process where atoms transition from random motion to an ordered crystalline structure. The onset of nucleation is crucial for

determining the structure and properties of the resulting solid, but it is challenging to capture, describe, and control. High-resolution transmission electron microscopy was used to image Pt nanoclusters. Using MEMS chips to control the temperature, Pt nanoclusters were molten in situ, allowing the investigation of the solidification mechanism. The electron beam can significantly increase the number of stationary atoms, which impacts the solidification process. When the number of stationary atoms is low, classical one-step nucleation mechanisms occur. However, an increase in stationary atoms drastically alters the solidification pathways. When the liquid nanodroplets are surrounded by a corral of stationary Pt atoms, crystallization is effectively halted. Surprisingly, these corralled nanodroplets remain liquid at temperatures several hundred degrees Celsius below the normal crystallization temperature of Pt nanoparticles before transforming into an amorphous solid instead of the usual face-centered cubic phase.

MON 44

Carbon layers with a regular lattice of holes

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Using a triphenylene derivative ($C_{18}H_6Br_6$) a two-dimensional monolayer was grown in an epitaxial synthesis. The Raman spectrum of the as grown sample shows two narrow bands at 255 cm^{-1} and at 281 cm^{-1} excited with laser energy of 1.94 eV. These “low-frequency bands” are reminiscent of the bands in to the one in covered-edged graphene nanoribbons. In addition to the sp^2 typical bands at 1586 cm^{-1} and 2602 cm^{-1} , a strong defect induced band appears at 1303 cm^{-1} . Resonant Raman investigation shows that both the “low-frequency bands” and the defect-induced bands (D- and 2D) vary their position and intensity with the excitation laser energy. High-resolution atomic force investigation reveals in the different areas in the monolayer with tetragonal and hexagonal structure. With polarized Raman measurements are anisotropic behavior of the D-, 2D- and the G-band was observed. This agrees with the tetragonal structure found in HR-AFM.

MON 45

Morphology Control for Functional Inorganic/Organic Heterostructures

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Morphology control is crucial for thin-film properties in printed nanoelectronics, as it directly impacts on the film characteristics. Recent advances enable the fabrication of mosaic-like nanosheet thin films, comprised of a monolayer of nanosheets with

minimal edge overlap facilitating a Langmuir-type approach. Control over the deposition parameters allows to fine-tune the nature of nanosheet junctions within the film and even to deposit suspended 2D-nanosheet thin films from nanosheet inks.

In our recent work, we developed an inorganic/organic heterostructure combining MoTe_2 with an imine-linked 2D polymer, synthesized at the liquid/air interface using the SMAIS (surfactant-monolayer-assisted interfacial synthesis) method.

In such a heterostructure we can exploit the pores of the 2D polymer as a channel which guides the reactive species for functionalization. This way, we introduce spatially controlled defects into the underlying TMD layer.

This novel approach provides a versatile pathway to pattern and to engineer defects in 2D nanomaterials with precisely tailored properties, enabling control over the local band structure through the chemical nature of the defects

MON 46

Revisiting Asymmetric Raman Lineshapes in Silicon Using Green's Function Analysis

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I am developing a time-resolved Raman spectroscopy system to probe electron-phonon interactions (EPI) and dynamics in semiconductors. To demonstrate its utility, we investigated photoexcited silicon, where coupling between continuum inter-valence band electronic transitions and discrete optical phonons creates an asymmetric Raman lineshape.

Traditionally, this asymmetric lineshape is analyzed using the Fano model, which describes the interference between discrete and continuum states. However, the Fano model fails to explain the transient evolution in Si from an asymmetric lineshape to a symmetric Lorentzian as photoexcited carriers decay. This limitation arises from the model's exclusion of intrinsic phonon lifetimes and anharmonic effects, significant at finite temperatures. To address this, we developed a Green's function-based coupled-modes model that incorporates phonon-phonon interactions, separating EPI from anharmonicity and clarifying Raman lineshape evolution.

Temperature-dependent Raman measurements validated this approach, demonstrating its ability to capture full spectral transition and provide deeper insights into the interplay between EPI and anharmonic effects.

MON 47

Ultra-high vacuum enabled study of novel layered dielectric CdI_2

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Studying the intrinsic properties of air-sensitive 2D materials presents challenges due to degradation upon exposure to oxygen or water vapour. Fabrication of het-

erostructures from these materials is therefore carried out in an inert atmosphere (e.g., argon) or under vacuum conditions. This work presents the first experimental characterisation of mechanically exfoliated CdI_2 , a novel 2D insulator with high water sensitivity. Sample fabrication was completed entirely within a glovebox or ultra-high vacuum environment. Thin CdI_2 flakes are encapsulated between few-layer hBN crystals and then characterised utilising a range of techniques including Raman spectroscopy and atomic force microscopy. Additionally, Hall bar devices with graphene were constructed and measured allowing investigation of CdI_2 's dielectric properties influence on graphene mobility. Understanding the dielectric properties of this new material could enable the fabrication of new graphene-based devices and new 2D material-based transistors.

MON 48

Optical Properties of Vanadium Doped WS_2 and WSe_2 Monolayers

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2D dilute magnetic semiconductors have been recently reported in transition metal dichalcogenides doped with spin-polarized transition metal atoms, for example vanadium-doped WS_2 and WSe_2 monolayers, which exhibit room-temperature ferromagnetic ordering. For V-doped WS_2 monolayers, power-dependent photoluminescence, resonant four-wave mixing, and differential reflectance spectroscopies are performed here to study optical transitions close to the A exciton energy of vanadium-doped WS_2 monolayers at three different doping levels. Density functional theory calculations show that the band structure is sensitive to the Hubbard U correction for vanadium, which is compared with experimental results. For V-doped WSe_2 monolayer, we report giant effective g-factors ranging between ~ -27 and -69 for the bound exciton at 4 K. This giant g-factor disappears at room temperature, suggesting that this response is associated with a magnetic ordering of the vanadium impurity states at low temperatures. *Ab initio* calculations for the vanadium-doped WSe_2 monolayer confirm the existence of magnetic ordering of the vanadium states.

MON 49

Insights on MnS Layered Heterostructures

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The ability to tune physical properties through layer composition, stacking order, and the relative rotation of adjacent layers makes van der Waals heterostructures highly attractive for advanced technological applications. Notably, the multiferroicity observed in monolayer and multilayer Transition Metal Dichalcogenides (TMDs) positions these materials as ideal candidates for composite multifunctional systems,

enabling significant advancements in next-generation memory devices. Despite extensive research in recent years, many of these systems still remain underexplored. In this work, we investigate the structural properties of MnS monolayers and bilayers using first-principles calculations. Our findings reveal that their ground state is antiferromagnetic, resembling the buckled bilayer structure of *h*-BN or MnSe monolayers. We also present the electronic band structure for these systems. Furthermore, we demonstrate the existence of sliding-driven reversible out-of-plane electric polarization. Finally, we compare our theoretical results with experimental observations of MnS multilayered heterostructures synthesized via Molecular Beam Epitaxy (MBE).

MON 50

Probing solitons of twisted homobilayer MoS₂ by tip-enhanced Raman spectroscopy

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Twisted moiré homobilayers, such as MoS₂, are rich playground to explore strain-induced phenomena at the nanoscale. Of particular interest are 1D shear solitons, which exhibit transitions in atomic stacking order within a few nanometers. These solitons occur in moiré crystals and are expected to host ultra-flat electronic bands and tensile strain, which allows the study of correlated electronic states and exciton guiding. Here we use tip-enhanced Raman spectroscopy (TERS) to directly probe and map the strain distribution in 1D solitons of ultra-clean twisted MoS₂ homobilayers at low twist angles (0.3 degrees) with nanoscale resolution. We show that solitons, where the strain is expected to be higher than the different stacking regions, give rise to broadening of the Raman peak widths, which is consistent with previous measurements in twisted bilayer graphene. Our results expand the possibilities of optical (TERS) measurements to probe different twisted two-dimensional materials other than graphene, opening a new perspective on how to study the optical properties with nanoscale resolution in twisted 2D heterostructures.

MON 51

Topological Darkness for Label-Free Biosensing

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Topological darkness (TD) is a new phenomenon that guarantees zero reflection/transmission of light from an optical sample and hence provides topologically non-trivial phase singularities. These arise from intersections between a constructed zero-reflection surface (ZRS) and the optical material's dispersion relation. These

intersections are topologically protected by the Jordan-Brouwer theorem and are therefore resilient to sample imperfection. The TD theory can be applied to a wide variety of structures such as self-assembled meta-materials [1], optical heterostructures [2], and 2D materials [3]. These phase singularities have many applications; here we highlight their use in ultra-sensitive label-free refractive index biosensing, (measuring the concentration of a molecule via its effect on refractive index at the surface of a sensor) for which single molecule detection has already been proven [4].

[1] Malassis, L. et al. *Adv. Mater.*, 26: 324-330. (2014).

[2] Cusworth, E. et al. *ACS Photonics* 10 (10), 3715-3722 (2023).

[3] Ermolaev, G. et al. *Nat Commun* 13, 2049 (2022).

[4] Kravets, V. et al. *Nature Mater* 12, 304–309 (2013).

MON 52

Dielectric Sheet Excitations of Graphene

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Graphene is the ultimate embodiment of a freestanding two dimensional dielectric sheet. In transmission electron energy-loss spectroscopy, the differential cross section of dielectric sheets is quenched by kinematic effects once the momentum transfer becomes smaller than a critical value set by q_z , the momentum loss parallel to the beam. A highly momentum ($\Delta q = 0.02 \text{ \AA}^{-1}$) and energy ($\Delta E = 45 \text{ meV}$) resolved setup is instrumental on delivering the unprecedented experimental verification of quenched 2D EELS spectra on freestanding graphene at momentum transfers q below 0.06 \AA^{-1} . Quantifying the kinematic suppression allows to retrieve the intrinsic dielectric response of graphene from measured spectra.[1]

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (MORE-TEM ERC-SYN project, grant agreement No 951215).

[1] A. Guandalini et al. *PRB letters*, accepted, doi.org/10.48550/arXiv.2406.02998

MON 53

Characterising Interlayer Excitons by Spectral Signature in Scattering Visible Near-Field Microscopy

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Interlayer excitons (IXs) in van der Waals heterostructures exhibit unique optical properties due to their spatially separated charge carriers. However, their weak oscillator strength and non-radiative broadening make them difficult to detect with conventional absorption spectroscopy. Here, we use scattering-type scanning near-field optical microscopy (s-SNOM) to directly probe their dielectric response at the nanoscale. We first validate this approach by measuring the B-exciton in a four-layer MoS₂ sample, where ion irradiation introduced defect-induced broadening. Extending this method to a MoSe₂/WSe₂ heterostructure, we observe a Lorentzian resonance at 1.35 eV, characteristic of interlayer excitons, with broadening dominated by non-radiative decay. These results demonstrate the capability of s-SNOM to image and characterize weak excitonic resonances at the nanoscale, overcoming the limitations of conventional techniques and providing new insights into localised exciton dynamics in 2D heterostructures.

MON 54

Understanding the morphology and bonding environments of small diameter B-doped SWCNT

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Tailoring the properties of SWCNTs via substitutional doping is a very powerful method to gain control on their physical behavior towards their applicability. Boron doping is however underexplored due to difficulties for production with traditional synthesis methods. We have pioneered the use of high vacuum chemical vapor deposition to enable the synthesis using a non-diluted feedstock containing C and B in the same molecule. Previous work has shown that using tri-isopropyl borate accounts for the production of very small diameter nanotubes but with low yield. In order to improve the SWCNT to impurity ratio, multiple catalysts were tested and an elemental analysis was done at the different phases of the synthesis. The overall sample morphology was inspected by Raman spectroscopy and SEM corroborating an increase of at least 60% in the yield of SWCNTs when using at least two types of catalyst. The catalyst-dependent B incorporation needs a mild-purification of the samples and combined capabilities of EDX in microscopy and high resolution XPS. Our target is to keep the small diameters characteristic of TIB with, very low dopant concentration, while maintaining the tube's stability.

MON 55**Disorder-Driven Topological Insulator Phases in Two-Dimensional Solids**Ksenija Kovalenka¹¹Department of Physics and Astronomy, The University of Manchester, Manchester

Topology in two-dimensional (2D) solid state systems is a rich field which describes a variety of unique properties and phenomena of electronic behaviour. We investigate the interplay of topology and disorder in the system widely used to study 2D Chern insulators - Haldane model, with the presence of onsite disorder. We use local Chern marker (LCM) to quantify the topology in a finite and disordered system [1]. We map out the phase landscape of the disordered Haldane model, identifying a rich array of phases, including trivial and topological Haldane phases, the Anderson localisation phase, and the recently proposed topological Anderson insulator (TAI) phase [2]. In the latter phase, disorder is responsible for creating extended edge states for a trivial set of parameters of the Haldane model. Additionally, we explore the multifractal nature of critical eigenstates within the TAI phase by calculating the dimensionality spectrum to get an insight into the scaling behaviour of the wavefunctions [3].

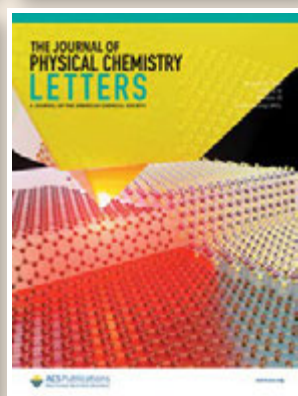
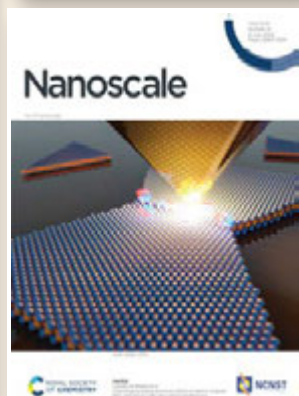
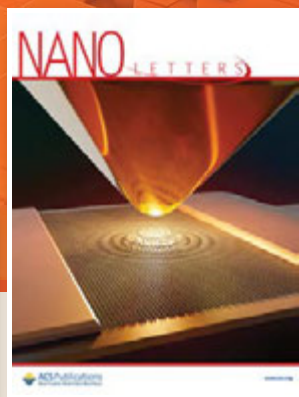
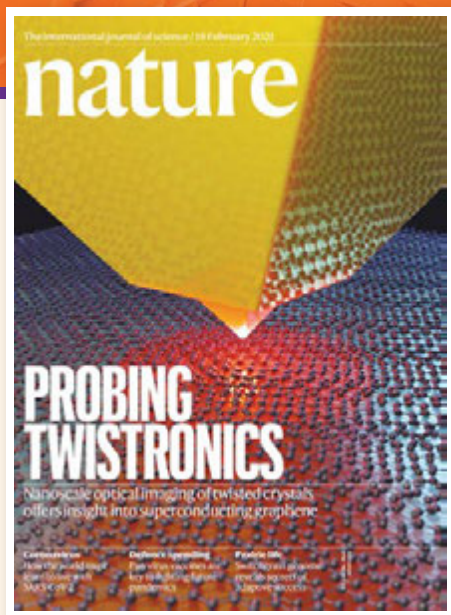
[1] R. Bianco, R. Resta, Phys. Rev. B 84, 241106 (2011) [2] J. Li et al., Phys. Rev. Lett. 102, 136806 (2009). [3] M. Schreiber, H. Grussbach, Phys. Rev. Lett. 67, 607 (1991)



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Tuesday, March 11th

- 08:30 – 09:30 **TUTORIAL: H. Seiler, Berlin**
Probing Electronic Disorder in Nanomaterials with 2D Spectroscopy
- 09:30 – 10:00 **L. Novotny, Zurich**
Exciton-Assisted Electron Tunneling in van der Waals Heterostructures
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **M. Calandra, Trento**
Phonon Mediated Superconductivity in Field-Effect Doped Molybdenum Dichalcogenides
- 11:00 – 11:30 **A. Castellanos-Gomez, Madrid**
High Throughput Mechanical Exfoliation for Large Area and Low Cost Production of 2D Materials
- 11:30 – 12:00 **X. Ling, Boston**
Designed Synthesis of non vdW 2D Materials for Advanced Electronics
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:30 **TUTORIAL: P. Jarillo-Herrero, Cambridge**
The Magic of Morie Quantum Matter
- 19:30 **Celebration 40 years IWEPNM**

Tuesday, March 11th

08:30

Probing electronic disorder in nanomaterials with 2D spectroscopy

Hélène Seiler¹

¹Physics, Freie Universität Berlin, Berlin

Static inhomogeneities and dynamic fluctuations are inherent to nanomaterials, and understanding their impact on the electronic properties is highly relevant for potential nanotechnology applications. Coherent two-dimensional (2D) electronic spectroscopy is a powerful tool to separate static and dynamic sources of disorder. Here we introduce our progresses towards a coherent two-dimensional spectrometer tunable over the 460-950 nm spectral range to investigate the exciton and polariton dynamics in 2D materials. A custom sample area has been designed specifically for 2D materials, typically featuring high degrees of spatial inhomogeneity and small sizes (few tens of micrometers). Linear spectroscopies can be performed at the same position as the 2D spectroscopy experiments, including angle-resolved spectroscopy to investigate polariton dispersion. With our setup we will be able to reveal insights into excitonic and polaritonic properties in 2D materials.

09:30

Exciton-assisted electron tunneling in van der Waals heterostructures

Lukas Novotny¹, Sotirios Papadopoulos¹, Lujun Wang¹, Jonas D. Ziegler¹

¹ETH Zürich, Photonics Laboratory, 8092 Zürich, Switzerland

We fabricate tunnel junctions consisting of graphene and gold electrodes separated by hexagonal boron nitride (hBN) tunnel barriers. The corresponding current-to-voltage (IV) curves feature a typical Fowler-Nordheim tunneling behavior. However, when a single layer of a transition metal dichalcogenide (TMD) is placed close by we observe resonant features in the IV curves. These resonant features match the TMD exciton energies. We thus observe *optical* modes in *electrical* transport measurements.

Tunneling spectroscopy has been utilized extensively in the field of 2D materials to explore electron-phonon coupling (Nature Physics **4**, 627, 2008), to address electronic defect states (Commun Phys **1**, 94, 2018), and to investigate resonant tunneling (Nature Nanotech **9**, 808, 2014). Moreover, excitons have been observed in transport measurements in semiconductor heterostructures (J. Appl. Phys. **81**, 6221, 1997). In all these studies the relevant states were excited by charge injection. On the other hand, in our work the TMDs are sitting outside the electrical path and no charge carriers are injected into the TMDs.

Tuesday, March 11th

10:30

Phonon mediated superconductivity in field-effect doped molybdenum dichalcogenides

Matteo Calandra¹, Giovanni Marini¹

¹Department of Physics, University of Trento, Italy

Superconductivity occurs in electrochemically doped molybdenum dichalcogenides samples thicker than four layers. While the critical temperature (T_c) strongly depends on the field effect geometry (single or double gate) and on the sample (MoS₂ or MoSe₂), T_c always saturates at high doping. The pairing mechanism and the complicated dependence of T_c on doping, samples and field-effect geometry are currently not understood.

In this talk, by performing fully relativistic first principles calculations accounting for the sample thickness, the field-effect geometry and anharmonicity, we rule out the occurrence of charge density waves in the experimental doping range and demonstrate a suppression of one order of magnitude in the electron–phonon coupling with respect to previous calculations, now in excellent agreement with transport data. We explain the behavior of T_c in different systems and geometries. As our first principles calculations [1] show an ever increasing T_c as a function of doping, we suggest that extrinsic mechanisms may be responsible for the experimentally observed saturating trend.

References.

[1] G. Marini and M. Calandra, *2D Materials*, 10, 015013 (2022)

11:00

High throughput mechanical exfoliation for large area and low cost production of 2D materials

Andres Castellanos-Gomez¹

¹Consejo Superior de Investigaciones Científicas, Madrid

Efforts in nanoscience have long sought scalable methods for producing van der Waals materials, following the landmark discovery of graphene via mechanical exfoliation. While this technique offers superior material quality, its scalability is limited by challenges in controlling thickness and lateral size. In this talk, we will introduce a novel approach utilizing a roll-to-roll setup and an automated, massive parallel exfoliation process to address these limitations. Our method yields adhesive tapes densely populated with nanosheets of van der Waals materials over large areas, achieving a notable balance between large lateral size, scalability, and cost-efficiency. Notably, our technique avoids harsh treatments and is compatible with air-sensitive materials. Through successful fabrication of field-effect transistors and flexible photodetectors in large batches, we demonstrate the practicality and versatility of our approach. By providing a low-cost, scalable pathway for producing large-area films, our method promises significant advancements in the fabrication of high-performance nanoscale devices.

Tuesday, March 11th

11:30

Designed Synthesis of non vdW 2D Materials for Advanced Electronics

Xi Ling^{1,2}

¹Department of Chemistry, Boston University, Boston, USA

²Division of Materials Science and Engineering, Boston University, Boston, USA

Extensive research has been conducted on 2D van der Waals (vdW) materials such as graphene, transition metal dichalcogenides (TMDs), and hexagonal boron nitride (hBN) in the past two decades. However, little attention has been given to non vdW materials, which make up the majority of materials in nature. One significant challenge is the lack of an effective synthesis method to access them. In this talk, I will introduce an atomic substitution approach that we have developed to convert vdW layered materials to nanometer-thin non vdW materials. This approach is universal, enabling the synthesis of diverse non vdW 2D materials with tunable thicknesses, desired dimensions, and properties for fundamental physics investigations and nanodevices. As a model system, we will demonstrate the conversion of transition metal dichalcogenides (e.g MoS₂ and WSe₂) to transition metal nitrides (TMN_x) (e.g. MoN_x and WN_x), investigate the conversion process and dynamics, and discuss the stacking configuration dependent chemical reactivity. Moreover, we will discuss the electronic properties of nanometer-thin TMNs and their potential as contacts for electronic devices.

18:30

The Magic of Moiré Quantum Matter

Pablo Jarillo-Herrero¹

¹MIT, Cambridge, USA

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

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Wednesday, March 12th

- 08:30 – 09:00 **M. Bockrath, Columbus**
Correlated Electron States in Multilayer Graphene: From Superconductivity to Half-Integer Quantum Hall Effects
- 09:00 – 09:30 **E. Andrei, Piscataway**
Moiré Periodic and Quasiperiodic Crystals
- 09:30 – 10:00 **N. Avraham, Rehovot**
Visualizing Incommensurate Inter-Valley Coherent States in Rhombohedral Trilayer Graphene
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **J. Folk, Vancouver**
Tales from Twisted Bilayer-Trilayer Graphene
- 11:00 – 11:30 **X. Xu, Seattle**
New Developments in Fractional Quantum Anomalous Hall Effect
- 11:30 – 12:00 **F. Mauri, Rome**
After 20 Years of Research, do we Really Know the Electron-Phonon Interaction of Graphene?
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **A. Luican-Mayer, Ottawa**
Visualizing Moiré Structures in Twisted Semiconducting TMDs and Multilayer Graphene
- 19:00 – 19:30 **S. Ilani, Rehovot**
The Interacting Energy Bands of Magic Angle Graphene Revealed by the Quantum Twisting Microscope
- 19:30 **Poster III**

Wednesday, March 12th

08:30

Correlated electron states in multilayer graphene: from superconductivity to half-integer quantum Hall effects

Marc Bockrath¹

¹Department of Physics, Ohio State University, Columbus

Thin graphite flakes behave as two-dimensional conductors in sufficiently high magnetic fields. I will discuss half-integer fractional quantum Hall states we observe at large filling factors. These single-component states likely stem from Pfaffian wavefunctions derived from those in graphene bilayers, which are predicted to host non-abelian quasiparticles. The facile integration of graphite with top and back surface gates makes this an excellent system to explore device geometries capable of manipulating such quasiparticles. Moreover, the extremely low velocity v_F of electrons in a flat band system results in quenched kinetic energy. Superconductivity thus appears impossible, as conventional theory implies a vanishing superfluid stiffness and coherence length. Using twisted bilayer graphene, we explore the profound effect of very small v_F . We find $v_F \sim 1000$ m/s near moiré superlattice filling fraction $\nu = -2$. This velocity yields a new limiting mechanism for the superconducting critical current. We estimate the superfluid stiffness, finding it is dominated by the interaction-driven superconducting gap, consistent with recent theories on quantum geometric contributions.

09:00

Moiré Periodic and Quasiperiodic Crystals

Eva Y. Andrei¹, Xinyuan Lai¹, Guohong Li¹, Angela Coe¹
¹, Rutgers University

Stacking two atomic crystals with a twist between their crystal axes produces moiré potentials that modify the electronic properties. Stacking three atomic crystals produces a double moiré potential leading to a new class of tunable 2D structures comprised of the two superposed lattices. By using scanning tunneling microscopy and spectroscopy to study the double crystal structures formed by superposing twisted bilayer graphene on hexagonal boron nitride, we observed a wide variety of commensurate periodic and incommensurate quasiperiodic 2D crystals. The incommensurate crystals include quasicrystals, which are quasiperiodic and feature a Bravais-forbidden dodecagonal symmetry, and intercrystals, which are also quasiperiodic but lack forbidden symmetries. These double moiré structures offer a synthetic platform which allowed us to explore the unique properties of quasiperiodic crystals and their profound effect on the electronic wavefunctions.

Wednesday, March 12th

09:30

Visualizing incommensurate inter-valley coherent states in rhombohedral trilayer graphene

Nurit Avraham¹, Yiwen Liu¹, Ambikesh Gupta¹, Youngjoon Choi², Yaar Vituri¹, Hari Stoyanov², Jiewen Xiao¹, Yanzhen Wang¹, Haibiao Zhou¹, Barun Barick¹, Takashi Taniguchi³, Kenji Watanabe³, Binghai Yan¹, Erez Berg¹, Andrea F. Young², Haim Beidenkopf¹

¹Condensed matter physics, Weizmann Institute of Science, Rehovot

²Department of Physics, University of California at Santa Barbara

³ National Institute for Materials Science, Tsukuba, Japan.

Rhombohedral graphene multilayers have emerged as a fascinating platform for exploring a wide range of correlated electronic phenomena due to the promotion of strong electron-electron interactions within gate-tunable van Hove singularities. Recently, indirect evidence of inter-valley coherent (IVC) order has been reported in rhombohedral trilayer graphene (RTG), with possible implications for the origin of superconductivity. In this state, the electronic wave functions in the two valleys form a superposition characterized by a macroscopically coherent phase. I will introduce the rhombohedral trilayer graphene system, its unique properties and the way we study it using scanning tunneling microscopy. Following that I will present the direct visualization of the IVC order in RTG. We observe a cascade of phase transitions associated with the formation of half- and quarter-metal states. IVC phases, distinguished by an enlarged real space unit cell, are directly imaged near both the high- and low-density boundaries of the half-metal phase. I will explain the nature of the observed phases and demonstrate that IVC phases are a widespread ground state within graphene systems.

10:30

Tales from twisted bilayer-trilayer graphene

Joshua Folk^{1,2}, Ruiheng Su^{1,2}, Dacen Waters³, Matthew Yankowitz³, Krystof Kolar⁴, Cyprian Lewandowski⁴

¹Department Physics and Astronomy, University of British Columbia, Vancouver

²Blusson Quantum Matter Institute, University of British Columbia, Vancouver

³Department of Physics, University of Washington, Seattle

⁴Department of Physics, Florida State University, Tallahassee

Twisted graphene structures derived from Bernal-stacked flakes host a rich variety of correlated and topological electronic states. This talk will present a recent discovery in twisted bilayer-trilayer graphene, where strong correlations and topology are deeply intertwined. When the electron density corresponds to simple fractions of the moiré site density, a topological electron crystal (TEC) emerges, akin to a Wigner crystal but carrying a finite Chern number $|C| = 1$, even when the metallic state it formed from had $C = 0$. Minute changes in experimental parameters switch the sign of the Chern number, offering insight into the TEC's underlying nature.

The phase transition to the isospin-polarized metal from which TEC states arise depended on only one of the two electrostatic gates used to tune the sample. This led us to uncover a fundamental effect overlooked since the earliest twisted graphene experiments. At a conceptual level, the moiré bands in Bernal-stacked systems decompose into two components: layer-polarized states, where strong correlations emerge, and delocalized states, which screen the layer-polarized states from one of the electrostatic gates.

Wednesday, March 12th

11:00

NEW DEVELOPMENTS IN FRACTIONAL QUANTUM ANOMALOUS HALL EFFECT

Xiaodong Xu¹

¹Department of Physics, University of Washington, Seattle

The interplay between spontaneous symmetry breaking and topology can result in exotic quantum states of matter. A celebrated example is the quantum anomalous Hall (QAH) effect, which exhibits an integer quantum Hall effect at zero magnetic field due to topologically nontrivial bands and intrinsic magnetism. In the presence of strong electron-electron interactions, fractional-QAH (FQAH) effect at zero magnetic field can emerge, which is a lattice analog of fractional quantum Hall effect without Landau level formation. In this talk, I will first briefly discuss the experimental observation of FQAH effect in twisted MoTe₂ bilayer, using combined magneto-optical and -transport measurements. Then I will present new developments in this direction, including the observation of nearly ideal FQAH effect, abundant Jain sequence of fractional Chern insulator states, as well as ferromagnetism and twist-angle dependent topology of higher energy flat Chern band. Direct observation of the FQAH and associated effects paves the way for researching charge fractionalization and anyonic statistics at zero magnetic field.

11:30

After 20 years of research, do we really know the electron-phonon interaction of graphene?

Francesco Mauri¹

¹Universita di' Roma - La Sapienza, Roma, Italy

The electron-phonon interaction rules electrical transport, relaxation dynamics after photoexcitation and many other properties. It determines the presence of Kohn anomalies in the phonon dispersion and can be investigated using resonant Raman spectroscopy. Recent results from Raman spectroscopy, that uses IR light, indicate that the magnitude of electron phonon interaction could have a strong momentum dependence, that has always been neglected [1]. Here I will present a novel theoretical first-principles framework capable of accounting for the effects of the electron-hole excitonic attraction on the phonon properties [2]. This allows us to reevaluate the graphene electron-phonon interaction and its impact on the phonon dispersion and lifetimes (Kohn-anomalies) near the Gamma (zone-center) and K points (zone-border) [2]. We found a huge, momentum-dependent, enhancement of the electron-phonon coupling with respect to the previous estimations based on DFT or GW theories, when the phonon approaches the zone-border. As a consequence, we predict that room-temperature the graphene mobility is dominated by optical zone-border phonons and that it can be tuned by the dielectric environment.

1. Venanzi et al, Phys. Rev. Lett. 130, 256901 (2023).
2. A. Guandalini, G. Caldarelli, F. Macheda, and F. Mauri, to be published.

Wednesday, March 12th

18:30

Visualizing Moiré Structures in Twisted Semiconducting TMDs and Multilayer Graphene

Adina Luican-Mayer¹

¹Physics , University of Ottawa, Ottawa

By spanning the full range of twist angles between two-dimensional (2D) layers, one can observe the formation of long-range moiré lattices or in-plane reconstructions into energetically favorable patterns. In this talk, I will discuss both phenomena in twisted transition metal dichalcogenides (TMDs) and graphene, as investigated through scanning tunneling microscopy (STM). In the first part of the talk, I will discuss the demonstration of reversible local response of domain wall networks in ferroelectric interfaces of marginally twisted WS_2 bilayers. Moreover, in the case of twisted WS_2 bilayers close to 60° , we observe signatures of flat bands and study the influence of atomic relaxation on their band structure. In the second part of the talk, I will discuss recent results exploring complex moire patterns in twisted multilayer graphene.

19:00

The Interacting Energy Bands of Magic Angle Graphene Revealed by the Quantum Twisting Microscope

Shahal Ilani¹

¹Weizmann Institute, Rehovot

One of the core mysteries of magic-angle twisted bilayer graphene (MATBG) lies in understanding the nature of its interacting energy bands. While MATBG has shown topological phenomena, explained by topological Chern bands in momentum space, the observation of giant entropy at low temperatures has suggested a seemingly contradicting, local moments behavior. This dichotomy has led to various theoretical models, including the topological heavy fermion model and the Mott semimetal framework, each attempting to reconcile how these contrasting features emerge within the flat bands of MATBG. Until now, no tool has been capable of imaging these energy bands at low temperatures and with high enough energy and momentum resolution to resolve these puzzles. Recently, we developed the Quantum Twisting Microscope (QTM), which utilizes momentum-resolved tunneling at a twisting van der Waals interface to directly map the energy bands of quantum materials. In this talk, I will present new measurements, done with the cryogenic QTM on MATBG, revealing the shape and evolution of the interacting energy bands in this canonical quantum system.



POSTER III

WED 1**ENGINEERING OF ADVANCED NANOCARBONS FOR MOF POST-SYNTHETIC MODIFICATION**

Ioanna K. Sideri¹, Georgia Basina¹, Giasemi K. Angeli¹, Nikos Tagmatarchis¹

¹Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens

Currently, MOFs, due to their tunable structural and functional characteristics, are emerging as a sustainable alternative for solar-driven H₂ production. Aiming in advancing their performance, hybridization of MOFs with nanocarbons e.g. fullerenes and carbon nanotubes, holds great promise. In this context, following the synthesis and characterization of engineered advanced nanocarbons, the in-situ or post-synthetic preparation of hybrid MOFs was realized. Emphasizing the tunable nature of MOFs, modified C₆₀ and CNTs bearing -COOH groups and bis-azafullerene (C₅₉N)₂ were prepared to explore their post-synthetic installation and/or impregnation, aiming to create hybrid materials with enhanced performance. All hybrid materials were characterized in detail using state-of-the-art spectroscopic, thermal and imaging techniques.

WED 2**Spin-on Nanocrystalline Graphenic Layers by Pyrolyzation of Polymer Films**

Natalie Galfe¹, Florian Herdl¹, Sebastian Klenk¹, Moritz Quincke², Cormac Ó Coileáin¹, Kangho Lee¹, Ute Kaiser², Georg S. Duesberg¹

¹Institute of Physics, EIT4 and SENS Research Center, University of the Bundeswehr Munich, Neubiberg, Germany

²Central Facility for Materials Science Electron Microscopy, University of Ulm, Ulm, Germany

A novel method for direct fabrication of graphenic carbon layers via a simple spin-on process followed by annealing is presented. The catalyst-free method uses pyrolysis of photoresist films (PPF) and is applicable on multiple substrates. Thus, large-area structured films with decreasing – down to nanometrically thin – thicknesses, as determined by atomic force microscopy, can be fabricated. X-ray photoelectron spectroscopy confirms the predominant *sp*²-nature of our films, and Raman spectroscopy shows signatures of evolving nanocrystallinity with decreasing film thickness. Transmission electron microscopy reveals domains with hexagonal nanocrystalline atomic structure. These films open a cost-efficient, reliable, and scalable integration route for directly grown two-dimensional graphenic carbon materials as an alternative to catalytically grown CVD-graphene requiring a transfer step. We demonstrate the use of PPF films as resistive gas sensing devices, which yields exciting results for NO₂ sensing. These versatile graphenic carbon films hold great promise for a plethora of novel scientific research and future applications, such as advanced optoelectronics and biointerfaces.

WED 3**Mechanically induced sliding of ferroelectric boron-nitride**Francisco Selles^{1,2}, Roman Gorbachev^{1,2}¹Department of Physics and Astronomy, University of Manchester, Manchester, UK²National Graphene Institute, University of Manchester, Manchester, UK

Parallel stacked boron-nitride (BN) crystals exhibit sliding ferroelectricity: a robust out-of-plane electric polarisation that can be reversed by the stacking order. These polarisation states are separated by a fraction of a unit cell, such that deterministic control of the stacking order could allow for displacement sensors with a precision of $< 1 \text{ \AA}$.

To induce sliding, it is necessary to overcome a high-friction commensurate stacking state, as well as pinning from edges, steps and defects. Here, we fabricate a parallel-stacked BN device on a piezoelectric substrate, which uniformly expands with applied voltage. Through clamping, we prevent slippage of the crystals as strain is applied, enabling sliding. The ferroelectric configuration of the BN stack is probed in-situ with electrostatic force microscopy (EFM).

WED 4**Single-Photon Emission and Collective Behaviour of Graphene Quantum Dots in Controlled Environments**Suman Sarkar¹, Hugo Levy-Falk¹, Huynh Thanh¹, Elsa Cassette¹, Loïc Rondin¹, Aurélie Pierret³, Christophe Voisin³, Baudin Emmanuel³, Gaëlle Allard¹, Emmanuelle Deleporte¹, Stéphane Campidelli², Jean-Sébastien Lauret¹¹LuMIn–Lumière, Matière et Interfaces, ENS Paris-Saclay, CentraleSupélec, CNRS, Université Paris-Saclay, Orsay, France²Université Paris-Saclay, CEA, CNRS, NIMBE, LICSEN, Gif-sur-Yvette, France³Laboratoire de Physique de l'École normale supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université de Paris, Paris, France

Bottom-up synthesized graphene quantum dots (GQDs) have emerged as exceptional single-photon emitters, boasting quantum yields (QY) approaching unity. Interestingly, GQDs also exhibit collective behaviour in aggregated states, characterized by sharply redshifted spectral signatures and shorter radiative lifetimes compared to their monomer counterparts. The choice of substrate or environmental conditions for GQD deposition plays a pivotal role in stabilizing monomers and controlling aggregate formation. Achieving absolute control over these factors is critical for exploring indistinguishable photon emission and attaining coherence in molecular aggregates. In this poster, we present the single-photon emission properties of GQDs, their collective behaviour and dynamics, the influence of environmental factors, and the preliminary results on the role of hexagonal boron nitride (hBN) as a high-performance dielectric substrate.

WED 5**Topological Thermal Hall Conductance of Even Denominator Fractional States**

Arup Kumar Paul¹, Priya Tiwari¹, Ron Melcer², Vladimir Umansky¹, Moty Heiblu¹

¹Braun Center for Submicron Research, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel

²Qedma Quantum Computing, Tel Aviv, Israel

The even denominator fractional quantum Hall (FQH) states $\nu = 5/2$ and $\nu = 7/2$ have been long predicted to host non-abelian quasiparticles (QPs). Their present energy-carrying neutral modes are hidden from customary conductance measurements and thus motivate thermal transport measurements, which are sensitive to all energy-carrying modes. While past ‘two-terminal’ thermal conductance ($k_{2t}T$) measurements already proved the non-Abelian nature of the $\nu = 5/2$ FQH state, they might have been prone to a lack of thermal equilibration among the counter-propagating edge modes. Here, we report a novel thermal Hall conductance measurement of the $\nu = 5/2$ and $\nu = 7/2$ states, being insensitive to equilibration among edge modes. We verify the state’s non-Abelian nature, with both states supporting a single upstream Majorana edge mode (hence, a particle-hole Pfaffian order). While current numerical works predict a different topological order, this contribution should motivate further theoretical work.

WED 6**Graphene-based room-temperature IR detector for phonon-enhanced near-field molecular sensing**

Andrei Bylinkin^{1,2}, Sebastián Castilla³, Tetiana M. Slipchenko^{4,5}, Kateryna Domina², Francesco Calavalle¹, Varun-Varma Pusapati³, Marta Autore¹, Fèlix Casanova^{1,8}, Luis E. Hueso^{1,8}, Luis Martín-Moreno^{4,5}, Alexey Y. Nikitin^{2,8}, Frank Koppens^{3,6}, Rainer Hillenbrand^{7,8}

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⁴Instituto de Nanociencia y Materiales de Aragon (INMA), CSIC-Universidad de Zaragoza, Zaragoza, Spain

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⁶ICREA—Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

⁷CIC nanoGUNE BRTA and EHU/UPV, Donostia-San Sebastian, Spain

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Phonon polaritons (PhPs), quasiparticles arising from the strong coupling of infrared (IR) light with lattice vibrations in polar materials, can be used for surface-enhanced infrared absorption (SEIRA) spectroscopy and even for vibrational strong coupling with minute amounts of molecules. Here, we present a compact phononic SEIRA platform using an h-BN/graphene/h-BN heterostructure on a metal split-gate that

forms a p-n junction in graphene. The split gate concentrates light and excites PhPs in the heterostructure, serving as a SEIRA substrate and a room-temperature IR detector. When thin organic layers are deposited directly on top of the heterostructure, we observe a photocurrent encoding the layer's molecular vibrational fingerprint, which is strongly enhanced compared to that observed in standard far-field absorption spectroscopy. The theory supports our findings, predicting further sensitivity gains for thin molecular layers of deep subwavelength scales. Our on-chip phononic SEIRA approach opens exciting possibilities for enhanced molecular sensing at the nanoscale, potentially paving the way for more sensitive and compact sensors in the IR frequency range.

WED 7

Covalent Patterning of Graphene with PAHs and Chiral Molecules for the Construction of Multilayer Materials

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Graphene is a one-atom-thick all-sp²-carbon honeycomb network with outstanding mechanical and electronic properties. However, the lack of an electronic band gap and the semimetal behavior of this material hampers its use in modern electronics. Among the available solutions to this problem, lithographic techniques allow the covalent chemical patterning of graphene with a plethora of molecules in a site-selective manner. These processes create surface defects which open graphene's band gap, while at the same time endow graphene with tailor-made functionalities, thus providing an added value to this material. Covalent patterning of graphene has recently played a relevant role in the construction of novel multilayer structures. Nonetheless, the molecules used to join these layers do not surpass the nanoscale. In addition, chirality is still unexplored in this field, which could open the door to chiral properties in these structures. Therefore, the study of the covalent patterning of graphene with Polycyclic Aromatic Hydrocarbons (PAHs) and chiral molecules will be presented, aiming towards the construction of graphene-based multilayer structures with unprecedented properties.

WED 8

Exciton-polaritons in van der Waals heterostructure metasurfaces

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Recent advances in metasurfaces and 2D materials have revolutionized light-matter interaction in ultrathin devices, yet integrating these fields remains challenging. Here, we introduce van der Waals (vdW) heterostructure metasurfaces, embedding multilayer 2D material stacks with nanophotonic functionalities into monolithic optical metasurfaces. By designing quasi-bound states in the continuum (qBIC) resonances

in vdW thin films, we achieve strong light confinement, enabling these structures to function as optical cavities. Using WS₂ monolayers encapsulated in hexagonal boron nitride (hBN) as a prototype, we pattern vdW stacks via electron beam lithography and dry etching. Hybridization of qBIC resonances with WS₂ excitons demonstrates strong coupling at room temperature. Back focal plane spectroscopy reveals polariton directionality influenced by grating modes, while significant nonlinearities emerge at ultralow fluences (<1 nJ/cm²), outperforming traditional systems. These vdW metasurfaces offer strong light-matter coupling without external cavities, paving the way for ultrathin, low-power photonic devices, including low-threshold lasers and polaritonic condensates.

WED 9

Micro-3D-printing of two-dimensional MoS₂/carbon 3D-electrodes by aerosol jet printing for green hydrogen from electrocatalytic water splitting

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Sustainably produced “green” hydrogen (H₂) is urgently needed as a key energy carrier for a fossil-fuel free future. Sustainable water splitting by electrochemical (EC) and photoelectrochemical (PEC) routes are key technologies for the realization of green H₂ production. Both EC and PEC critically rely on the availability of suitable catalyst electrodes. Currently, it is unclear how EC/PEC catalyst electrodes will bridge macroscopic, complex-shaped three-dimensional (3D) form with nanoscopic, catalytic materials functionality, which is hard to achieve with traditional fabrication methods. Even currently available 3D printing techniques are limited for 3D EC/PEC electrode manufacturing. However, the scientific community has overseen the potential of aerosol jet printing (AJP) to produce such (photo-)electrocatalytic active structures. Here, we demonstrate 3D-AJP of functional 2D+ material inks, as promising (photo-)electrocatalysts for water splitting. We show that not only 3D grid structures are possible, but also pillars of up to 1 mm in height. This study thereby establishes a framework for the parameter space towards rational process development of functional 2D+ material AJP.

WED 10

Compact On-Chip Reflector for Broadband Out-of-Plane Light Collection from Carbon Nanotube Quantum Emitters

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A wide range of nanomaterials have been shown to be promising on-chip emitters of both classical and quantum light for integrated photonics. However, out-of-plane collection of such light remains challenging, particularly for broadband light or when no predefined emitter wavelength exists, as in the case of aryl sp^3 -functionalized carbon nanotubes. Light outcoupling is typically achieved using grating couplers or 3D-printed polymer couplers. The former operates efficiently only within narrow wavelength bands, while the latter requires additional fabrication equipment and lacks thermal stability. We propose a broadband, thermally stable reflector for out-of-plane light collection that can be fabricated with standard laboratory equipment. L-shaped metal reflectors positioned at the end of a waveguide are designed and investigated. Geometrical parameters, such as the waveguide-to-reflector distance and the reflector dimensions, are shown to be critical. To optimize these parameters, we model light propagation using the FDTD method. We believe the proposed method offers a novel solution to the challenge of efficiently and broadly collecting out-of-plane light from on-chip emitters.

WED 11

Tuning the proximity induced spin-orbit coupling in bilayer graphene/WSe₂ heterostructures with pressure

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To probe the interlayer interactions in van der Waals heterostructures, the pressure is an ideal tool, as it changes the interlayer distance and thus the interlayer tunneling.

Here, we show how the proximity induced spin-orbit coupling (SOC) is changed with applied hydrostatic pressure in graphene and transition-metal dichalcogenide based devices. In monolayer graphene based heterostructures it was already shown with weak anti-localization measurements that the pressure increases the SOC strength. To demonstrate this, we measured bilayer graphene (BLG) and WSe₂ based heterostructures[1]. From magnetotransport measurements, we extracted Landau level crossings, which is used to obtain the strength of the Ising-type SOC. On the other

hand, we performed Shubnikov-de Haas measurements to obtain the strength of the Rashba-type SOC.

Furthermore, we measured WSe₂/BLG/WSe₂ heterostructures, where we used the closing of the inverted phase to extract the SOC strength[2]. This phase occurs when the sign of the induced SOC is opposite for the top and bottom graphene layers.

[1] Szentpeteri, B., et al. arXiv:2409.20062

[2] Kedves, M. et. al. Nano lett 23 (2023), 20, 9508–9514

WED 12

Highly efficient photocatalytic functionalization of single-wall carbon nanotubes with luminescent quantum defects for bioimaging

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Semiconducting single-wall carbon nanotubes (SWCNTs) functionalized with luminescent quantum defects are a promising material platform for next-generation in-vivo imaging, metabolite sensing and single-photon emission in the near-infrared (nIR). With growing interest to apply SWCNTs with quantum defects in new imaging and sensing applications, it is crucial to develop efficient and selective functionalization methods leading to high photoluminescence quantum yields. Here, we introduce a photocatalytic procedure to functionalize SWCNTs with bright oxygen quantum defects in aqueous environments, organic solvents, and in thin films. Based on inexpensive chemicals and proceeding under mild conditions, this method simultaneously offers high scalability and precise control of the defect density, as determined by Raman spectroscopy.[1,2] The functionalization protocol is applicable to nanotubes with different diameters, and perfectly suited to prepare bright and biocompatible SWCNTs for high-contrast biological imaging in the nIR.

[1] Sebastian et al., J. Phys. Chem. Lett. 2022, 13, 3542-3548.

[2] Sebastian et al., Nanoscale Horiz. 2024, DOI: 10.1039/D4NH00383G.

WED 13**Optical Properties of TMDCs/Plasmonic Supercrystal Heterostructures**

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Plasmonic supercrystals, which are highly ordered three-dimensional assemblies of metallic nanoparticles, are promising materials for tailoring exquisite optical properties that enable applications in analytical chemistry, bioimaging, optical coatings and waveguiding. Their excitation spectrum is characterized by the formation of hybrid light-matter states, 3D plasmon polaritons, transverse propagations which form standing waves within the crystal, leading to optical resonances across a broad spectral range.

In this work we combine nanoparticle supercrystals with transition metal dichalcogenides in order to enhance their optical response. Flakes of tungsten diselenide were deposited on top of gold nanoparticle supercrystals to create a heterostructure. The results of the absorption experiments with different thickness of TMDCs layers were compared with FDTD simulations in order to understand the underlying processes.

WED 14**Universal vibrational anharmonicity in carbyne-like materials**

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Carbyne, an infinite linear chain of carbon atoms, is the truly one-dimensional allotrope of carbon. While ideal carbyne and its fundamental properties have remained elusive, carbyne-like materials like carbyne chains confined inside carbon nanotubes are available for study. Here, we probe the longitudinal optical phonon (C-mode) of confined carbyne chains by Raman spectroscopy. We observe a strong vibrational anharmonicity that increases with decreasing C-mode frequency, reaching up to 8% for the third overtone. Comparing with carbon atomic wires, we find that this relation between vibrational anharmonicity and C-mode frequency is universal to carbyne-like materials. This establishes experimentally that carbyne and related materials have pronounced anharmonic potential landscapes which must be included in the theoretical description of their structure and properties.

WED 15**Rabi Splitting in Quantum Wells and TMDCs: Influence of Many-Particle Coulomb Correlations**

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Ultrafast coherent manipulation of matter with light remains a highly active field. Here, in a joint theory-experiment collaboration, we study the Rabi splitting of excitons under simultaneous strong light-matter and Coulomb interaction on ultrafast timescales.

In particular, we develop a model based on Heisenberg equations of motion and apply a correlation expansion of many-body interactions to discuss these signatures in measured pump-probe spectra of (Ga,In)As multi quantum wells (MQW) and MoSe₂ monolayers.

It turns out, that in a setting, where Coulomb and optical interaction are comparable (MQW in co-circular excitation), the Rabi splitting almost linearly follows the optical field amplitude similar to an ideal two-level system.

On the other hand, in a setting with dominating Coulomb interaction (MoSe₂ in co-linear excitation), the Rabi splitting depends sublinearly on the optical field strength and it significantly deviates from an ideal two-level system. Within the developed many-body approach, we identify the origin of this sublinear trend due to the presence of six-particle exciton-to-biexciton transitions.

WED 16**Tuning WS₂ Epitaxy: Insights into High- and Low-Temperature Mechanisms**

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The evolution of semiconductor technology relies on precise thin film and nanostructure control, critical for nanoelectronics, optoelectronics, and sensors. While traditional epitaxy has been central to this progress, the concepts of "van der Waals" (vdW) and "quasi-vdW (Q-vdW) epitaxy," introduced decades ago, provide new frameworks for the oriented growth of vdW layers on 2D and 3D substrates. This

study introduces a novel WS₂ growth method using a metal-organic chemical vapor deposition (MOCVD) system with sequential metal and chalcogen precursor introduction. A pre-growth metal-seeding step facilitates the formation of an ordered WO₃ mono- or few-layer on c-plane sapphire, which critically enables quasi-vdW epitaxy. This reveals a new mechanism of epitaxial growth. Additionally, we demonstrate WS₂ epitaxial growth at relatively low temperatures, down to 300 °C, and provide new insights into temperature-dependent processes. These findings enable the rational design of epitaxial growth for a broader range of material systems.

WED 17

Sum-Frequency Spectro-Microscopy to Image Infrared Materials Excitations

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Nonlinear optical microscopy and spectroscopy are powerful tools to characterize interfaces and lower-dimensional materials. Here, I show two examples how we use infrared + visible sum-frequency generation to image mid-infrared materials excitations with wide-field optical microscopy. The techniques provide combined spatial and spectral information, with sub-diffractive spatial resolution. 1. We visualize the propagation patterns of infrared phonon polaritons in a metasurface of silicon carbide [1]. Through a combination of microscopy and spectroscopy, we observe the hybridization and strong coupling of propagating and localized polaritons. 2. We visualize monolayers of hexagonal boron nitride on an insulating substrate. This material is usually optically invisible because of its large band gap. Resonant infrared excitation of phonons and heterodyne sum-frequency imaging enable us to image, both, its topography and crystal orientation.

[1] Niemann, Mueller et al. *Advanced Materials* 36, 2312507 (2024)

WED 18

Dual role of gold on MoS₂ in aqueous environment: proximity-dependent degradation catalysis versus protection

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Many applications of MoS₂ in sensing, catalysis, or electrochemistry rely on the interactions of MoS₂ with solvents or wet chemical functionalization. Gold substrates are important due to the gold-assisted exfoliation, which enables the preparation of exceptionally large MoS₂ flakes, facilitated by the strong interaction between MoS₂ and Au. While MoS₂ is generally considered stable in water and other solvents, the stability and reactivity of MoS₂ on gold substrates in aqueous environments remain unclear. The presence of gold likely alters local conditions, potentially affecting the material's properties and behavior.

In this work, we report on the dual role of gold in the degradation of MoS₂ in water under laser irradiation. We demonstrate that gold catalyzes the degradation of MoS₂, leading to a layer-by-layer breakdown. Simultaneously, the strong interaction with gold protects the closest MoS₂ layer from this degradation. Additionally, we observe that the degradation process is accompanied by intriguing time-dependent photoluminescence events, which provide potential tools for real-time monitoring of the degradation processes.

WED 19

Towards Far-field Light Coupling to Hyperbolic Polaritons in CrSBr through Nanoscale Patterning

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Two-dimensional Van der Waals materials have proven an interesting platform to study the coupling of light to different dipolar excitations, leading to polariton formation in different coupling regimes. In particular, hyperbolic polaritons are exotic modes showing interesting physical phenomena in anisotropic materials with permittivities having different signs along different crystallographic axes, which combined with the advances in twist angle control of the 2D materials, has been used to control light propagation via the shaping of its dielectric function, showing topological behavior, polariton canalization or sub-diffractive wave guiding.

Here we show our progress on far-field light coupling to self-hybridized hyperbolic exciton-polaritons in a 2D magnetic semiconductor CrSBr, through a nanopatterned structure in its crystallographic structure that provides the necessary momentum to couple to in-plane hyperbolic modes. Such technique overcomes the limitations imposed by near-field techniques, and is compatible with recent developments in the in-situ angle control of 2D materials towards the development of twist angle dependent optical phenomena in the NIR-VI range.

WED 20**Mid-infrared optoelectronics of graphene-based devices**

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We use a tuneable femtosecond mid-IR laser to probe the photocurrent response and charge carrier dynamics in graphene-based devices from 4 μm to 20 μm . For monolayer graphene, we demonstrate that two-terminal devices allow determining the pulse shape of a femtosecond mid-IR pulse with a pulse duration of about 100 fs in the wavelength regime of 5.5-14 μm via an autocorrelated photocurrent at the metal-graphene interface [1]. For near-magic angle twisted bilayer graphene, recent THz studies demonstrated a polarization-resolved shift-current response which can access the underlying quantum geometry of the correlated bands [2]. We discuss how to extend the experimental regime to a femtosecond mid-IR excitation to access also the carrier dynamics after a near-resonant excitation. We present first results, fabrication, and characterization of twisted bilayer devices close to the magic angle.

[1] Pettinger et al., App. Phys. Lett. (2024)

[2] Kumar et al., arXiv:2406.16532 (2024)

WED 21**Beyond First-Order: Unlocking the Potential of Higher-Order Moiré Patterns in 2D Materials**

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Higher-order moiré patterns in 2D materials open new possibilities for tuning electronic properties beyond first-order moiré systems. While first-order patterns arise from fundamental lattice periodicities, higher-order structures result from harmonic contributions that dominate at specific twist angles [1]. We investigate different model systems (MoTe₂/graphene, graphene/Au(111)) using density functional theory (DFT) and molecular dynamics (CMD), supported by STM. We show that these patterns can generate large-wavelength periodic potentials in heterobilayers for modulating electronic states, akin to those observed near the 0° twist angle in homobilayers. Our analysis reveals unique properties of this new class of patterns, including large-wavelength effects (8–10 nm) with electron localization relevant to flat-band

physics and coexisting higher-order textures, in which STM bias voltage can selectively enhance specific moiré patterns, enabling electronic switching between them [2]. These phenomena present exciting opportunities for novel electronic devices.

[1] Zeller, P. & Günther, S., *New J. Phys.* 16, 083028 (2014)

[2] Pham, T. T. et al. *npj 2D Mater. Appl.* 6, 1–11 (2022)

WED 22

Infrared photodetection in graphene-based heterostructures and twisted bilayer graphene

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Stacking of van der Waals materials enables various degrees of freedom for properties control. We study two types of devices based on graphene for enhanced infrared photodetection. The first one is the small-angle twisted bilayer graphene (tBLG). It attracts much attention due to appearance of low-energy flat bands. We demonstrate the gate-tunable photoresponse and find the peculiarities at integer band fillings upon linear and circular excitation. The origin of the photodetection may stem from the bulk photovoltaic effect.

The second type is graphene/hBN/graphene tunnel device that offers promise as sensitive mid-infrared photodetector. We demonstrate that the photocurrent is proportional to the second derivative of the tunnel current with respect to the bias voltage, peaking during tunneling through the hBN impurity level. We revealed that the origin of the photocurrent generation lies in the change of the tunneling probability upon radiation-induced electron heating in graphene layers [1]. The photocurrent can be used for accurate measurements of the electronic temperature.

[1] *npj 2D Mater. Appl.* 8, 34 (2024)

WED 23

Twist angle dependent interlayer transfer of valley polarization from excitons to free charge carriers in WSe₂/MoSe₂ heterobilayers

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Transition metal dichalcogenides (TMDs) have attracted much attention in the fields of valley- and spintronics due to their property of forming valley-polarized excitons when illuminated by circularly polarized light. In TMD-heterostructures it was shown that these electron-hole pairs can scatter into valley-polarized interlayer exciton states, which exhibit long lifetimes and a twist-angle dependence. However, the question how to create a valley polarization of free charge carriers in these heterostructures after a valley selective optical excitation is unexplored, despite its relevance for opto-electronic devices. Here, we identify an interlayer transfer mechanism in twisted $WSe_2/MoSe_2$ heterobilayers that transfers the valley polarization from excitons in WSe_2 to free charge carriers in $MoSe_2$ with valley lifetimes of up to 12 ns. This mechanism is most efficient at large twist angles, whereas the valley lifetimes of free charge carriers are surprisingly short for small twist angles, despite the occurrence of interlayer excitons.

WED 24

Carbon Nanotube Network Memory Enabling Ultrafast Memory Operations

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Emerging non-volatile memory (NVM) promises computing-in-memory, a brain-like computing framework transcending the current von Neumann architecture. However, the development of NVM with high-speed write and erase operations thus far remains challenging. Here, we propose enabling ultrafast memory operations in NVM employing the Maxwell-Wagner effect. Complying with this effect, we demonstrate wafer-scale charge trapping memories with polymer sorted single-walled carbon nanotube networks. The memories exhibit an ultrafast write and erase speeds of 100 ns, approaching the limit of the Maxwell-Wagner effect. Notably, the memories are 1000 times faster than the conventional silicon-based flash memories. Via opto-electrical characterisations, we prove the ultrafast memory operations arise

from the ultrafast charge trapping behavior in the ultrathin heterogeneous interfaces in the carbon nanotube networks, as the Maxwell-Wagner effect dictates. The understanding suggests the ultrafast memory operations are universal for devices with similar network structures, and can enable high-performance computing-in-memory.

WED 25

Towards Probing Topological Superconductivity via Josephson Radiation in Cd_3As_2 Nanowire Junctions

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Topological superconductivity is a key topic in condensed matter physics for its potential to host stable states for Majorana fermions, which can arise in 3D Dirac materials with strong spin orbit coupling. One such topological material is Cd_3As_2 , where superconductivity was successfully induced in nanowire Josephson junctions. These junctions demonstrate strong gateability, missing first order Shapiro steps, and magnetic field induced opening and closing of the Dirac gap. Although these phenomena are signs of a topological phase transition, we aim to strengthen this claim by measuring 4π periodic Josephson radiation arising from the ac Josephson effect.

We develop a state-of-the-art radiation detector inside a 20 mK cryogenic environment, where the ac Josephson radiation generated by a Nb- Cd_3As_2 -Nb junction couples to a nearby RF-line for amplification and readout. This provides the radiation spectrum arising from the junction, which can identify the present transport modes. Using this, we increase the understanding of the topological nature of Cd_3As_2 , but also develop an infrastructure for Josephson radiation spectroscopy.

WED 26

Generation of broadband entangled photon pairs with Raman and electronic interactions in centrosymmetric materials

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In Raman scattering, when a Stokes and an anti-Stokes photon are created via the same phonon, a correlated Stokes-anti-Stokes (SaS) photon pair is created. It is known that quantum correlations between the two photons can arise in such a setting [PRL 119, 193603 (2017)], and even polarization entanglement [PRA 108, L051501 (2023)], while the spectrum of the correlated SaS scattering exhibits a characteristic asymmetry with respect to the phonon resonance frequency [PRB

99, 100503(R) (2019)]. This phenomenon lacked until now a proper theoretical description that could explain these features in a unified way. Here we present a fully quantum theory [arXiv:2408.11602], and we show that a coherent contribution of an electronic and a phononic (Raman) four-wave mixing process explains both the polarization entanglement and the correlation spectrum. The theory allows us to predict how to build experiments to generate photon pairs that could maximally violate a Bell-type CHSH inequality, opening the path to use SaS scattering in quantum information tasks, having Raman scattering of centrosymmetric materials as the basis for a new kind of broadband source of entangled photon pairs.

WED 27

Tip assisted Fourier space nonlinear images of 2D materials

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Fourier space images reveal the angular emission distribution of a source, i.e., its radiation pattern. We show that the images generated by Fourier second harmonic generation (FSHG) imaging provide valuable information on the crystal symmetry and orientation of 2D materials [1]. However, the SHG process is limited to non-centrosymmetric materials. One way to overcome this limitation is to use third-order nonlinear techniques such as four-wave mixing (FWM). We then present Fourier space FWM images and the particular case of Coherent anti-Stokes Raman scattering (CARS). Moreover, we introduce a tip in order to amplify our signal [2] and observe the effects of the tip confinement of nonlinear processes to a coherently emitting nanoscale area with a strongly heterogeneous polarization distribution. We demonstrate the influence of the tip on the Fourier space images using plasmon-tunable tip pyramids (PTTP) for monolayers of transition metal dichalcogenides.

[1] L. Lafeta et al. Probing Symmetry of Noncentrosymmetric 2D Materials by Fourier Second Harmonic Imaging. (Under Review).

[2] A. Jorio et al. Nano-Raman Spectroscopy of 2D Materials. 2D Materials, 11, 033003.

WED 28

Fingerprinting perfect and mixed stackings of rhombohedral graphite

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In recent years, rhombohedral graphite gained prominence, because it can host a multitude of strongly correlated electronic phenomena in its surface flat electronic band. However, the identification of rhombohedral graphite samples is getting more

challenging as the layer number increases because traditional Raman identification methods become unreliable. Furthermore, the number of possible stacking configurations in these thicker crystals increases exponentially with N . Recently, using a conventional confocal Raman spectrometer at room temperature, we were able to unambiguously identify the perfect rhombohedral stacks by measuring their Electronic Raman Scattering signal which directly fingerprints the flawless stacking [1]. In this paper we extend this method for mixed stackings (partial rhombohedral and Bernal), and we show that the mixed stackings can be fingerprinted as well, what configurations are elemental weak ferroelectric materials. Furthermore, based on DFT and TB calculations, we give the full landscape of the ERS spectra of the possible stacking configurations to establish a solid background for their identification.

[1] Pálinkás et al. Carbon 230, 119608 (2024)

WED 29

In-Situ Heating and Growth Experiments on a Copper-Benzenhexathiol Coordination Polymer in High-Resolution (Liquid-Phase) Transmission Electron Microscopy

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Two-dimensional polymers, as layer-stacked conjugated metal-organic frameworks (2D c-MOFs) and conjugated coordination polymers (2D c-CPs) spark enormous interest nowadays due to their structure-dependent properties. By linking different node molecules with metal atoms, a manifold of structures and hence, a large variety of properties is possible. We found that the hydrogen free c-CP $\text{Cu}_3(\text{BHT})$ (BHT = benzenehexathiol), expresses high electron beam resilience unlocked through its high electrical conductivity. Furthermore, utilizing this highly stable c-CP enables us to perform in-situ HRTEM studies, capturing the heat-induced structural dynamics of $\text{Cu}_3(\text{BHT})$. In addition, we study the formation process of $\text{Cu}_3(\text{BHT})$ and perform in-situ liquid-cell transmission electron microscopy (LC-TEM) experiments. Surprisingly, the growth here results in the formation of $\text{Cu}_4(\text{BHT})$ instead of the expected $\text{Cu}_3(\text{BHT})$. We explain this difference by considering radiolysis taking place during the interaction of the electron beam with the solutions inside the liquid cell.

WED 30**Novel Ultra-High Vacuum Fabrication for Magnetic 2D Material Heterostructures**

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The novel properties observed in heterostructures of 2D materials rely on clean, atomically flat interfaces. Investigations into the crystallographic and electronic properties of many 2D materials, especially monolayers of magnetic materials, has been limited due to the difficulty of fabricating clean monolayer samples caused by their degradation in ambient conditions.

This work presents novel techniques for the fabrication of 2D heterostructures in ultra-high vacuum (UHV) conditions, using a polymer free, SiN_x membrane based transfer method. The full fabrication process, including material exfoliation, is carried out within the UHV environment. The benefits of the system are demonstrated by the fabrication of heterostructures from air sensitive materials including CrI₃ for ARPES measurements and the first characterisation of VBr₃ monolayers for NV scanning magnetometry. The clean, high-quality devices produced showcase the advantages of UHV sample fabrication for highly sensitive materials. The NV scanning magnetometry results obtained confirm that the VBr₃ monolayer is an out of plane ferromagnet.

WED 31**Photoluminescence and resonant Raman scattering of MoTe₂ in the IR regime**

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Raman scattering with infrared excitation can be useful to study graphene [1] and semiconductors with band gap in the infrared [2]. Here we report on PL and Raman scattering spectroscopy of MoTe₂ with IR excitation energies.

At 1.16 eV we excite monolayer MoTe₂ in resonance with the A exciton. We observe the typical valley selection rule in the PL spectra of TMD monolayers and the appearance of several Raman modes, switched on by the resonant excitation.

In bulk MoTe₂, at 0.8 eV, below the energy of the direct optical gap, we observe an enhancement of the second order modes and an inversion of the intensities of the

first order modes (A_{1g} and E_{2g}) when reducing the excitation energy from visible to the IR, as predicted in [3].

Through symmetry analysis and ab-initio calculations of the exciton-phonon scattering matrix elements, we study the allowed Raman-scattering pathways which lead to the observed resonant enhancements of certain 2nd order peak and quenching of the first order E_{2g} mode.

[1] T. Venanzi et al., PRL 130, 2023, 25690

[2] S. Sotgiu et. al., PRB 106 2022, 085204

[3] H.P.C. Miranda et al., Nano Lett 17 2017,2381

WED 32

Excitation-dependent Raman Mode Polarization Switching in CrSBr

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Semiconducting CrSBr is a layered A-type antiferromagnet, with individual layers antiferromagnetically coupled along the stacking direction. Due to its unique orthorhombic crystal structure, CrSBr exhibits highly anisotropic mechanical and optoelectronic properties acting as a quasi-1D material. CrSBr demonstrates complex coupling phenomena involving phonons, excitons, magnons, and polaritons. Here we show through polarization-resolved resonant Raman scattering the intricate interaction between the vibrational and electronic properties of CrSBr. For samples spanning from few-layer to bulk thickness, we observe that the polarization of the A_g^2 Raman mode can be rotated by 90 degrees, shifting from alignment with the crystallographic a (intermediate magnetic) axis to the b (easy magnetic) axis, depending on the excitation energy. In contrast, the A_g^1 and A_g^3 modes consistently remain polarized along the b axis, regardless of the laser energy used. We access real and imaginary parts of the Raman tensor in our analysis, uncovering resonant electron-phonon coupling.

This work has been preprinted as [P. Mondal, et al., "arXiv preprint arXiv:2410.22164" (2024)].

WED 33**Spatially resolved 2D Laser Writing of Graphene with Diazonium Salts**Johanna Krüger¹, Tamara Nagel¹, Frank Hauke¹, Andreas Hirsch¹¹Lehrstuhl für Organische Chemie II, FAU, Erlangen

Modifying graphene via covalent functionalization by introducing various functional moieties and therefore tuning the chemical properties has established itself as a key field in graphene research.¹ Modern 2D patterning techniques, which combine highly efficient, covalent functionalization with precise spatial resolution, allows a dimensional and quantitative control over the addend binding.² Herein, we present an optimized protocol for the laser activated spatially resolved functionalization of graphene using various diazonium salts exhibiting different functional groups, where the laser writing behavior of 4-tertbutylbenzenediazonium tetrafluoroborate (4-TBBD) is presented in detail.

References

¹ T. Wei, F. Hauke, A. Hirsch, *Adv. Mater.* 2021, 33, 2104060.² K. F. Edelthammer, D. Dasler, L. Jurkiewicz, T. Nagel, S. Al-Fogra, F. Hauke, A. Hirsch, *Angew. Chem. Int. Ed.* 2020, 59, 23329-23334.**WED 34****Optical properties of phthalocyanine monolayers**José A. Arcos Pareja¹, Jiajun Dai¹, Sabrina Juergensen¹, Beate Paulus¹, Eduardo B. Barros¹, Stephanie Reich¹,¹Freie University Berlin, Germany²Universidade Federal do Ceara, Brazil

Highly ordered monolayers of organic molecules show intriguing optical properties, arising from the interaction of their transition dipole moments in the lattice. The coupling of these transition dipole moments gives rise to a delocalized collective optical state [1]. The nature of the transition dipole moment has a strong impact on the optical properties of the system. Here we grow two-dimensional monolayers of metal free phthalocyanine and copper phthalocyanine and study their optical properties. Phthalocyanine molecules are compelling due to their two degenerate transition dipole moments. Polarization dependent measurements reveal a clear difference between the metal-based and the metal-free phthalocyanine. DFT calculations indicate, that this is caused by the interaction of the metallic molecules with the substrate, resulting in the degeneracy breaking of the molecular eigenstate.

[1] S. Juergensen & S. Reich et al., *Collective States in Molecular Monolayers on 2D Materials*, *ACS nano* 17(17), 17350-17358 (2023).

WED 35**Time-resolved spectroscopy of the spin-valley blockade in a bipolar double quantum dot in bilayer graphene**

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Pauli blockade is an established read-out mechanism for quantum dot (QD)-based spin qubits hosted in semiconductors. Bilayer graphene (BLG) is a novel platform offering tunable valley degree of freedom, weak spin-orbit coupling and hyperfine interaction, as well as a gate-tunable band gap. Recently, a strong spin-valley blockade in a single electron-single hole double quantum dot (DQD) with a near perfect symmetry, was shown, where only time-averaged transport measurements were performed. This method leaves out low-probability tunnel processes. Here, we report on time-resolved measurements by applying a dual pulse between the (0 electron, 0 hole) to (1 electron, 1 hole) charge configurations. By comparison with rate equation simulations, we find that unconventional higher order tunneling processes mainly lift the blockade, where the timescale depends on lead-QD coupling and the amount of contributing states, which vary with applied magnetic fields. Extracting the timescales of blockade lifting and investigating the main mechanisms in this rarely studied strong lead-QD coupled system, allows us to understand the importance of tunable coupling strengths for the read-out of QD states.

WED 36**Graphene Nanoribbons as Atomically Precise Light Emitters**

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of Bern, Bern, Switzerland.

Owing to graphene nanoribbons (GNRs) structural descent from graphene, combined with an opening of the electronic/optical bandgap (1D-electron confinement), GNRs are expected to be stable yet atomically precise light emitters that can be triggered electronically (electroluminescence) or by photon absorption (photoluminescence) (1). In my poster, I discuss the concept of localized electron density by extensions, electron donor-acceptor groups or atom-doping as possible approaches to provide a robust platform for luminescence in GNRs, without relying on reactive terminal end states (2). To incorporate luminescent GNRs into opto-electronic devices, a transfer step from the growth-surface onto a non-metallic substrate is necessary, as well as to study their optical properties in an STM junction by STML spectroscopy and in the far-field by means of PL/Raman spectroscopy (prevent luminescence quenching). As a first step, we investigate how the Raman spectra differ between various GNR modifications and their evolution with external parameters (oxygen, temperature) to monitor the transfer of GNRs between surfaces.

(1) Nature 466, 470–473 (2010)

(2) Science 379, 1049-1054 (2023)

WED 37

Strain-dependent properties of free-standing PtSe₂: Towards 2D MEMS

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Two-dimensional (2D) layered materials have attracted considerable attention due to their exceptional mechanical, electrical, and thermal properties. PtSe₂ is a prime candidate for next-generation micro- and nano-electromechanical systems (MEMS/NEMS) due to its high piezoresistivity. In our work, we demonstrate the scalable fabrication of free-standing 2D materials, including PtSe₂ and other novel nanomaterials. The devices provide a universal platform for fundamental research on 2D materials under strain and pathways to applications in next-generation MEMS. In-depth characterization methods, including Raman spectroscopy, scanning transmission electron microscopy (STEM), and electrical characterization, are employed to evaluate the structural, electronic, and micromechanical properties of the material. Our free-standing devices exhibit potential applications in novel 2D MEMS, with

advantages in terms of scalability, enhanced sensitivity, and improved performance over conventional materials.

WED 38

Van der Waals engineering of one-transistor-one-memristor architecture for energy-efficient neuromorphic array

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2D-material-based memristor arrays are a promising innovation with considerable potential for data-centric applications. Here, we propose a van der Waals engineering approach to create one transistor one-memristor (1T1M) cells using atomic-thick CuCrP2S6, MoS2 and h-BN. Through MoS2 transistor gating effect, the CuCrP2S6-based memory cell exhibits a high resistance tunability of up to 10⁶, which enables the memory to switch on or off to a record-low sneak current of 120 fA with an ultralow static power of 12 fW. Using the designed 1T1M architecture, a neuromorphic array with greatly reduced crosstalk issues is experimentally demonstrated. Furthermore, the nonvolatile resistance switching observed in the device is attributed to electric field-driven polarization reversal, which is confirmed by the electrical measurements and first principles calculations. The proposed approach of van der Waals engineering offers a universal solution for creating compact 2D in-memory computation systems with a higher degree of gate control freedom toward next-generation artificial neural networks.

WED 39

Electrochemical hydrogen peroxide production by metal-free functionalized graphene featuring electrostatically associated polyacrylate chains

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Graphene-based materials hold a strong potential for electrocatalysing the oxygen reduction reaction (ORR) owing to their modification capability.[1] Herein, oxidized graphene was initially covalently decorated with amphoteric imidazole rings, which were then converted to the corresponding imidazolium counterparts. Anion exchange allowed the immobilization of polyacrylate chains on the imidazolium cations via electrostatic interactions. The electrocatalytic performance of the so-formed graphene-based ensemble towards ORR was evaluated, unveiling the 2e⁻ reduction of oxygen selectively producing hydrogen peroxide. The importance and effect of the bulky polyacrylate anions' presence, as part of the graphene-based electrocatalyst towards ORR, are highlighted, providing valuable insights for tuning the electrocatalytic performance of graphene-based ensembles as metal-free elec-

trocatalysts.

[1] I. K. Sideri, N. Tagmatarchis, *Chem. Eur. J.* 2020, 26, 15397.

WED 40

Ordered Au Membranes for Bulk-suppressed and surface-sensitive Raman scattering

Gonca Aras¹, Roman M Wyss^{1,2}, Pietro Marabotti¹, Aleksei Tsarapkin³, Jonas Henning³, Katja Höflich³, Maximilian Oezkent⁴, Chen-Hsun Lu⁴, Kevin-P Gradwohl⁴, Sebastian Heeg¹

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Raman spectroscopy is a powerful characterization technique that is rarely applied to study surfaces due to their weak Raman response and dominating bulk Raman signals. We recently overcame this limitation by using nanoporous gold membranes (PAuM) to enhance the surface Raman signal by plasmonic enhancement from the membrane's nanopores while suppressing the bulk Raman signal [1]. Here, we develop substrate-assisted strategies to fabricate ordered PAuM which outperform PAuM with entirely random nanopores. We tailor the substrate surface energy using a photo-resist to control the nanopore morphology. Using Raman spectroscopy and electron energy-loss spectroscopy, we studied the wavelength dependence of nanoslot plasmonic enhancement on their shapes at the single-pore level, revealing maximum plasmonic efficiency in high aspect ratio pores. By tuning the surface energy, we obtained optimized PAuMs which outperform FIB-fabricated membranes in terms of signal-to-bulk ratio enhancement. [1] R. Wyss et al. *Nat. Comm.* 15, 7546 (2024)

WED 41

Integrated Chemical and Field Effect Doping for Controllable Charge Transfer in Graphene

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Graphene has outstanding properties and can play an important role in a wide range of applications. Precise control over its electronic structure is essential in order to fully exploit its potential for targeted applications. Charge transfer doping is a key technique for modulating the charge carrier density in materials. This study unveils the doping efficiency of the strong molecular dopant hexacyano-trimethyl-

cyclopropane (CN6-CP) on graphene measured by in situ Raman spectroscopy. The deposition of CN6-CP shifts the G peak by 13 cm^{-1} , indicating a charge carrier density of $0.8 \times 10^{13} \text{ cm}^{-2}$ in the graphene lattice. To achieve further control we integrate molecular doping with a graphene field effect transistor (GFET). This dual approach leverages the interplay between chemical and field-effect doping, enabling precise tuning of the charge carrier density. These findings provide a deeper understanding of the charge transfer process, paving the way for integrated molecular-graphene based electronic devices.

WED 42

Control over magnon spin transport in van der Waals antiferromagnetic CrPS₄

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Magnon based spintronic devices require the modulation of magnon spin transport for their operations. We investigate the injection, modulation of transport and detection of magnon spins in the van der Waals antiferromagnet chromium thiophosphate (CrPS₄). We electrically, via the spin Hall effect (SHE), and thermally, via the spin Seebeck effect (SSE), inject magnon spins by platinum contacts and examine the non-local resistance as a function of in-plane magnetic field up to 12 Tesla. We observe a large magnon spin transport signal and we extract a magnon relaxation length of 800 nm and a typical magnon conductivity of $1 \cdot 10^4 \text{ S/m}$, which is only one order of magnitude smaller than in yttrium iron garnet (YIG) films, the “workhorse” of magnonics. Furthermore, we provide a proof-of-principle of two unconventional magnon transistor devices where we modulate the diffusive magnon transport by a gate contact that increases or decreases the magnon chemical potential. These results open the way towards fully two-dimensional magnon based devices.

WED 43

Progress in Confined Carbyne: cryogenic behavior and yield determination

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Carbyne is an infinitely long chain of carbon atoms, with theoretically calculated outstanding mechanical, optical and electronic properties. It is highly unstable and has only ever been successfully synthesized inside carbon nanotubes, known as confined carbyne(CC). Based on our recent progress in the synthesis of CC[1-2] and new methodology in yield determination[3] in combination with the huge resonance

Raman cross section[4] there is a great application potential for thermometry[5-6]. In this contribution we will show recent progress in unravelling the details of the temperature dependent carbyne response in the 10-300K region and recent insights on resonance independent yield determination of carbyne using Raman spectroscopy.

[1]L. Shi et al. Nano Lett.(2021), Vol.21, No.2, p.1096-1101 [2]W. Cui et al. Adv. Funct. Mater.(2022), Vol.32, No.41, p.2206491 [3]C. Schuster et al. submitted to Carbon(2024) [4]C. D. Tschannen et al. NanoLett.(2020), Vol.20, No.9, p.6750-6755 [5]L. Shi et al. Nat. Mat.(2016), Vol.15, No.6, p.634-639 [6]C.D. Tschannen et al. ACS Nano(2021), Vol.15, No.7, p.12249-12255

WED 44

Feedstock-dependent growth of small diameter B-SWCNTs and their optical properties

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The electronic properties of SWCNTs are intrinsically dependent on their structure, making a synthesis method which provides a narrow diameter distribution very attractive. Additionally, these properties can be tuned through the incorporation of heteroatoms. In this context, we have shown that using Tri-isopropyl Borate as C and B feedstock in a HV-CVD system, the synthesis results are consistently small diameter SWCNTs with a narrow distribution, almost regardless the type of catalyst, over a temperature range of 300 °C. Thus the properties of the final product are mainly determined by the feedstock.

To better understand the influence of boron on the material, we have adapted our setup to synthesize suspended SWCNTs to characterize individual tubes. Both the bulk and the individualized material have been studied to understand the diameter distribution, quality and optical properties of the synthesized SWCNTs. These measurements provide deeper insights into the impact of low boron doping on the electronic structure, enabling the chemical modulation of the properties of SWCNTs, which could potentially eliminate the need for the synthesis of single-chirality samples.

WED 45

Growth and Characterization of PtTe₂ and PdTe₂ Thin Films: Insights into Dirac Semimetals

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Dirac topological semimetals (DSMs) exhibit nontrivial band structures. In a DSM, pairs of Dirac cones are formed at the crossing points of bands with linear dispersion. These cones are located at opposite corners of the Brillouin zone. Depending on the presence or absence of Lorentz invariance, DSMs are classified as type I or type II, respectively. In type II DSMs, tilted Dirac cones appear at the Dirac points. Platinum and palladium ditellurides, members of the transition metal dichalcogenide family, are proposed to host tilted Dirac cones in their electronic structure. We present recent results on the growth of PtTe₂ and PdTe₂ thin layers achieved through the tellurization of metallic films. Raman and optical measurements were performed at various sample temperatures and thicknesses. The goal is to determine key optical parameters, such as refractive indices and optical conductivity in the mid and far-IR ranges, and to correlate these quantities with the electrical conductivity observed in temperature- and thickness-dependent measurements. Support from the APVV project 23-0564 and VEGA project 2/0046/23 is acknowledged.

WED 46

Material selective Nonlinear Optics on Transition-metal Dichalcogenide - ZnO Nanowire Hybrid Structures

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The nonlinear optical (NLO) properties of any material are described by the complex tensor $\chi^{(n)}$, where, for each element of the tensor, the imaginary part mainly appears close to optical resonances. A direct measurement of the complex NLO susceptibility is challenging because any NLO measurement is proportional to $|\chi^{(n)}|^2$. A second harmonic generation (SHG) interference measurement from two different materials with $\chi_{1,2}^{(2)}$, is also proportional to $|\chi_1^{(2)}| |\chi_2^{(2)}| \cos \theta$, where θ is the phase mismatch. For non overlapping resonances, if the SH photon energy is off-resonant for one material and resonant for the other, the interference term directly probes the complex NLO susceptibility of the resonant material. In this work, we study a transition-metal dichalcogenide (TMD) ZnO-nanowire (NW) hybrid structure, and we characterize the complex NLO susceptibility of the TMD close to the A-exciton resonance. The ZnO NW needs to be placed along the armchair direction of the TMD, (WSe₂). Preliminary measurements and the results of SH polarization and wavelength dependent measurements will be presented in this talk.

WED 47

Transparent and reproducible contacts to MoS₂ nanotube quantum dots

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MoS₂, a prominent member of the transitional metal dichalcogenide family, has exceptional optical and electronic properties. However, the large effective electron mass requires narrow confinement potentials for single quantum level transport.

To overcome these constraints, MoS₂ nanotubes are used, since they naturally confine electrons in two dimensions. Using the "classical" Scotch tape method, we have achieved single level transport in a QD matching the active device area.¹ So far the nanotubes exhibited significantly larger contact resistance variations than their flat counterparts, a major fabrication challenge for more complex devices. This was likely caused by the small, curved surface area, leading to the formation of nanogaps between the contact material on top of the tubes and on the chip surface.²

Here, we present an optimized contact deposition approach that significantly improves contact yield, with reproducible results. This enables us to fabricate nanotube QDs on top of 2D material heterostacks.

¹R. T. K. Schock et al., Adv. Mat. 35, 13 (2023); ²R. T. K. Schock et al., PSSb, 2400366 (2024)

WED 48

Towards Floquet-type phenomena in a suspended magnonic cavity

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Two dimensional materials host a zoo of quasiparticles that can interact with each other. Two examples are phonons and magnons – excitation of lattice and magnetization texture of the material, which can couple to so called magnetoelastic waves. We demonstrate that a suspended flake of a van der Waals antiferromagnet CrSBr can serve as a magnonic cavity, a controllable platform to study interactions between phonons and magnons. In CrSBr, magnons resonances, around 20-30 GHz, can be tuned by external magnetic field in and out of resonance with out of plane phonons, with frequency dependence on flake's thickness. Using an ultrafast laser pulse, we excite and probe both coherent phonons and magnons. This configuration could potentially provide a platform for exploring Floquet-type phenomena, such as the AC Stark effect, magnon-phonon Rabi oscillations and other "cavity-electromagnonics" experiments with large coupling strength. Magnonic cavities can shed light on debated magnon generation mechanisms, interaction phenomena at high magnon density and potential for controlling and switching the magnetic state of a nearby 2D ferromagnet.

WED 49**MoS₂ and WS₂ synthesized in Graphene Oxide at ambient conditions**

Viera Skakalova^{1,2,3}, Peter Kotrusz^{2,3}, Thi Thuy An Bu¹, Marian Precner³, Artem Parshin^{2,3}, Lenka Pribusová Slušná³, Martin Hulman^{2,3}, Kimmo Mustonen¹

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In a previous work [1] we introduced a simple chemical synthesis of 2D metal iodides (2D-MI) embedded between graphene sheets where the desired 2D-MI is formed in graphene oxide at ambient conditions. Recently we succeeded to extend the method to synthesize 2D transition metal dichalcogenide, MoS₂ and WS₂, encapsulated in graphene. The chemical reaction also runs under ambient conditions. In this work, flakes of single-layer MoS₂ and WS₂ embedded between graphene sheets were widely characterised by Raman and electron energy loss spectroscopy, confirming presence of WS₂ or MoS₂ with reduced graphene oxide, whereas scanning transmission electron microscopy images show a dense appearance of single layer crystals of WS₂ or MoS₂ apparently separated by graphene. The results of electrical conductivity measured in the temperature range from 4.2 up to 340 K indicate that the electronic transport is mediated through graphene flakes percolated network significantly doped by 2D crystals of MoS₂ and WS₂. We also measured negative magneto-resistance at low temperatures typical for weak localization mechanism in disordered systems.

[1] Mustonen, K. et al., Advanced Materials 2106922 (2022)

WED 50**Strong Electrostatic Control of Excitonic Features in MoS₂ by a Free-Standing Ultrahigh-k Ferroelectric Perovskite**

Thomas Pucher¹, Sergio Puebla¹, Victor Zamora², Estrella Sanchez Viso¹, Victor Rouco², Carlos Leon², Mar Garcia-Hernandez¹, Jacobo Santamaria², Carmen Munuera¹, Andres Castellanos-Gomez¹

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²GFMC, Department Fisica de Materiales, Facultad de Fisica, Universidad Complutense

Research interest in freestanding complex oxides has grown rapidly recently. These oxides are offering advanced functionalities unthinkable for standard 2D dielectrics, such as hBN. Combining them with 2D semiconductors gives rise to rich new physics and improved electronic device systems. Specifically, the high-k ferroelectric perovskite BaTiO₃ (BTO) has drawn attention as a novel freestanding material for future transistor and memory applications.[1,2]

After growth of BTO and its delamination we can transfer the freestanding material of desired thickness to any substrate. By combining it with MoS₂, we are able

to largely control excitonic behavior of the monolayer MoS₂ by electrostatic gating through BTO. Photoluminescence measurements at room temperature reveal highly tunable emission between the A exciton and its trion, as well as tunable trion binding energy over a small range of gate voltage with considerably lower power consumption compared to the same structure with hBN dielectric.[3]

[1] S Puebla et al. Nano Letters 22.18 (2022), [2] G Sánchez-Santolino et al. Nature 626.7999 (2024), [3] T Pucher et al. Adv. Funct. Mater. 2409447 (2024)

WED 51

Controlling spin transport in NPG materials with hydrogen defects.

Alan Ernesto Anaya Morales¹, Mads Brandbyge¹

¹Physics, Denmark Technical University, Kongens Lyngby

Graphene based materials have a great potential for developing spintronic devices due their small spin-orbit coupling, interaction responsible of spin relaxation and decoherence. Among these materials, bottom-up Nanoporous Graphene (NPG) and Nitrogen-Doped hybrid Nanoporous Graphene (hNPG) offer the potential of controlling the spatial electron propagation through their unique an-isotropic electronic structure. On the other hand, hydrogen defects are known to give rise to local magnetic moments in graphene and graphene nanoribbons. Here, we explore the use of hydrogen defects as a mean of controlling the spin transport in these NPG materials. For this, we employ a multi-scale approach to first-principles electron transport. We employ the spin polarization map of bond currents to observe the role of single hydrogen adatoms in electron transport. We hypothesize that the electron confinement in NPG together with localized magnetic defects, can give rise to spin-filtering in the bond-currents.

WED 52

Reconfigurable physical unclonable functions from carbon nanotube transistors for secure vehicle communications

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Hardware security is critical in the era of information and IoT, as the hardware is now transmitting and processing exponential amounts of data. Physical unclonable functions (PUF) are an emerging technology to secure hardware communications. Here we report scalable PUF design and implementation using wafer-scale carbon nanotube charge-trapping transistors. Arising from the unique electronic properties of carbon nanotubes and the intrinsic dynamics of charge trapping, the transistors exhibit trivial yet robust transferring dynamics in their non-volatile memory states,

thereby enabling reconfigurable PUFs. Notably, a PUF consisting of 9 transistor arrays allows secure and stable 32^9 mathematically and physically unclonable primitives. Our analyses prove an excellent resilience of the PUFs against attacks. For example, a 108-bit PUF may take up to 10^{16} years to attack in brute force method. Given this unclonable capability, as well as the scalability, the PUFs hold great potential in enabling hardware security in, for instance, vehicle communications. As an example, we demonstrate secure key exchange in autonomous vehicle communications on OMNET++ using the PUFs.

WED 53

Three-dimensional imaging of bulk twisted interfaces

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Atomic reconstruction of twisted two-dimensional interfaces offers a unique way of controlling optical, electronic and mechanical properties at the atomic level. Despite substantial recent progress in understanding both the structure and properties of twisted bilayers, their thicker counterparts remain largely unexplored. Here we employ multi-slice electron ptychography to perform the first high-resolution depth sectioning of a twisted multilayer transition metal dichalcogenide reconstructed interface. We achieve tracking of over 40,000 atomic locations individually across 20 layers. Position tracking with 6 pm uncertainty allows us to describe how the lattice reconstruction effects evolve as a function of distance from the twisted interface. Coupled with our bespoke theoretical modelling, our work creates a foundation for future experimental and computational discoveries in multi-layer heterostructures across several disciplines from nanoscale tribology to quantum science.

WED 54

Ultrafast switching of trions in 2D materials by terahertz photons

Tommaso Venanzi¹, Marzia Cuccu², Edith Wietek², Raul Perea-Causin³, Xiaoxiao Sun⁴, Samuel Brem⁵, Daniel Erkensten⁵, Takashi Taniguchi⁶, Kenji Watanabe⁶, Ermin Malic⁵, Manfred Helm^{2,4}, Stephan Winnerl⁴, Alexey Chernikov²

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Here we report the observation of transient trion-to-exciton conversion in hBN-encapsulated MoSe₂ monolayer induced by intense THz pulses on picosecond time-scales, generated at the infrared Free-Electron Laser facility (FELBE). The exciton dynamics is monitored at liquid helium temperature by recording time-resolved photoluminescence spectra with a streak camera. Pulses in the visible spectral range

excite a population of both excitons and trions. The THz pulses induce a transient quenching of the trion emission and a simultaneous brightening of the exciton emission, demonstrating an ultrafast trion-to-exciton population transfer. We find that the trion-to-exciton conversion is maximized when the THz photon energy is equal or higher than the trion binding energy. Finally, the THz-induced conversion of excitonic complexes is shown to equally apply to biexcitons in WSe₂ monolayers and interlayer excitons in MoSe₂/WSe₂ heterostructures. Altogether, the results open promising pathways towards ultrafast external control of many-particle states in low-dimensional materials.

[1] Venanzi, T., Cuccu, M. . . , and Chernikov, A. (2024). Nature Photonics.

WED 55

Advancing Techniques to Image the Moiré Electrostatic Potential Landscape of Magic-Angle Twisted Bilayer Graphene using the Atomic SET

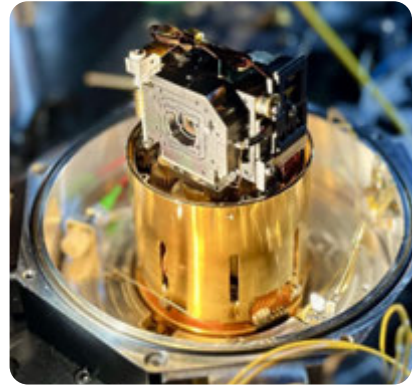
Yuval Yechiel Zamir¹, Shuichi Iwakiri¹, Dahlia R. Klein¹, Uri Zondiner¹, John Birkbeck¹, Jiewen Xiao¹, Alon Inbar¹, Shahal Ilani¹

¹Condensed Matter, Weizmann Institute of Science, Rehovot

Magic-angle twisted bilayer graphene (MATBG) has emerged as a canonical system in condensed matter physics, exhibiting a range of correlated phenomena. A key feature governing these phases is the electrostatic potential landscape of the moiré cell, which alters the electronic wavefunctions. Existing measurement techniques lack the spatial resolution to probe this potential at scales finer than the moiré periodicity (14nm), while allowing density control. In my poster, I present a novel technique to overcome these challenges: the Atomic Single Electron Transistor (SET). The Atomic SET utilizes a van der Waals (vdW) heterostructure of an electrode (graphene) and tunnel barrier (WSe₂) placed on a cantilever and a vdW sample (MATBG) placed on a flat substrate. As we scan the sample with the cantilever, we monitor the single electron tunneling through an atomic defect in the barrier. The defect's energy levels are sensitive to its local electrostatic environment, providing a mean to measure the moiré potential. We currently turn to apply this technique to reveal the electrostatic potential of MATBG. Our work aims to contribute insights into the underlying physics of this system.

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Mode volume

1-100 λ^3

Lateral scanning range

10 x 10 μm at LT

Customisable and

exchangeable mirrors

Thursday, March 13th

- 08:30 – 09:30 **TUTORIAL: P. Kim, Cambridge**
Searching for Anyon in Quantum Materials
- 09:30 – 10:00 **H. Vignaud, Barcelona**
Evidence for Chiral Supercurrent in Quantum Hall Josephson Junctions
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **R. Queiroz, New York**
Quantum Geometry: How to Picture Bound Electrons in Periodic Lattices
- 11:00 – 11:30 **F. Tabataba-Vakili, Munich**
Doping-Control of Excitons and Magnetism in Few-Layer CrSBr
- 11:30 – 12:00 **A. Loiseau, Chatillon**
Spectroscopic Properties of Black Phosphorus and Layers
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 17:30 **C. Kastl, Munich**
He-Ion Beam Modified van der Waals Materials: From Functional Defects to Nanostructured Quantum Matter
- 17:30 – 18:00 **I. Niehues, Münster**
Tip-Assisted and Tip-Enhanced Photoluminescence of Single Color Centers in hBN
- 18:00 – 18:30 **A. Jorio, Belo Horizonte**
Summary - 40 years IWEPNM
- 19:00 – 20:30 **Farewell Dinner (Bauernbuffet)**

08:30

Searching for Anyon in Quantum Materials

Philip Kim¹

¹Physics, Harvard University, Cambridge

The search for anyons, quasiparticles with fractional charge and exotic exchange statistics, has inspired decades of condensed matter research. Moreover, it has been predicted that exchange braiding of these particles, especially non-abelian anyons, can produce topologically protected logic operations that can serve as building blocks for fault-tolerant quantum computing. In this talk, I will discuss the progress of research on two quantum materials platforms to realize these exotic particles. In the first example, we will discuss anyons arising in fractional quantum Hall (FQH) effects, using quantum Hall interferometers for direct observation of the anyon braiding phase around a confined cavity. In the second example, we will discuss our recent experimental efforts to realize non-abelian anyons in proximitized topological insulator surfaces by controlled manipulation of magnetic vortices containing non-abelian anyons.

Thursday, March 13th

09:30

Evidence for chiral supercurrent in quantum Hall Josephson junctions

Hadrien Vignaud¹

¹ICFO - The Institute of Photonic Sciences, Castelldefels, SPAIN

Hybridizing superconductivity with the quantum Hall (QH) effect holds significant potential for designing novel circuits capable of inducing and manipulating non-Abelian states. In this talk, we will present our results on quantum Hall Josephson junctions based on graphene nanoribbons. We will show that with suitably designed junctions, a robust supercurrent can develop on the quantum Hall plateau of normal state resistance $h/2e$ and withstand up to 8 teslas. The particular feature of those junctions is a chiral supercurrent with an unusual $2\Phi_0$ -flux periodicity [1], indicating that the Andreev bound states propagate in a chiral fashion via the quantum Hall edge channels and form a loop along the sample periphery. The key parameters that limit the supercurrent in the quantum Hall regime and their consequences for more exotic quantum Hall states will also be discussed [2].

[1] Ma, M. & Zyuzin, A. Y., Europhys. Lett., 21 (1993) 941-945

[2] Vignaud H., Perconte D., Yang W., Kousar B., Wagner E., Gay F., Watanabe K., Taniguchi T., Courtois H., Han, Z., Sellier H., and Sacépé B., Nature, 624 (2023) 545-550

10:30

Quantum geometry: how to picture bound electrons in periodic lattices

Raquel Queiroz¹

¹Physics, Columbia University, New York

The concept of quantum geometry has been at the forefront of condensed matter physics, starting from how quantized Berry curvature leads to quantized Hall conductivity, anomalous velocities in Dirac metals, or other topological responses in a growing list of so-called topological materials. Recently, the real part of the quantum geometric tensor - the quantum metric - has also been suggested to play an important role, both in response and in the tendency for materials to assume correlated ground states at low temperatures. In this talk, I will give a local picture of quantum geometry to create an intuition about what it is and when it is essential, relating it to how bonds are formed in infinite lattices.

Thursday, March 13th

11:00

Doping-control of excitons and magnetism in few-layer CrSBr

Farsane Tabataba-Vakili¹

¹Institute of Condensed Matter Physics, TU Braunschweig, Braunschweig, Germany

In two-dimensional (2D) magnets, phenomena distinct from bulk magnetism have been revealed, such as sensitivity to charge doping and electric field in few-layer CrI₃. Within the class of 2D magnets, air-stable CrSBr stands out as an antiferromagnetic semiconductor with a high Néel temperature, excitons coupled to the magnetic order, and exciton-magnon coupling. In this talk, I will present our work on doping-control of excitons and magnetism in few-layer CrSBr [1]. We demonstrate that both exciton and magnetic transitions are sensitive to field-effect charging, exhibiting bound exciton-charge complexes and doping-induced metamagnetic transitions. We further visualize magnetic domain formation induced by magnetic field or charge-doping at the metamagnetic transition all-optically by raster-scan reflectance imaging. Our work identifies few-layer CrSBr as a rich platform for exploring collaborative effects of charge, optical excitations, and magnetism.

[1] F. Tabataba-Vakili et al., Nat. Commun. 15, 4735 (2024).

11:30

Spectroscopic properties of black phosphorus and layers

Etienne Carré^{1,2}, Lorenzo Sponza¹, Alain Lusson², Frederic Fossard¹, Pierre Sénéor³, Bruno Dublak³, Julien Barjon², Etienne Gaufres⁴, Annick Loiseau¹

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BP stands out from other 2D materials by the thickness dependent band gap energy that sweeps a large optical Vis-IR wavelengths window, and offers promising perspectives. However, the fast thickness dependent photooxidation in ambient condition is a serious obstacle for studying intrinsic properties (Nature Mat. 14 826 (2015)). This talk will report our comprehensive studies for investigating intrinsic spectroscopic properties of BP crystal (2D Mater. 8 021001 (2021)) passivated and free standing flakes (Phys. Rev. B 109 035424 (2024)). By combining micro-Raman and photoluminescence (PL), the mechanical exfoliation used for fabricating flakes is shown to induce defects which open new radiative recombination paths replacing those of the bulk. The evolution of the PL energy versus flake thickness in the range 700-4 nm, is shown to follow an inverse square law that we relate to a quantum well model and justify in an intermediate thickness range. Further, in this range, the emission energy is weakly modulated by the dielectric environment in contrast to ultra thin free standing layers as evidenced by their dielectric response studied using EELS in a STEM (Nanolett.19 8303 (2019)).

Thursday, March 13th

17:00

He-ion beam modified van der Waals materials: from functional defects to nanostructured quantum matter

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²Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

The helium ion microscope is a versatile tool for both nanoanalytics and nanoscale fabrication of atomically thin van der Waals materials. Focused He-ion beam exposure can create functional defects, such as single photon emitters, with a spatial resolution well below 10 nm (Nano Lett. 2020, 20, 4437). For monolayer MoS₂, I will discuss the optical properties of sulfur vacancy defects. There, the defect excitons exhibit a mixed localized-delocalized character resulting in hybridized electron-hole transitions, which manifest as a varying exciton g-factor (npj 2D Mater. Appl. 2023, 7, 30) and a broadband sub-gap absorption (J. Phys Chem. Lett. 2022, 13, 10291 & Nano Lett. 2023, 23, 11655). For multilayer hBN, I will discuss defect creation using focused He-ions and, in particular, the quantification of optically active, negatively charged boron vacancies (A. Carbone et al., under review, 2025). Lastly, I will provide an outlook on the application of He-ion beam milling for creating nanoscale patterned superlattices in van der Waals materials.

17:30

Tip-assisted and tip-enhanced photoluminescence of single color centers in hBN

Iris Niehues¹, D. Wigger², K. Kaltenecker³, A. Klein-Hitpass¹, P. Roelli⁴, A. K. Dabrowska⁵, K. Ludwiczak⁵, P. Tatarczak⁵, J. O. Becker¹, R. Schmidt¹, M. Schnell^{4,6}, J. Binder⁵, A. Wysmolek⁵, R. Hillenbrand^{4,6,7}

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Color centers in hexagonal boron nitride (hBN) have emerged as interesting quantum light sources due to their stable and bright single-photon emission at room temperature. We utilize a scattering-type near-field optical microscope (s-SNOM) to study the photoluminescence (PL) emission characteristics of such quantum emitters in metalorganic vapor phase epitaxy grown hBN[1]. In our specific experiments, we employ the near-field optical microscope, to detect PL signals influenced by the presence of the metallic tip. On the one hand, we demonstrate direct near-field optical excitation and emission through interaction with the nanofocus of the tip resulting in a sub-diffraction limited tip-enhanced PL hotspot. On the other hand, we observe a more pronounced ‘arc’ around the dot. We explain this feature by constructive interference between direct beams to/from the color center and those scattered from the tip (indirect beam) leading to a significant increase of the recorded PL intensity (TAPL). We apply the TAPL method to map the in-plane dipole orientations of the hBN color centers on the nanoscale.

[1] I. Niehues et al., Nanophotonics, under review (2025)

Author Index

18:00

IWEPNM Summary

Ado Jorio¹

¹Physics, UFMG, Belo Horizonte

Summary of the last 40 years IWEPNM.

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