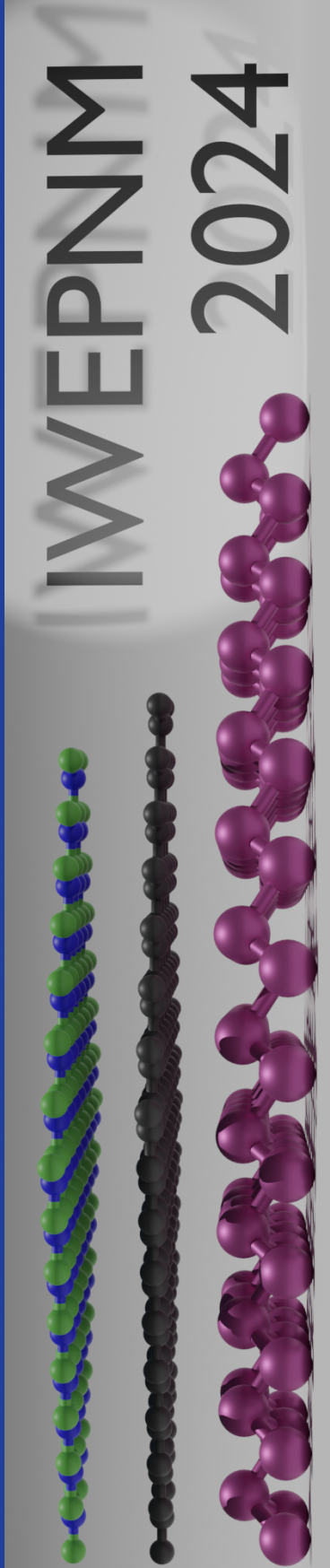
XXXVIth International Winterschool on Electronic Properties of Novel Materials

Molecular Nanostructures

Program



Hotel Sonnalp
Kirchberg/Tirol
Austria

09 - 15 March, 2024

SUPPORTERS

Verein zur Durchführung der International Winterschool on Electronic Properties of Novel Materials
Verein zur Förderung der Internationalen Winterschulen in Kirchberg Austria

PATRONAGE

Helmut Berger
Mayor of Kirchberg

LAYOUT

María Machón, Felix Herziger

Logo designed by Stefan Wolff.
This year's Logo of the IWEPNM shows a schematic image of a heterostructure out of three materials: hBN (top), graphene (middle), and antimonene (bottom).

SPONSORS

neaspec GmbH
Eglfinger Weg 2
85540 Haar (Munich), Germany

HÜBNER GmbH & Co. KG
Heinrich-Hertz-Straße 2
34123 Kassel, Germany

Nanosurf
Gräubernstrasse 14
4410 Liestal, Switzerland

Wiley VCH
Boschstrasse 12
69469 Weinheim, Germany

Financial assistance from the sponsors and supporters is greatly acknowledged.

Dear Friend:

Welcome to the 36th International Winterschool on:

Electronic Properties of Novel Materials!

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

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

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

Program	Janina Maultzsch
Accommodation	Tobias Dierke, Eileen Schneider & Britta Maib
Finances	Antonio Setaro
Accommodation Finances	Kati G.-Hubmann
Credit Card Maintenance	Eileen Schneider
Website & Database	Roland Gillen
Abstract Book & Giveaways	Sabrina Juergensen
Technique	Patryk Kusch, Oisín Garrity & Charlotte Berrezueta
Announcements	Stefan Wolff
Daily Information Poster	Gabriela Luna Amador
Conference Publications	Antonio Setaro
Visa	Angelin See

We want to thank our colleagues who helped in organizing this winterschool: Chantal Müller und Mira Kreßler.

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

E. Andrei (US)
A. Bachtold (ES)
C. Backes (DE)
H. M. Cheng (CN)
J. Fink (DE)
M. Glazov (RU)
R. Gorbachev (UK)
I. Grigorieva (UK)
S. Haigh (UK)
T. Heine (DE)
T. F. Heinz (US)
A. Hirsch (DE)
S. Ilani (IL)
A. Jorio (BR)
H. Kataura (JP)
R. Krupke (DE)
H. Kuzmany (AT)
Y. H. Lee (KR)
Y. Li (CN)
F. Libisch (AT)
A. Loiseau (FR)
S. Maruyama (JP)
J. Maultzsch (DE)
F. Mauri (IT)
K. S. Novoselov (UK)
E. Obraztsova (RU)
A. Penicaud (FR)
T. Pichler (AT)
M. Prato (IT)
S. Reich (DE)
J. Robertson (UK)
S. Roth (DE)
P. Rudolf (NL)
C. Schönenberger (CH)
P. Sheng (CN)
F. Simon (HU)
C. Stampfer (DE)
M. Strano (US)
K. Suenaga (JP)
A. Swan (US)
C. Voisin (FR)
J. Zaumseil (DE)
A. Zettl (US)

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 2024 starts on Saturday, 9 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Friday, 15 March, breakfast. There will be a reception party on Saturday, 9 March, after dinner, and a farewell party including dinner on Thursday, 14 March.

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

Addresses
The address of the Winterschool is:
IWEPNM 2024 Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria
e-mail: info@hotelsonnalp.info, web: `www.hotelsonnalp.info`

All questions concerning the IWEPNM 2024 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 2024 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 IWEPNM 2024 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 "IWEPNM: Electronic Properties of Novel Materials. If you intend to submit a "Rapid Research Letter", a "Feature Article" or a manuscript to Advanced Electronic Materials, please consult with the editors at
iwepnm-publication@physik.fu-berlin.de.

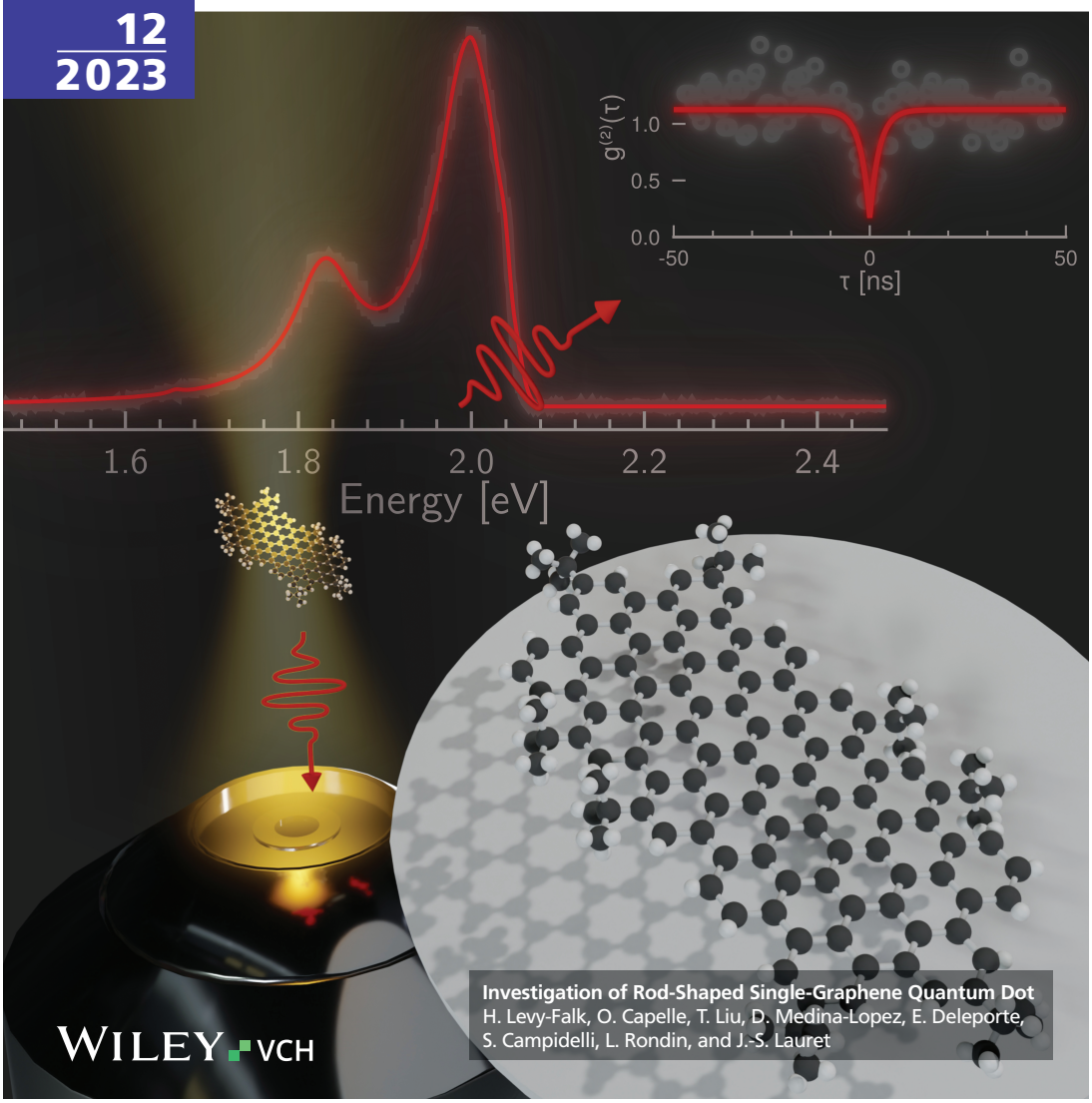
ISSN 1521-3951
Phys. Status Solidi B
260 · No. 12 December
(2023)

physica status solidi b

www.pss-b.com

basic solid state physics

12
2023



Investigation of Rod-Shaped Single-Graphene Quantum Dot
H. Levy-Falk, O. Capelle, T. Liu, D. Medina-Lopez, E. Deleporte, S. Campidelli, L. Rondin, and J.-S. Lauret

WILEY VCH

IWEPNM 2024
CHAIRPERSONS FOR THE ORAL SESSIONS

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

Sunday, 10.03.	morning	Stephanie Reich
	morning, after coffee break	Hans Kurzmany
	evening	Andreas Hüttel
Monday, 11.03.	morning	Lutz Waldecker
	morning, after coffee break	Otakar Frank
	evening	Christoph Stampfer
Tuesday, 12.03.	morning	Janina Maultzsch
	morning, after coffee break	Tobias Hertel
	evening	Viera Skakalova
Wednesday, 13.03.	morning	Annick Loiseau
	morning, after coffee break	Claudia Backes
	evening	Ursula Wurstbauer
Thursday, 14.03.	morning	Ralph Krupke
	morning, after coffee break	Carlo Casari
	evening	Florian Libisch

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

08:30 – 09:30	TUTORIAL: J. Zaumseil, Heidelberg *Creating and Quantifying Different Luminescent Defects in Single-Walled Carbon Nanotubes*
09:30 – 10:00	C. Voisin, Paris *Organic Color Centers Grafted on Carbon Nanotubes Coupled to a High finesse Micro-Cavity*
10:00 – 10:30	Coffee Break
10:30 – 11:00	H. Liu, Beijing *Milligram-Scale Production and Property Detection of Multiple Single-Chirality Carbon Nanotubes*
11:00 – 11:30	S. Maruyama, Tokyo *One-Dimensional vdW 'Double' Heterostructures Based on Single-Walled Carbon Nanotubes*
11:30 – 12:00	Y. Miyata, Tokyo *Growth and Characterization of 1D Transition Metal Chalcogenides*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	K. Franke, Berlin *Diode Effect in Josephson Junctions with a Single Magnetic Atom*
19:00 – 19:30	L. Venkataraman, New York *Ultrahigh Conductance in One-Dimensional Topological Insulators*
19:30 – 20:00	A. Stern, Rehovot *Electrons and Composite Fermions at the Half Filled Chern Band*
20:00	Poster I

08:30
Creating and Quantifying Different Luminescent Defects in Single-Walled Carbon Nanotubes
Jana Zaumseil[1]
[1]Angewandte Physikalische Chemie, Universität Heidelberg, Heidelberg

The functionalization of semiconducting single-walled carbon nanotubes (SWCNTs) with luminescent oxygen or sp^3 defects leads to new red-shifted emission features and increased photoluminescence (PL) quantum yields in the near-infrared. The selection of reactants and parameters allows for a precise control of the type of defect, thus tailoring their emission wavelength. Here we will discuss different functionalization methods and introduce a new highly scalable reaction scheme for creating very bright oxygen defects for bioimaging in the second biological window.
For the application of luminescent defects in SWCNTs, their quantification is required. We have recently introduced an absolute quantification method for sp^3 defects in (6,5) SWCNTs by correlating the change of the integrated D/G ratio in Raman spectra with the calculated sp^3 defect densities obtained from PL quantum yield measurements. We expand this approach to other semiconducting SWCNT species and show that it remains valid. Furthermore, the dependence of the Raman D-mode intensity on excitation wavelength is examined to enable an excitation energy independent quantification of luminescent defects in SWCNTs.

09:30

Organic color centers grafted on carbon nanotubes coupled to a high finesse micro-cavity

Federico Rapisarda[1], Antoine Borel[1], Yannick Chassagneux[1], Christophe Voisin[1]
[1]LPENS, Laboratoire de Physique, Ecole Normale Supérieure, PSL, UPC, Paris

The low-temperature spectroscopy of individual organic color centers covalently grafted on carbon nanotubes reveals a rich photo-physics. The coupling to a high finesse micro-cavity is a powerful tool to study the population dynamics, to manipulate the strength of light-matter interaction including absorption and emission enhancement or inhibition. We investigate more specifically the case of pairs of color centers that are dynamically coupled, exploiting correlations in the spectral diffusion, photon bunching at various time-scales and super-resolved microscopy. We propose a modeling of the system dynamics based on simple photo-induced electrostatic fluctuations and we put forward the potential use of such system as a sensitive near field electro-meter with interesting specificity as compared to related proposals with NV centers in diamonds.

10:30
Milligram-scale production and property detection of multiple single-chirality carbon nanotubes

Huaping Liu[1], Dehua Yang[1], Wei Su[1], Xiao Li[1], Linhai Li[1], Xiaojun Wei[1], Weiya Zhou[1]
[1]Institute of Physics, Chinese Academy of Sciences, Beijing

The diverse properties of an as-synthesized single-wall carbon nanotubes (SWCNT) mixture will definitely hinder their property detection and application in high-performance electronic devices. In recent decades, impressive progress in the structural separation of SWCNTs has been made. In particular, the gel chromatography technique has developed rapidly in the mass separation of single-chirality SWCNTs due to the simplicity, high efficiency, and low cost of this technique. The chirality separation of SWCNTs by gel chromatography is based on their selective adsorption onto and desorption from the gel medium. In recent years, we have greatly improved the separation efficiency of single-chirality SWCNTs and their enantiomers by temperature control, mixed surfactants, high-concentration solution and even their combination. With these techniques, a variety of single-chirality SWCNTs and even their enantiomers have been produced on milligram scale. Based on this, we further systematically explore the relationship between the electrical transport properties of SWCNTs and their chiral structures.

11:00

One-dimensional vdW 'double' heterostructures based on single-walled carbon nanotubes

Shigeo Maruyama[1], Yongjia Zheng[1,2], Wanyu Dai[1], Keigo Otsuka[1], Rong Xiang[1,2]
[1]Department of Mechanical Engineering, The University of Tokyo, Tokyo
[2]School of Mechanical Engineering, Zhejiang University, Hangzhou

We have demonstrated the atomically precise one-dimensional (1D) van der Waals (vdW) heterostructure based on single-walled carbon nanotubes (SWCNTs) in 2020. One of the obvious extensions of this work is the use of boron nitride nanotube (BNNT)-SWCNT, which has superior semiconductor properties such as field effect transistors. We have developed various characterization techniques for BNNT-SWCNT for the growth optimization and quality control of BNNT in various kinds of SWCNT. Yet another extension is the various kinds of transition metal dichalcogenides (TMD) nanotubes. We have optimized CVD conditions for various metal dichalcogenides such as tungsten disulfide (WS2), niobium disulfide (NbS2), and molybdenum diselenide (MoSe2) so far, in addition to the original MoS2. Here, we further broaden the concept of 1D vdW heterostructure by combining 2 transition metal species. The outermost tube can be axially combined with the monolayer MoS2 to form a MoS2 - WS2 axial junction. Such nanotube structure is proven to be both radially and axially hetero, and the whole structure is only confined to a width of 5 nm.

11:30
Growth and Characterization of 1D Transition Metal Chalcogenides
Yasumitsu Miyata[1]
[1]Department of Physics, Tokyo Metropolitan University, Tokyo

Transition metal chalcogenides are attractive materials with various nanostructures and physical properties. In particular, recent advances in growth techniques have facilitated the fabrication of various one-dimensional (1D) configurations of both transition metal monochalcogenides (TMMs) and transition metal dichalcogenides (TMDs). In this talk, we will present our recent progress in the fabrication and characterizations of such nanostructures, including nanowires, nanoribbons, nanotubes, nanoscrolls, and 1D interfaces. In addition, we highlight the utility of TMD-based 1D interfaces in device applications, such as color-tunable light-emitting diodes (LEDs) and tunnel field-effect transistors (TFETs). These developments pave the way for exploring low-dimensional physics and potential applications in advanced devices.

18:30
Diode effect in Josephson junctions with a single magnetic atom
Martina Trahms[1], Larissa Melischek[1], Jacob F. Steiner[1], Bharti Mahendru[1], Idan Tamir[1], Nils Bogdanoff[1], Olof Peters[1], Gael Reecht[1], Clemens B. Winkelmann[2], Felix von Oppen[1], Katharina J. Franke[1]
[1]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany
[2]Université Grenoble Alpes, CNRS, Institut Néel, Grenoble, France

Diode behavior in superconducting junctions describes the phenomenon of dissipationless current flow in one direction, while the current in the other direction underlies dissipation. Such non-reciprocal behavior has been found in Josephson junctions where inversion and time-reversal symmetry are broken. So far, most realizations are made of layered structures.
Here, we create atomic-scale Josephson junctions in a scanning tunneling microscope and investigate their transport properties in current-biased mode. This allows characterization of the switching and retrapping currents, which separate the dissipationless from the dissipative branch. Plain Pb-Pb junctions show hysteretic and reciprocal behavior. By insertion of single magnetic adatoms the retrapping current adopts nonreciprocity, mimicking diode behavior.
We show that the nonreciprocity of the retrapping current depends on the particle-hole asymmetry of the Yu-Shiba-Rusinov (YSR) states inside the superconducting energy gap. Aided by theoretical modelling, we ascribe the non-reciprocity to dissipative quasiparticle currents flowing via Yu-Shiba-Rusinov (YSR) states inside the superconducting energy gap.

19:00
Ultrahigh Conductance in One-Dimensional Topological Insulators
Latha Venkataraman[1]
[1]Applied Physics and Chemistry, Columbia University, New York

Molecular one-dimensional topological insulators (1D TIs), which conduct through energetically low-lying topological edge states (or radical states), can be extremely highly conducting and exhibit a reversed conductance decay, affording them great potential as building blocks for nanoelectronic devices. In this talk, I will present experimental results from recent works where we demonstrate that molecular wires can behave as one-dimensional topological insulators. I will first focus on a family of oligophenylene-bridged bis(triarylamines). These wires can undergo one- and two-electron chemical oxidations. The oxidized wires exhibit high reversed conductance decay with increasing length, consistent with the expectation for the Su-Schrieffer-Heeger-type 1D TIs. I will then show how we can extend the length at which these anomalously high conductance can be observed in topological oligo[n]emeraldine wires where we use short 1D TIs as building blocks. For this series, we find that as the wire length increases, the number of topological states increases, enabling an increased electronic transmission along the wire.

19:30
Electrons and composite fermions at the half filled Chern band
Ady Stern[1]
[1]Weizmann Institute (Israel)

In this talk I will describe electronic properties of two possible states that may occur at the half-filled Chern band - a Fermi liquid of electrons and a Fermi liquid of composite fermions. I will give an introduction to all these terms before focusing on the problem at hand, and will make connections to recent experiments.

SUN 1
Infrared correlation nanoscopy for organic and inorganic material analysis at the nanoscale

A.J. Huber[1], B. Sava[1], C. Reckmeier[1], A. Govyadinov[1]
[1]attocube systems AG, Haar (Munich), Germany

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 resolved 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.

[1] F. Keilmann, and R. Hillenbrand, Phil. Trans. R. Soc. Lond. A 362, 787 (2004).
[2] D. Kurouski, A. Dazzi, R. Zenobi, and A. Centrone, Chem. Soc. Rev., 49, 3315 (2020).
[3] T. L. Cocker, V. Jelic, R. Hillenbrand, and F. A. Hegmann, Nature Phot. 15, 558 (2021).

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

SUN 2
Spectroscopic Characterization of (Electro-)Chemically Doped Graphene Nanoribbon films in the SWIR-region

Sebastian Lindenthal[1], Justin Earley[2], Finn L. Sebastian[1], Nicolas F. Zorn[1], Jeffrey L. Blackburn[2], Andrew J. Ferguson[2], Jana Zaumseil[1]
[1]Heidelberg University, Heidelberg, Germany
[2]National Renewable Energy Laboratories, Golden, United States of America

Graphene Nanoribbons (GNRs) are quasi-one-dimensional nanomaterials exhibiting unique optical and electronic properties, that depend on width and edge type. In addition, structural defects, introduced during GNR synthesis, influence the optical properties of GNRs. Upon molecular doping in dispersion, pristine and defective armchair GNRs form polaronic states, observable as new features in the absorption spectra, that appear above 1000 nm. In dispersion, however, a systematic investigation of these new bands in the short-wavelength infrared (SWIR) region (1.5 - 3.5 µm) proves to be difficult, due to strong solvent and dopant absorption. Here we chemically and electrochemically dope thin films of solution-synthesized 9-armchair GNRs and investigate the emerging spectroscopic features up to the mid-IR region by absorption, photoluminescence and infrared spectroscopy. We further characterize local and macroscopic charge carrier mobilities in these GNR films depending on charge carrier density and defect density.

SUN 3
Two-dimensional magnetic metal-iodides encapsulated in graphene

Viera Skakalova[1]
[1]Institute of Electrical Engineering of SAS, Bratislava, Slovakia

Recently, we developed a simple chemical method that, under ambient conditions, can provide novel two-dimensional (2D) materials in a macroscopic scale [1]. The method called SinGO (Synthesis in Graphene Oxide) opens an avenue to a new class of 2D magnetic and non-magnetic metal-iodides (2D-MI) encapsulated between impermeable graphene layers. At the same time, utilizing chemically clean interfaces in the vdW stack, it would represent a novel platform for devices in which graphene, as an ideal conducting channel of Dirac electrons, can guide encoded technologically-relevant information. Even though the weak spin-orbit coupling in graphene limits its applicability for spintronics, the encapsulated 2D-MI magnets might, by proximity, induce spin-orbit coupling in graphene enabling spin transport with unexplored yet physical mechanisms. Here we will present the wide range characterization of the synthesized 2D magnetic metal-iodides: 2D CrI2, FeI2, CoI2, NiI2 and MnI2, including their atomic structures (STEM), magnetization characteristics, X-ray circular magnetic dichroism and electrical transport properties.

[1] K. Mustonen et al., Advanced Materials 34, 2106922 (2022).

SUN 4
Enhanced infrared photoresponse in bilayer graphene

D. Mylnikov[1], I. Mazurenko[1], A. Parappurath[3], S. Bhowmik[4], D. Bandurin[5], A. Ghosh[3], A. Chernov[1,2]
[1]Center for Photonics and 2D Materials, MIPT, Dolgoprudny
[2]Russian Quantum Center, Skolkovo
[3]Department of Physics, Indian Institute of Science, Bangalore
[4]Department of Instrumentation and Applied Physics, Indian Institute of Science, Bangalore
[5]Department of Materials Science and Engineering, National University of Singapore

Small-angle twisted bilayer graphene (tBLG) has attracted much attention due to appearance of low-energy flat bands of the emerging moiré superlattice [1]. Strong electron-electron interactions within the bands lead to correlation-driven phenomena, realization of correlated phases, and result in new devices. In particular optoelectronic devices such as infrared and THz detectors have been recently demonstrated. Here we have performed the photoresponse measurements at 5 – 10 um in the tBLG, where the mis-orientation angle is close to the magic one. We detect the 8 times enhanced bolometric response compared to the previous works. We demonstrate the gate-tunable photoresponse and find the peculiarities at integer and half-integer band fillings. The obtained results can be further used for tunable mid-infrared optoelectronics.

[1] https://arxiv.org/pdf/2309.08938.pdf

SUN 5
Exciton condensation in $TiSe_2$ detected by screening of single-layer WSe_2

Adrián Dewambrechies[1], Ben Weintrub[1], Kirill I. Bolotin[1]
[1]Physics, FU Berlin, Berlin

Two-dimensional materials and the recent progress in their manipulation have provided a platform to study highly correlated phenomena, a relevant case being the condensation of the excitons dominating their optical response. Recent advances show that the exciton properties, and their tunability in such systems, offer the observation of high temperature condensation, and allows the study of the crossover between different types of condensates including the Excitonic Insulator. However, a definitive proof of the exciton condensation and superfluidity is still missing mainly due to the charge of excitons being zero, and new experimental techniques are being explored in this direction. Here, we present our latest results in the detection of exciton condensation in two-dimentional semimetal $TiSe_2$. We study its effect in

the dielectric environment of a nearby sensor layer of WSe_2, by tracking the emission and absorption of its excitons to understand charge transfer between the two materials and the potential transition to an excitonic insulating state in $TiSe_2$.

SUN 6
Filling carbon nanotubes with phosphorus, sulfur and their compounds: structural features and properties

Alexander Okotrub[1], Anna Vorfolomeeva[1], Olga Gurova[1], Vitalii Sysoev[1], Olga Sedelnikova[1], Lyubov G. Bulusheva[1]
[1]Nikolaev Institute of Inorganic Chemistry, Novosibirsk

In this work, we synthesized and studied SWCNTs from OKSIAL Company modified with sulfur, phosphorus and their compounds. The synthesis was carried out using the ampoule method. We found that moderate heating of filled nanotubes can be used to decrease capsulation nanotubes, tuning the local composition and hence the functional properties of SWCNT-based materials. Hybrid structures changes electronic structure of nanotubes and can be used in Li- ionic batteries as electrodes, for the manufacture of highly sensitive sensors, and in other applications. Extensive study of materials using transmission electron microscopy, X-ray photoelectron spectroscopy and quantum chemical modeling has led to an understanding of the factors influencing the properties being studied. S@SWCNTs have been shown to have exceptional sensitivity to ppb levels of nitrogen dioxide in the gas phase due to increased charge transfer between the nanotubes and adsorbed molecules. The work was carried out with financial support from the Russian Science Foundation (project No. 2

SUN 7
Extremely Efficient Light Absorption by Acoustic Graphene Plasmons

Michael Klein[1], Dongjea Seo[2], Sang-Hyun Oh[2], Itai Epstein[1]
[1]School of Electrical Engineering, Department of Physical Electronics, Tel Aviv University
[2]Department of Electrical and Computer Engineering, University of Minnesota, Twin Cities, USA

Acoustic graphene plasmons are highly confined electromagnetic modes carrying large momentum and low loss in the mid-infrared and terahertz spectra. Acoustic graphene plasmons are difficult to interact with from the far field due to the large momentum mismatch, making it challenging to couple with free space light. Here, we show that by constructing a heterostructure composed of a nanometric graphene resonator and an optical cavity we can drastically enhance the far field MIR light absorption of acoustic graphene plasmons, reaching up to 70% efficiency. This has potential for applications in optoelectronics, sensing, and energy harvesting, where high light absorption and strong light-matter interaction are required.

SUN 8
Nano-Schottky junction in AgPt@GO composite and their role in ppb-level NO2 gas sensor

Dariusz Łukowiec[1], Marcin Procek[1], Adrian Radoń[2], Jerzy Kubacki[3], Tomasz Wasiak[1], Stanisław Wacławek[4]
[1]Silesian University of Technology, Gliwice, Poland
[2] Łukasiewicz Research Network - Institute of Non-Ferrous Metals, Gliwice, Poland
[3]A. Chelkowski Institute of Physics, University of Silesia, Katowice, Poland
[4]Technical University of Liberec, Liberec, Czech Republic

Challenges in the area of gas sensors: low sensitivity, long reaction times and working at elevated temperatures can be solved by designing sensors composed of various active materials. In the present study, the nature of the interface between core-shell AgPt nanoparticles and carbon structures (graphene oxide, graphene oxide doped with nitrogen, reduced graphene oxide) was analysed, followed by their sensing properties towards NO2. The best sensing properties showed the AgPt@GO, which responded to NO2 concentrations below 1 ppm at room temperature (RT). In addition, the tested material was characterised by stability and quick response (in the range of 1-50 ppm at RT). The excellent characteristics of AgPt@GO are attributed to the generated nano-Schottky junction, as demonstrated by dielectric spectroscopic experiments. The existence of a p-n junction was verified for the other material. In the sensor investigations, the impact of variations in humidity (RH 3–50%) and temperature (RT-250 C) on the response of the manufactured sensor systems and their selectivity (H2, CH4, H2S) was examined. Furthermore, the electronic structure of obtained composites was studied in detail.

SUN 9
Interlayer distance of twisted bilayer graphene measured through interferometric 4D-STEM

Clara Kofler[1], Jani Kotakoski[1]
[1]University of Vienna, Faculty of Physics, Vienna

Although (scanning) transmission electron microscopy ((S)TEM) can routinely resolve structures down to individual atoms, it is typically limited to 2D projections. However, measuring the 3D structure is in many cases necessary for fully understanding material properties, even for 2D materials such as graphene [1]. This becomes still more important when 2D layers with different lattice parameters [2] or orientations are combined. In this contribution, twisted bilayer graphene samples are created by folding monolayer graphene using heat treatment in vacuum, and subsequently measured using interferometric 4D-STEM, similar to the implementation in Ref. [3] to gain information on the interlayer distance variations. The experimental results are compared to image simulations carried out with abTEM [4]. The average interlayer distance agreed with expectations, however the structure de-

pendence could not be reproduced using this method.

[1] Meyer et al., Nature 446, 60 (2007)
[2] Argentero et al., Nano Lett. 17, 1409 (2017)
[3] Zachman et al., Small 17, 2100388 (2021)
[4] Madsen et al., Open Res Europe 1, 24 (2021)

SUN 10
The three Fermi pockets of NbSe2 - Investigating a Kohn-Luttinger like mechanism in TMD monolayers.

Julian Siegl[1], Magdalena Marganska[1], Milena Grifoni[1]
[1]Institute of Physics, University of Regensburg, Regensburg

We investigate a possible superconducting pairing generated by competing Coulomb repulsion processes in monolayer NbSe2. The two spin-orbit split Fermi surfaces (FS) of ML NbSe 2 in the K and K' valley can support a superconducting gap, with predominant f-wave symmetry, when the short-range intervalley scattering is stronger than the long-range intravalley one. Upon inclusion of the third FS centered at the Gamma point an additional competing pairing channel favoring s-wave symmetry opens for strong interpocket scattering. The competition between these two channels is governed by the relative strengths of the three processes involved, resulting either in one, two or three symmetry related values of the gaps at the FSs. We estimate the relevant interactions by calculating the dielectric susceptibility and the screened Coulomb potential in the RPA approximation for a DFT-based tight-binding model. The multi-orbital nature of the valence band results in preferential screening of short-range scattering processes, favoring the interpocket scattering. Far from being a spectator, the third Fermi pocket turns out to be a powerful player, even to the point of changing the symmetry.

SUN 11
Ultra-steep slope cryogenic FETs based on bilayer graphene

Christoph Stampfer[1,2], Eike Icking[1,2], David Emmerich[1], Kenji Watanabe[3], Takashi Taniguchi[4], Bernd Beschoten[1], Max Lemme[5,6], Joachim Knoch[7]
[1]JARA-FIT and 2nd Institute of Physics A, RWTH Aachen University, Aachen
[2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany
[3]esearch Center for Functional Materials, National Institute for Mate
[4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan
[5]Chair of Electronic Devices, RWTH Aachen University, Aachen, Germany
[6]AMO GmbH, Aachen, Germany
[7]IHT, RWTH Aachen University, Aachen, Germany

Cryogenic field-effect transistors (FETs) offer great potential for a wide range of applications, the most notable example being classical control electronics for quantum

information processors. In the latter context, on-chip FETs with low power consumption are a crucial requirement. This, in turn, requires operating voltages in the millivolt range, which are only achievable in devices with ultra-steep subthreshold slopes. However, in conventional cryogenic MOSFETs based on bulk material, the experimentally achieved inverse subthreshold slopes saturate around a few mV/dec due to disorder and charged defects at the MOS interface. FETs based on two-dimensional materials offer a promising alternative. Here, we show that FETs based on Bernal stacked bilayer graphene encapsulated in hexagonal boron nitride and graphite gates exhibit inverse subthreshold slopes of down to 250 μV/dec at 0.1 K, approaching the Boltzmann limit. This result indicates an effective suppression of band tailing in van-der-Waals heterostructures without bulk interfaces, leading to superior device performance at cryogenic temperature.

SUN 12
Ultrafast Dynamics in p-Doped Single-Wall Carbon Nanotubes at Cryogenic Temperatures

Heiko Lackinger[1], Klaus H. Eckstein[1], Friedrich Schöppler[1], Tobias Hertel[1]
[1]Julius-Maximilians-Universität Würzburg (JMU) - Würzburg, Germany

The doping of low-dimensional semiconductors and the precise quantification of doping levels pose significant technological challenges critical to advancing new technologies based on semiconductors. Therefore, understanding the dynamics of excitons and charged excitons (trions) is crucial for improving our knowledge of the doping process [1-3]. The coupling between excitons and trions of doped semiconducting single-wall carbon nanotubes (s-SWNTs) can be investigated by studying their temperature dependence, to the best of our knowledge lacking any reported data so far. Here, we report preliminary findings derived from transient absorption measurements that explore the correlation between doping levels and the dynamics of excitons and trions in thin films of polymer-wrapped (6,5) s-SWNTs as a function of the temperature.

[1] K.H. Eckstein, et al., J. Phys. Chem. C 127, 19659-19667 (2023).
[2] K.H. Eckstein, et al., J. Phys. Chem. C 123, 30001-30006 (2019).
[3] K.H. Eckstein, et al., ACS Nano 11, 10401-10408 (2017).

SUN 13
Mechanical tuning of magnetic interactions in nanographenes

Goncalo Catarina[1]
[1]nanotech@surfaces Laboratory, Empa—Swiss Federal Laboratories for Materials Science and Technology, Dubendorf, Switzerland

Phenalenyl is an open-shell spin-1/2 nanographene with triangular shape. Using inelastic electron tunneling spectroscopy, covalently-bonded phenalenyl dimers have been shown to feature inelastic conductance steps compatible with spin excitations

of a spin-1/2 dimer with antiferromagnetic exchange. Here we address the possibility of tuning the magnitude of the exchange interactions by controlling the dihedral angle between the two molecules. By means of first principle calculations, we propose strategies to induce sizeable rotations. Our theory, in agreement with experimental results, paves the way toward controlling magnetic couplings in carbon-based spin lattices.

SUN 14

Towards a microscopic understanding of photoluminescence quenching in monolayer MoSe2/n-layer graphene heterostructures

Aditi Raman Moghe[1], Loïc Moczko[1], Delphine Lagarde[2], Maxime Mauguet[2], Michelangelo Romeo[1], Takashi Taniguchi[3], Kenji Watanabe[3], Arnaud Gloppe[1], Xavier Marie[2], Cedric Robert[2], Stéphane Berciaud[1]
[1]Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, Strasbourg, France
[2]Université de Toulouse, INSA-CNRS-UPS, LPCNO, Toulouse, France
[3]National Institute for Materials Science, Tsukuba, Ibaraki, Japan

The van der Waals heterostructure consisting of transition metal dichalcogenide (TMD) and graphene is an interesting system as it provides an opportunity to understand the microscopic charge and energy transfer processes occurring at their heterointerfaces. The coupling between graphene and TMD gives rise to intriguing effects such as the neutralization of the TMD and the quenching of its PL [1,2]. Whether these effects occur through short-range charge tunneling or longer-range dipole-dipole interactions still remains unclear [1]. Here, the heterostructure made of monolayer $MoSe_2$ covering thin graphene of different thicknesses is studied to reveal details about transfer mechanisms, exciton dynamics and their dependence on incident laser energy and graphene thickness. For this, we have used photoluminescence and Raman spectroscopy. The results obtained in our work reveals efficient exciton transfer from $MoSe_2$ to graphene and short range ($\sim$1 nm) charge transfer mechanism as dominant process between the layers.

[1] G. Froehlicher et al., PRX 8, 011007 (2018)
[2] E. Lorchat, L. E. Parra Lopez, et al., Nature Nanotechnology, 15, 283 (2020)

SUN 15

Collective Optical States of Encapsulated Alpha-Sexithiopene Chains in Boron Nitride Nanotubes

Sabrina Juergensen[1], Jean-Baptiste Merceau[2], Chantal Isabel Mueller[1], Antonio Setaro[1], Patryk Kusch[1], Etienne Gaufrès[2], Stephanie Reich[1]
[1]Physics, Freie Universität Berlin, Berlin, Germany
[2]Laboratoire Photonique Numérique et Nanosciences, Institut d'Optique, Université de Bordeaux, Bordeaux, France

Molecules inside nanotubes form chains, aligning their transition dipole. The Coulomb coupling between the molecular dipoles leads to a collective state with characteristic optical properties like strong and narrow emission, shifted emission and absorption, and a vanishing Stokes shift. Depending on the inner tube diameter the molecules inside the nanotubes form single chains that show pure J-aggregate characteristics. Multi-file chains or randomly aligned molecules can be found in larger diameter tubes leading to a mixture of J- and H-aggregate behavior. In the past it was also shown that parts of tubes might contain no molecules. [1,2]
Here, we used a bundle of boron nitride nanotubes that are filled with α-sexithiophene molecules to study molecular aggregates by various spectroscopic and microscopic techniques to understand how the synergy of coexisting J- and H-aggregates influence their optical properties.

[1] Allard et al., Adv. Mater. 32 (2020)
[2] Badon et al., Mater. Horiz. 10 (2023)

SUN 16
High-Precision Recognition of Left- and Right-Handed Carbon Nanotubes Using Chiral Molecules

Xiaojun Wei[1,2], Shuang Ling[1,3], Lin Liu[1], Shilong Li[1], Xin Luo[1], Linfan Duan[4], Xiao Wang[4], Feibing Xiong[3], Weiya Zhou[1,2], Sishen Xie[1,2], Huaping Liu[1,2]
[1]Institute of Physics, Chinese Academy of Sciences, Beijing, China
[2]University of Chinese Academy of Sciences, Beijing, China
[3]Xiamen University of Technology, Xiamen, Fujian, China
[4]Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, Shenzhen, China

High-precision enantiomeric recognition and characterization of chiral single-wall carbon nanotubes (SWCNTs) with opposite handedness remain a challenge, compared with electrical type and chirality recognition [1,2]. Herein, we systematically investigated the enantioselective interactions of chiral sodium hyodeoxycholate surfactant molecule with two enantiomers of 12 distinct single-chirality SWCNTs and found a type mod(2n + m, 3)-dependent rule in which the E11 transition wavelength of the left-handed enantiomer was larger than that of the right-handed enantiomer for Type I SWCNTs; this trend was the opposite for Type II SWCNTs. Based on the spectral difference from chiral surfactant modulation, a type-dependent rule was successfully established for enantiomeric recognition of SWCNTs with various handedness characteristics. Furthermore, the present method could achieve enantiomeric recognition of SWCNTs at concentrations as low as the ng/mL scale. The detection precision was approximately two orders of magnitude higher than that of traditional circular dichroism spectroscopy.

[1] X. Wei et al., Nat. Commun. 7, 12899 (2016).
[2] X. Wei et al., Adv. Sci. 9, 2200054 (2022).

SUN 17

Signatures of efficient intervalley scattering by acoustic phonons in WSe_2/$MoSe_2$ heterostructure

Hendrik Lambers[1], Nihit Saigal[1], Jonas Kiemle[2], Alexander W. Holleitner[2], Ursula Wurstbauer[1]
[1]Institute of Physics, University of Münster, Münster, Germany
[2]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany

The ability to host excitonic phenomena and correlated phases gives rise to many recent studies on TMDC bilayers. In particular interlayer excitons in heterobilayers are promising candidates to form coherent many body states [1]. The role of exciton-phonon interaction for the thermalization process of these interlayer excitons and the dominant type of involved phonons are of ongoing interest [2]. We employ resonant Raman scattering at cryogenic temperatures to study the exciton phonon coupling in WSe_2/$MoSe_2$ heterostructures. The resonance profiles of degenerated WSe_2 A_1'/E' phonon modes are significantly affected by the assembly into heterobilayers. The profiles cannot be explained only by an incoming and an outgoing resonance of a first order Raman process. Our findings indicate a higher order Raman scattering process involving acoustic M or K point phonons of WSe2 and therefore strong interaction of acoustic phonons with electronic states, that results in efficient intervalley scattering of charge carriers.

[1] M. Troue et al., Phys. Rev. Lett. 131, 036902 (2023).
[2] M. Katzer et al., Phys. Rev B 108, L121102 (2023).

SUN 18

Patterning of covalent and non-covalent functionalization of graphene and twisted bilayer graphene

Tobias Dierke[1], Stefan Wolff[1], Roland Gillen[1], Tamara Nagel[2], Daniela Dasler[2], Sabine Maier[1], Milan Kivala[3], Frank Hauke[2], Andreas Hirsch[2], Janina Maultzsch[1]
[1]Chair of Experimental Physics, FAU Erlangen Nürnberg, Erlangen
[2]Department of Chemistry and Pharmacy, FAU Erlangen Nürnberg
[3]Organisch-Chemisches Institut, Centre for Advanced Materials, Universität Heidelberg

We present an experimental study on the degree of covalent functionalization of graphene exfoliated on top of hBN stripes on Si/SiO_2 as well as on other two-dimensional (2D) materials. The underlying substrate has a strong effect on the degree of functionalization of graphene. Our results show that the functionalization of graphene is less effective on hBN than on SiO_2, as shown by higher defect-induced modes in the graphene Raman spectra on SiO_2. Other underlying 2D materials like MoS_2, WS_2, and MoO_3 show less contrast in functionalization density than hBN or lead to even higher degree of functionalization than the Si substrate. Further-

more, we show an innovative approach to achieve spatial variations in the degree of non-covalent functionalization of twisted bilayer graphene (tBLG). The tBLG was non-covalently functionalized with carbon based molecules. Our results shows a correlation between the degree of functionalization and the twist angle of tBLG. This correlation was determined through Raman spectroscopy, revealing that areas with larger twist angles exhibited lower molecule peak intensity compared to areas with smaller twist angles.

SUN 19

Order of magnitude improvement of transport performances of carbon nanotube films by completely removing surfactants

Xiao Li[1,2,3], Wenke Wang[1,2,3], Hongshan Xiao[4], Yuejuan Zhang[1,2,3], Chang Liu[1], Shilong Li[1], Linhai Li[1,2,3], Wei Su[1], Xiaojun Wei[1,2,3,5], Yunliang Li[1], Honggang Liu[4], Weiya Zhou[1,2,3,5], Huaping Liu[1,2,3,5]

[1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences

[2]Center of Materials Science and Optoelectronics Engineering, and school of Physical Sciences, University of Chinese Academy of Sciences

[3]Beijing Key Laboratory for Advanced Functional Materials and Structure Research

[4]Research Center for Carbon-based Electronics, School of Electronics, Peking University

[5]Songshan Lake Materials Laboratory

Surfactant-based separation techniques have been developed for the high-efficiency production of high-purity semiconducting single-wall carbon nanotubes (s-SWCNTs), which establish an important material foundation for the preparation of high- performance carbon-based electronic devices. However, surfactant molecules wrapping around SWCNTs during structural separation inevitably degrade the resulting device performances due to increasing contact resistance between the SWCNTs and electrodes and between individual SWCNTs. Here, we developed a simple and effective strategy for completely removing the surfactant molecules around separated s-SWCNTs by annealing and rinsing. With this technique, defects were not clearly increased in the crystal structure of SWCNTs, and the transport performances of SWCNT-based thin film transistors (TFTs), including the on-state current and mobility, were improved by approximately an order of magnitude, while the on-off ratio increased by nearly 1.5 orders of magnitude. The present technique provides an important foundation for promoting the development of carbon-based electronic devices.

SUN 20

Multipolar plasmonic modes in cylindrical nanoparticles

Muhammad Shoufie Ukhtary[1,2], Charles Downing[1]

[1]Department of Physics and Astronomy, University of Exeter, Exeter

[2]Research Center for Quantum Physics, National Research and Innovation Agency

(BRIN), South Tangerang, Indonesia

We investigate multipolar plasmonic modes in a metallic nanocylinder with a finite dimension. By employing Rayleigh's variational principle, we calculate frequency of the plasmonic modes for both polarizations: longitudinal and azimuthal polarizations. This method allows us to calculate the frequency of plasmonic modes as a function of aspect ratio of the cylinder, which is defined as the ratio of its length (L) to its radius (a). Therefore, we can investigate how the frequency changes due to the shape varying between nanodisk $(L/a \ll 1)$ to nanowire $(L/a \gg 1)$. Furthermore, we consider not only dipolar plasmonic modes, but also multipolar ones. We found an opposite behaviour of the frequency between both polarizations, where frequency for longitudinal (azimuthal) mode decreases (increases) when we move from nanodisk to nanowire. Our calculation not only recovers the frequency of spheroidal particles for the asymptotic cases of nanodisk and nanowire, but also provides the frequency within intermediate aspect ratio that differs from the case of spheroidal particle due to the sharp edges of the cylinder.

SUN 21
Structural evolution and transformation of a few-layer graphene under high shear stress

Alexander V. Soldatov[1]
[1]Center for High-Pressure Science, State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, China

Graphene and its derivatives have been in the focus of materials research over a decade due to the superior physical properties they exhibit. Yet its behaviour under high pressure and shear stress still not well understood. We exposed a few-layer graphene (FLG) powder to shear stress after pre-compression in a rotational diamond anvil cell. The recovered from high pressure samples were characterized by HRTEM and multi-wavelength excitation Raman. Spectral mapping revealed high inhomogeneity of the Raman spectra reflecting difference in shear- and normal stress distribution across the sample: a minor change in the spectra in the centre vs very high increase of the D-band (defect concentration) on the sample periphery whereas the long-range graphene structure was totally ruined in between [1]. Remarkably, we observed formation of diamond nano-domains coherently connected to the parent graphene structure in certain parts of the sample with disordered structure [2]. Evolution of the FLG structure and its transformation to nanocrystalline diamond under shear deformation are discussed.

1. M. Yuan et al. Appl. Phys. Lett. 118, 213101 (2021).
2. A.V. Soldatov et al., unpublished.

SUN 22
Determining the Crystal Orientation of TMDs by Angular-Resolved Second-Harmonic Generation

Lucas Lafeta[1], Sean Hartman[1], Bárbara Rosa[2], Stephan Reitzenstein[2], Leandro M. Malard[3], Achim Hartschuh[1]
[1]Department of Chemistry and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität, Munich, Germany
[2]Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany
[3]Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, Minas Gerais, Brazil

Second-harmonic generation (SHG) is a unique tool for the investigation of transition metal dichalcogenide (TMD) flakes and can even be used to determine their orientation in an experiment [1,2]. We present our studies on the angular-resolved detection of the SHG in the back-focal plane (BFP) of a microscope objective in monolayer WSe2 and MoSe2. We first analyze the signal produced by the center and edges of monolayer flakes and demonstrate how edges influence the angular SHG radiation pattern. Moreover, we find that we can determine the crystal orientation of the flake from the ellipticity of the detected SHG back-focal plane image. We compare these BFP images with the 6-fold pattern recorded while simultaneously rotating the incident polarization and analyzer. We observe that when the incident field is polarized in the armchair direction, the ellipticity of the SHG-BFP pattern is increased compared with the zig-zag direction.

[1] B. R. Carvalho *et al.* Nano Letters, 20, 284 (2020)
[2] L. M. Malard *et al.* Physical Review B, 87, 201401(R) (2013)

SUN 23
Room temperature gas sensing based on substitutional atom doped MoS_2

David Lamprecht[1,2], Mate Capin[1], Anna Benzer[1], Manuel Längle[2], Clemens Mangler[2], Jani Kotakoski[2], Lado Filipovic[1,3]
[1]Vienna University of Technology, Institute for Microelectronics, Vienna, Austria
[2]University of Vienna, Faculty of Physics, Physics of Nanostructured Materials, Vienna, Austria
[3]CDL for Multi-Scale Process Modeling of Semiconductor Devices and Sensors at the Institute for Microelectronics, Vienna, Austria

2D materials like MoS_2 are a promising alternative to state-of-the-art chemiresistive gas sensors which require high operating temperatures. However, pristine MoS_2 exhibits low sensitivity, long response times and poor selectivity [1]. Ab-initio studies have shown that substitutional doping can be applied to improve these factors significantly [2]. We utilize a helium plasma to induce controlled defects in monolayer-MoS_2, subsequently filling these sites with heteroatoms (e.g. Au, Pt) via evaporation [3], unwanted defects like sulfur monovacancies are removed by resulfurization [4].

The dopants are characterized using scanning transmission electron microscopy. Simulations are conducted to determine the optimal dopant atoms by assessing their adsorption properties to environmental pollutants like NO_2. Further we are building a gas sensor test setup to evaluate the sensing performance of the resulting structures.

[1] Filipovic et al., Nanomaterials 12, 20, 3651 (2022)
[2] Tang et al., J. Mater. Chem. A 8, 24943-24976 (2020)
[3] Zagler et al., 2D Mater. 9, 035009 (2022)
[4] Li et al., Phys Chem Chem Phys. 8(22), 15110-7 (2016)

SUN 24

Scaling of Coulomb Defects in Low-D Semiconductors from Variational and Modified Hückel Calculations

Tobias Hertel[1], Klaus H. Eckstein[1]
[1]Institute of Physical and Theoretical Chemistry, Julius-Maximilians University Würzburg, Germany

Understanding doping is critical for advancing nanoscale technologies, particularly those using semiconducting single-wall carbon nanotubes (s-SWNTs), where doping levels can be controlled by adsorbed counterions. However, modeling low doping levels is challenging due to large unit cells required to represent such 'Coulomb defects'. This study thus utilizes modified Hückel calculations of s-SWNTs measuring 120 nm to explore the properties of shallow Coulomb defects near the valence band edge and of quantum well (QW) states in the conduction band. The QW states could explain frequently observed shifts in exciton bands of inhomogeneously doped semiconductors. A variational approach reveals the scaling properties of Coulomb defects with counterion distance, effective band mass, relative permittivity, and counterion charge [1]. Our findings thus offer new insights into the interactions of exohedral charges with low-dimensional semiconductors having delocalized band states.
[1] K.H. Eckstein and T. Hertel, J. Phys. Chem. C (in press).

SUN 25

Extended spatial coherence of interlayer excitons in $MoSe_2$/WSe_2 heterobilayers

Mirco Troue[1,2], Johannes Figueiredo[1,2], Lukas Sigl[1,2], Christos Paspalides[1,2], Manuel Katzer[3], Takashi Taniguchi[4], Kenji Watanabe[5], Malte Selig[4], Andreas Knorr[4], Ursula Wurstbauer[6], Alexander W. Holleitner[1,2]
[1]Walter Schottky Institute and Physics Department, Technical University of Munich, Germany
[2]Munich Center of Quantum Science and Technology (MCQST), Germany
[3]Institute for Theoretical Physics, Nonlinear Optics and Quantum Electronics, Technical University of Berlin, Germany
[4]International Center for Materials Nanoarchitectonics, National Institute for Materi-

als Science, Japan
[5]Research Center for Functional Materials, National Institute for Materials Science, Japan
[6]Institute of Physics, Münster University, Germany

Our work advances the study of coherent interlayer exciton ensembles in $MoSe_2$/WSe_2 heterobilayers by utilizing a spatially resolved point-inversion Michelson-Morley interferometer. We report on the spatial coherence of a dense interlayer exciton ensemble for a wide range of temperatures and exciton densities. Below 10K, we detect a spatial coherence length of interlayer excitons limited only by the lateral expansion of the exciton ensembles. In this regime, the emission of the excitons is homogeneously broadened and features a coherence visibility of up to 90%. Both the spatial and temporal coherence decrease with increasing temperature, most likely due to thermal processes. We also consider further coherence-limiting processes and exciton diffusion dynamics to explain our findings. Our research sheds new light on the physics of coherent exciton phases in the proposed heterostacks and paves the way toward quantum devices based on many-body quantum phenomena in two-dimensional materials [1,2,3].

[1] M. Katzer *et al.*, PRB 108, L121102 (2023)
[2] L. Sigl *et al.*, PRR 2, 042044(R) (2020)
[3] M. Troue and J. Figueiredo *et al.*, PRL 131, 036902 (2023)

SUN 26

Ultrafast exciton trapping dynamics in oxygen-doped single walled carbon nanotubes

Timofei Eremin[1], Rakesh Dhama[2], Humeyra Caglayan[2], Petr Obraztsov[1]
[1]Department of Physics and Mathematics, University of Eastern Finland, Joensuu, Finland
[2]Faculty of Engineering and Natural Science, Tampere University, Tampere, Finland

Artificial zero-dimensional quantum defects within single-walled carbon nanotubes hold immense promise for diverse optoelectronic applications. This study delves into the temporal behavior of excitons within oxygen-doped single-walled carbon nanotubes, employing ultrafast transient absorption spectroscopy. Our investigation unveils the emergence of doping-induced excitonic states, distinguished by a long-lasting induced transmittance signal. Even at low doping densities, we observe a reduction in the lifetime of band-edge excitons. In contrast, the population dynamics of deep-band excitons exhibit resilience against low and moderate doping densities, with a pronounced reduction only at high doping levels. Our findings align with a kinetic model that accounts for an additional relaxation channel prompted by doping. Thus we establish that the formation of defect-localized excitonic states within oxygen-doped single-walled carbon nanotubes is a consequence of the diffusive trapping of free band edge excitons. These insights shed light on the intricate

dynamics of excitons within nanotube defects, advancing our understanding and potential applications in the realm of optoelectronics.

SUN 27
Ultrafast Phase-Control of the Non-Linear Optical Response of TMDs

Lucas Lange[1], Kunliang Wang[1], Lucas Lafeta[1], Bárbara Rosa[2], Stephan Reitzenstein[2], Sebastian Bange[3], Achim Hartschuh[2]
[1]Department of Chemistry and CeNS, LMU Munich, Munich, Germany
[2]Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany
[3]Department Physik, University of Regensburg, Regensburg, Germany

Monolayer semiconducting transition metal dichalcogenides (TMDs) feature particularly strong nonlinear light-matter interactions, which result from the large oscillator strength of tightly bound excitons. We investigate the third- and second-order nonlinear response of TMDs using phase-shaping of broadband laser pulses resonant with the lowest excitonic state. We find that the four-wave mixing response of TMDs can be coherently controlled and enhanced by manipulating the spectral phase profile of the laser pulse. Here, the optimum spectral phase profile crucically depends on the exciton resonance energy of the TMD and the laser fluence. Sum-frequency generation, on the other hand, is maximized for shortest laser pulses at the same experimental conditions. We then show that upon increasing the pump fluence pulsed laser excitation can induce a Mott transition from an excitonic regime to an electron–hole plasma in TMDs [1].

[1] F. B. Sousa et al., Nanoscale 15, 7154 (2023)

SUN 28
Ferroelectric domain writing in misfit layer compound $(PbS)_{1.11}VS_2$ using electron-beam lithography

Jiří Volný[1], Cinthia Antunes Corrêa[1,2], Klára Uhlířová[1], Kateřina Tetalová[1], Jan Honolka[2], Martin Vondráček[2], Tim Verhagen[1,2]
[1]Department of Condensed Matter Physics, Charles University, Prague
[2]FZU-Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic

Sliding (moiré) ferroelectricity exists only in 2D materials where the out-of-plane polarization is switched by in-plane interlayer sliding and thus breaking the inversion symmetry. So far, sliding ferroelectrics have been mostly observed in artificially created van der Waals multilayers with a small twist angle Θ between the individual layers.
Misfit layer compounds (MLC) are naturally grown materials that consists of alternating stacking of two different 2D materials forming an ordered superstructure. We focus on MLC $(PbS)_{1.11}VS_2$, formed by alternating layers of transition metal dichalcogenide VS_2 and transition metal monochalcogenide PbS. Bulk $(PbS)_{1.11}VS_2$

is stable at ambient conditions, shows semiconducting behaviour and exhibits sliding ferroelectric behaviour at room temperature. Ferroelectric domains with sizes varying between tens of nm up to tens of µm were observed using scanning electron microscopy (SEM) and scanning probe microscopy (SPM). We show that using electron-beam lithography, ferroelectric domains of arbitrary shape can be written. The written domains are thermodynamically stable and can be imaged using both SEM and SPM.

SUN 29
Ferroelectricity in twisted 2D semiconductors

Astrid Weston[1,2], Elisa Castanon[3], Volodya Enaldiev[1,2], Andre Geim[1,2], Vladimir Falko[1,2], Roman Gorbachev[1,2]
[1]School of Physics and Astronomy, University of Manchester, Manchester
[2]National Graphene Institute, University of Manchester, Manchester, UK
[3]National Physical Laboratory, Teddington, UK

A room-temperature ferroelectric semiconductor can be assembled using two vertically stacked layers of MoS2 with a relative twist angle close to zero degrees. Below a critical angle, twisted bilayers of MoS2 atomically reconstruct to generate an energetically favourable triangular domain structure in the case of the 3R stacking polytype. These heterostructures feature broken inversion symmetry, which, together with the asymmetry of atomic arrangement at the interface of the vertically stacked layers, enables ferroelectric domains with alternating out-of-plane polarisation arranged into a twist-controlled network. Through domain-wall sliding, polarised states can be 'switched' by applying out-of-plane electrical fields. This mechanism has been visualized in-situ using channelling contrast electron microscopy for better understanding of the switching mechanism. The electrical properties were further investigated using Kelvin probe force microscopy, electrical transport measurements as well as varying device device geometries (e.g. tunnelling junctions).

SUN 30
Temperature Dependent Light-matter Interaction in 2D polar metals at Cryogenic Temperatures

Jakob Henz[1], Siavash Rajabpour[2], Alexander Vera[2], Joshua A. Robinson[2], Su Ying Quek[3], Ursula Wurstbauer[1]
[1]Institute of Physics, University of Münster, Germany
[2]MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA
[3]Centre for Advanced 2D Materials, National University of Singapore, Singapore

Spectroscopic Imaging Ellipsometry (SIE) is a powerful and versatile optical measurement technique, combining the ability of an ellipsometer to determine layer thicknesses and optical properties of thin film samples to the monolayer limit with the lateral resolution of a microscope. The resolution enables the investigation of

the homogeneity of the dielectric response on the micrometer scale in such various systems such as TMDCs [1] and their heterostructures [2], or 2D polar metals [3].
Using a cryostat with free beam optical access, we established a unique setup for SIE at cryogenic temperatures, allowing us to investigate the temperature-dependence of the local dielectric function of two-dimensional materials from room temperature down to 800 mK. We demonstrate temperature changes in the dielectric function of 2D polar gallium that are interpreted to indicate structural phase transitions.

[1] S. Funke et al., J. Phys.: Condens. Matter **28** 385301 (2016).
[2] F. Sigger et al. Apl. Phys. Lett. **121**, 071102 (2022).
[3] K. Nisi et al., Adv. Funct. Mater. **31** 2005977 (2020).

SUN 31
Interaction of 2D materials with laser-written waveguide circuits

Alina Schubert[1], Karo Becker[1], Marco Kirsch[1], Jakob Kuhlke[1], Rico Schwartz[1], Andreas Thies[2], Alexander Szameit[1], Matthias Heinrich[1], Tobias Korn[1]
[1]Institute of Physics, University of Rostock, Rostock
[2]Ferdinand Braun Institut, Leibnitz Institut für Höchstfrequenztechnik, Berlin

The remarkable optical properties of monolayer transition metal dichalcogenides (TMDCs) are determined by strongly bound excitons. Currently, most of the micro--photoluminescence measurements are performed with light polarized in the plane of the TMDC layer. However, so-called dark excitons that emit z-polarized light propagating along the TMDC layer require detection from the side [1, 2].
Our intention is to probe TMDCs in this direction by depositing them onto a fused silica glass substrate containing femtosecond laser direct written waveguides [3]. By defining the waveguide near the surface of the glass, interactions of the waveguide's evanescent field and the TMDC are enabled.
Our micro-photoluminescence setup that couples into the sides of the waveguide and simultaneously detects light perpendicular to the TMDC layer has the potential to excite and detect the x,y and z polarization of the PL signal, allowing for direct observations of dark excitons.

[1] X.-X. Zhang et al., Phys. Rev. Lett., 115 257403 (2015).
[2] G. Wang et al., Phys. Rev. Lett., 119 047401 (2017).
[3] A. Szameit et al., J. Phys. B.: At. Mol. Opt. Phys., 43 163001 (2010).

SUN 32
Wafer-Scale Growth of Sb2Te3 Films via Low-Temperature Atomic Layer Deposition for Self-Powered Photodetectors

Amin Bahrami[1], Jun Yang[1], Sebastian Lehmann[1], Kornelius Nielsch[1]
[1]IFW-Dresden, Dresden

In this work, we demonstrate the performance of a silicon-compatible, high-performance, and self-powered photodetector. A wide detection range from visible (405 nm) to near-infrared (1550 nm) light was enabled by the vertical p–n heterojunction between the p-type antimony telluride (Sb2Te3) thin film and the n-type silicon (Si) substrates. A Sb2Te3 film with a good crystal quality, low density of extended defects, proper stoichiometry, p-type nature, and excellent uniformity across a 4 in. wafer was achieved by atomic layer deposition at 80 ℃ using (Et3Si)2Te and SbCl3 as precursors. The processed photodetectors have a low dark current (∼20 pA), a high responsivity of (∼4.3 A/W at 405 nm and ∼150 mA/W at 1550 nm), a peak detectivity of ∼1.65 × 1014 Jones, and a quick rise time of ∼98 μs under zero bias voltage. Density functional theory calculations reveal a narrow, near-direct, type-II band gap at the heterointerface that supports a strong built-in electric field leading to efficient separation of the photogenerated carriers. The devices have long-term air stability and efficient switching behavior even at elevated temperatures. These high-performance and self-powered p-Sb2Te3/n-

SUN 33
Nanoscrolls of Janus Monolayer Transition Metal Dichalcogenides

Masahiko Kaneda[1], Wenjin Zhang[1], Zheng Liu[2], Yanlin Gao[3], Mina Maruyama[3], Yusuke Nakanishi[1], Hiroshi Nakajo[4,5,6], Soma Aoki[4,5], Kota Honda[7], Tomoya Ogawa[1], Kazuki Hashimoto[1], Takahiko Endo[1], Kohei Aso[8], Tongmin Chen[8], Yoshifumi Oshima[8], Yukiko Yamada-Takamura[8], Yasufumi Takahashi[7,9], Susumu Okada[3], Toshiaki Kato[4,5], Yasumitsu Miyata[1]
[1]Department of physics, Tokyo metropolitan university, Tokyo
[2]Innovative Functional Materials Research Institute, AIST, Nagoya
[3]Department of Physics, University of Tsukuba, Tsukuba
[4]Graduate School of Engineering, Tohoku University, Sendai
[5]Advanced Institute for Materials Research (AIMR), Tohoku University, Sendai
[6]KOKUSAI ELECTRIC CORP., Toyama
[7]Department of Electronics, Nagoya University, Nagoya
[8]School of Materials Science, JAIST, Ishikawa
[9]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa

Tubular structures of transition metal dichalcogenides (TMDCs) have attracted attention due to their emergent physical properties, such as giant bulk photovoltaic effect and chirality-dependent superconductivity. To understand and control these properties, it is highly desirable to develop a sophisticated method to fabricate the TMDC tubular structures with smaller diameters and uniform crystalline orientation. For this purpose, the rolling up of TMDC monolayers into nanoscrolls is an attractive approach to fabricate such a tubular structure. However, monolayer TMDC generally makes its tubular structure energetically unstable due to considerable lattice strain in curved monolayers. Here, we report the fabrication of narrow nanoscrolls by using Janus TMDC monolayers. The multilayer tubular structures of Janus nanoscrolls were revealed by scanning transmission electron microscopy (STEM) observations.

Atomic resolution elemental analysis confirms that the Janus monolayers were rolled up with the Se-side surface on the outside. We found that the present nanoscrolls have the smallest diameter of about 5 nm, which is almost the same as the value predicted by the DFT calculation.

SUN 34
Signatures of Josephson force in a vibrating carbon nanotube junction

Andreas K. Hüttel[1,2], Jukka-Pekka Kaikkonen[2], Keijo Korhonen[2], Pertti Hakonen[2]
[1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg
[2]Low Temperature Laboratory, Dept. of Applied Physics, Aalto University, Espoo, Finland

A carbon nanotube suspended between superconducting electrodes acts simultaneously as nanomechanical resonator and as a Josephson junction. Its energy-dependent density of states and with that displacement-dependent critical current further adds to the complexity of the system, as does both mechanical and electronic nonlinearity.
Measurements on such a system display complex behaviour of the vibrational resonance with respect to junction biasing. Strikingly, the resonance frequency appears to decrease in a distinct parameter region where the biasing is similar in size to the junction switching current.
Using parallelized Julia [1] code, we numerically solve the coupled differential equation system of the driven (via an ac gate voltage and ac current or voltage bias) system for realistic device parameters and characterize the evolving steady state. Specific attention is given to the impact of the Josephson junction behaviour on the mechanical resonance frequency and the vibration amplitude, and on the ac signal simultaneously acting on gate and bias.

[1] https://julialang.org/

SUN 35
Interplay of energy transfer and charge carrier thermalization in WS_2 - graphene heterostructures

David Tebbe[1], Marc Schütte[1], Kenji Watanabe[4], Takashi Taniguchi[5], Christoph Stampfer[1,2], Bernd Beschoten[1,3], Lutz Waldecker[1]
[1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Germany
[2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany
[3]JARA-FIT Institute for Quantum Information, Forschungszentrum JülichGmbH and RWTH Aachen University, Aachen, Germany
[4]Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan
[5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan

In two-dimensional heterostructures, materials in proximity couple via near-field interactions, which can result in the transfer of energy from one material to the other. We investigate the mechanism of energy transfer in heterostructures of the two-dimensional semiconductor WS_2 and graphene with variable interlayer distances, achieved through spacer layers of hexagonal boron nitride. By analyzing the emission and absorption line widths, we find that the energy transfer is dominated by states outside the light cone, indicative of a Förster transfer process. An increase of the line width at 0.5 nm interlayer distance of (0.7 ± 0.3) meV reveals an additional, but small, component from a Dexter process. We find that the measured dependence of the luminescence intensity on interlayer distances above 1 nm can be quantitatively reproduced using calculated values of the Förster transfer rates of thermalized charge carriers. At smaller interlayer distances, our experiments reveal the transfer rates to be much higher than the calculated values. Using different excitation conditions, we show that these transfer rates result from non-thermalized charge carrier distributions.

SUN 36

Layer Hybridisation and Exciton-Phonon Coupling in in $MoSe_2$/WSe_2 Heterobilayers

Oisín Garrity[1], Annika Bergmann[2], Tobias Korn[2], Stephanie Reich[1], Patryk Kusch[1]
[1]Freie Universität Berlin, Berlin, Germany
[2]Institut für Physik, Universität Rostock, Rostock, Germany

Transition metal dichalcogenides (TMDCs) have garnered strong interest for their robust excitonic properties and potential applications in valleytronics and mixed light-matter states like exciton-polaritons. Stacking TMDC monolayers to create heterobilayers opens doors for tailored material properties, vital for diverse applications from biosensors to solar cells and transistors. Two-dimensional heterostructures inherit their physics from the monolayers, but in addition to the combined properties of the respective monolayers there are often strong cross-layer processes. This study demonstrates cross-layer interactions in exciton-phonon coupling in a WSe2/MoSe2 heterobilayer using resonant Raman spectroscopy. We show that the WSe2 monolayer induces an additional cross-layer optical resonance in the cross-section of the MoSe2 A1g Raman process. Calculations using the frozen phonon method and density functional theory (DFT) reveal a strong exciton-phonon coupling between the A exciton in WSe2 and the A1g phonon mode in MoSe2. This highlights the importance of understanding stacked TMDCs in all their excitations and quasiparticles, going beyond the sum of their constituent parts.

SUN 37

Linear Graphdiynes: the evolution from metalorganic to covalent carbon networks

Alice Cartoceti[1]
[1] Department of Energy, Politecnico di Milano, Milan, Italy

[2]Department of Physics, Engineering Physics and Astronomy, Queen's University, Kingston ON, Canada
[3]Department of Chemistry, Università di Pavia, Pavia, Italy
[4]Department of Physics, Università degli Studi di Milano, Milan, Italy

Graphdiynes (GDYs) are novel 2D carbon materials with mixed sp-sp^2 hybridization, whose atomic arrangement consists of benzene rings connected by diacetylenic bonds in different possible configurations. Their predicted high electrical conductivity and tunability of electronic properties (e.g. bandgap), made possible by an extended π-electron conjugation and easy functionalization, suggest them as highly promising materials for a wide range of applications [1-3].

In this work, linear GDY nanoribbons were grown on Au(111) via on-surface synthesis (OSS), starting from 1,4-bBEB powdered precursors deposited via organic molecular beam epitaxy. The effect of the deposition and annealing temperatures on the atomic structure and vibrational properties of the obtained networks was investigated in situ, by Scanning Tunnelling Microscopy (STM) and Raman spectroscopy respectively, revealing a transition from metalorganic to disordered covalent organic systems.

[1] P. Serafini et al., Phys. Chem. Chem. Phys. 24.17 (2022):10524-10536.
[2] Y. Xue et al., Science China Chemistry 61 (2018):765-786.
[3] G. Li et al., Chemical Communications 46.19 (2010):3256-3258

SUN 38
Efficient Algebraic Method for Flat Bands Construction and EBRs-based Topological Characterization

Ivan Damnjanovic[1,2,3], Milan Damnjanovic[4], Ivanka Milosevic[5], Dragan Stevanovic[6]
[1]Faculty of Electronic Engineering, University of Niš, Niš, Serbia
[2]Diffine LLC, San Diego, CA, USA
[3]Faculty of Mathematics, Natural Sciences and Information Technology, University of Primorska, Koper, Slovenia
[4]Serbian Academy of Sciences and Arts, Belgrade, Serbia
[5]Faculty of Physics, University of Belgrade, Belgrade, Serbia
[6]Mathematical Institute of the Serbian Academy of Sciences and Arts, Belgrade, Serbia

Flat bands (FBs) are generating high attention from researchers in the condensed matter — topological materials and superconductivity, in particular. Various methods for constructing FBs have been proposed. E.g. generalized Lieb's method [1,2] and the refinement of existing techniques within graph theory — exploiting latent symmetry and isospectral reduction of the underlying effective Hamiltonian [3].

Here, we use a powerful yet simple and elegant algebraic method for FB construction which utilizes the Bloch Hamiltonian eigen-determinant functional to identify conditions guaranteeing the existence of non-dispersive eigenvalues (i.e. FBs).

For illustration, we examine both natural and artificial 2D lattices with layer group (LG) symmetry and investigate, using elementary band representations (EBRs) for LGs [4], whether the constructed FBs fall under trivial categories (such as flat or obstructive atomic bands) or possess topological nontrivial characteristics.

[1] E.H. Lieb, PRL 62 (1989) 1201.
[2] D. Calugaru et al. Nat. Phys. 18 (2022) 185.
[3] C.V. Morfonios et al. PRB 104 (2021) 035105.
[4] M. Damnjanovic and I. Milosevic, Bull. Sci. Math. Nat., SASA 47 (2022) 85.

SUN 39

Revisiting momentum-space indirect interlayer excitons in TMD heterostructures

Pablo Hernández López[1], Luka Pirker[2], Adrián Dewambrechies[3], Álvaro Rodríguez[2], Astrid Weston[4], Roman Gorbachev[4], Kirill I. Bolotin[3], Otakar Frank[2], Sebastian Heeg[1]
[1]Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany
[2]J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic
[3]Physics Department, Freie Universität Berlin, Berlin , Germany
[4]Department of Physics and Astronomy and National Graphene Institute, University of Manchester, Manchester, UK

Interlayer excitons (IX) in transition metal dichalcogenide heterostructures have attracted much attention recently because of their permanent dipole and longer lifetimes compared to their intralayer counterparts. IX are generally only visible in the near-IR range and for twist angles of the heterobilayers close to 0°. These restrictive conditions for optical detection have motivated the search for twist-independent, momentum-indirect IX. Here, we discuss the common assignment of the photoluminescence (PL) feature around 1.6 eV in MoS2 - WSe2 heterostructures to such a momentum-indirect IX. We discuss room and cryogenic temperature PL and reflectivity measurements on heterostructures with different stacking orders and twist angles and find no evidence of interlayer emission. Charge transfer and momentum-space direct IX fingerprints indicate good coupling of the heterobilayers. We use tip-enhanced PL to show that an intralayer WSe2 exciton strained by pockets of contaminants trapped in the interface may produce a similar PL band to the one assigned to the momentum indirect IX. These pockets offer in turn an interesting strain engineering landscape for various excitonic species.

SUN 40

Lightwave electronics induced interlayer tunneling in FG-FET

Hieu Duc Nguyen[1], Christoffer Vendelbo Soerensen[1], Mattias Rasmussen[2], Binbin Zhou[2], Peter Uhd Jepsen[2], Peter Bøggild[1]

[1]Department of Physics, Danmark Tekniske Universitet
[2]Department of Electrical and Photonics Engineering, Danmark Tekniske Universitet

Previous investigations have shown that strong light pulses may manipulate quick transition currents in solid electrical fields. Studies have shown current tunneling across a thin hBN insulator barrier wrapped in two monolayer graphene. Based on the above, what would happen if a graphene channel and a graphite floating gate were separated by a thin layer of hBN and subjected to a powerful laser pulse? To answer the question, we researched extensively. Right now, the topic matter is misinterpreted. Using cutting-edge nanofabrication techniques, we developed a unique Graphene Floating gate – Field Emission Transistor (FG-FET) for Lightwave electronics. Using high-intensity broadband THz technology, we construct a low-energy memory Graphene device foundation for future applications. In our study, we observed an unusual phenomenon when samples are irradiated under THz pulses. The electrical results before and after the samples were interacted with THz pulses suggest that a significant amount of are transferred and trapped into the floating gate layer and discharge slowly over time.

SUN 41
SWNTs Charge Management Through Controlled Functionalization

Antonio Setaro[1], Alphonse Fiebor[1], Mohsen Adeli[1], Stephanie Reich[1]
[1]Physics, Freie Universität Berlin, Berlin

Gaining control of the doping level of SWNTs at the single particle level opens up new possibilities for their applications. Electrochemical gating allows fine tuning of the desired position of the Fermi level but can be implemented on ensembles of tubes. Filling the tubes with charge-transfer molecules, on the other side, allows doping at the single nanotube level but lacks fine control over the amount of charges transferred. Here we report our approach based on covalently attached ad-hoc synthesized charge-transfer compounds. This approach does not perturb the pi-conjugation of the carbon network, preserving their optoelectronic properties. By controlling the number of groups attached onto the SWNTs, we can set the amount of charges transferred into them, spanning from p-doping to n-doping in a straightforward way.

SUN 42
Cobalt-doped molybdenum disulfide: Electronic structure and performance in sodium-ion batteries

Lyubov G. Bulusheva[1], Alena A. Zaguzina[1], Alexander Okotrub[1]
[1]Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

To incorporate cobalt into the molybdenum disulfide (MoS_2) lattice, we decomposed a mixture of $(NH_4)_2MoS_4$, a source of molybdenum and sulfur, and cobalt acetate under thermal shock conditions. An EXAFS study of nanomaterials detected that cobalt has four sulfur atoms in its nearest environment. Such coordination is possi-

ble when cobalt is located at the edge of the layers. Co-MoS_2 samples were tested as anode materials in sodium-ion batteries. It was found that a sample containing 5 percent of cobalt has better stability and higher specific capacity at current densities from 0.5 to 2 A/g than other doped samples and undoped MoS_2 prepared in a similar way. The stability of the $5Co - MoS_2$ sample can be explained by its increased conductivity. Indeed, XANES S K-edge spectrum of this sample showed the appearance of a pre-edge peak which may correspond to p-type MoS_2 doping resulting from cobalt incorporation. DFT calculations found that cobalt has a negligible effect on sodium diffusion along the MoS_2 surface, however, charge transfer increases when Na is adsorbed near a cobalt defect. The work was funded by the Russian Science Foundation (grant 23-73-00048).

SUN 43

Crystal structure of the incommensurate composite structure of the sliding ferroelectric misfit layer compound (PbS)1.11VS2

Cinthia Antunes Corrêa[1,2], Jiří Volný[1], Klára Uhlířová[1], Tim Verhagen[1,2]
[1]Faculty of Mathemtics and Physics, Charles University, Prague, Czech Republic
[2]Institute of Physics of the Czech Academy of Sciences, Department of Structure Analysis, Prague, Czech Republic

Sliding ferroelectricity in 2D materials has been recently shown theoretically [1] and experimentally [2]. However, sliding ferroelectricity was mostly observed on artificially prepared layered materials. The layered compound (PbS)1.11VS2 naturally grows as a van der Waals superlattice, consisting of alternated stacked layers of the transition metal dichalcogenide VS2 and the transition metal monochalcogenide PbS [3].
We will present the crystal structure of (PbS)1.11VS2, an incommensurate modulated composite elucidated using single-crystal X-ray diffraction (SCXRD). The interaction between the two subsystems works as a perturbation potential, creating satellite reflections on the diffraction patterns. Intrinsic twin formation with a relative rotation of less than one degree leads to sliding ferroelectricity at room temperature. Using several imaging techniques, triangular and lamellar ferroelectric domains varying from a few nanometers up to tens of micrometers are observed. We will show that SCXRD can be a powerful tool to study moire physics.

1.Li, L. and Wu, M. ACS Nano 11, 6382, 2017
2.Zhang, D. et al., Nat Rev Mat 8, 25, 2023
3.Corrêa, C.A. et al., arXiv:2306.14446

SUN 44

Strain, bandgap, and photoluminescence in TMDC nanobubbles on Au films

Michele Gastaldo[1], Javier Varillas[1,2], Álvaro Rodriguez[3], Luka Pirker[1], Matěj Velický[1], Martin Kalbáč[1], Otakar Frank[1]
[1]J.Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, Prague,

Czech Republic
[2]Institute of Thermomechanics, Czech Academy of Sciences, Prague, Czech Republic
[3]Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Madrid, Spain

Nanobubbles form naturally at the interfaces of 2D materials and their substrate due to air-borne contamination trapped between them in the preparation process. The photoluminescence (PL) signal from the bubbles is strongly red-shifted because of tensile deformation. Its intensity is considerably increased in cases where the substrate otherwise causes PL quenching due to charge transfer [1]. In the present work, by combining (tip-enhanced) PL and Raman spectroscopy, scanning tunneling microscopy and spectroscopy, and molecular dynamics, we study the relations between size, strain, bandgap, and PL and Raman signatures of MoS_2 nanobubbles exfoliated on Au films. Among others, we demonstrate that below a critical radius of $\approx$10 nm, the aspect ratio and strain increase with increasing size, and the bandgap decreases accordingly [2].

[1] Rodriguez et al. 2D Mater. 8, 025028 (2021).
[2] Gastaldo et al. NPJ 2D Mater. Appl. 7, 71 (2023).

SUN 45
Strain response of moire excitons in a 2D semiconductor heterostructure

Denis Yagodkin[1], Sviatoslav Kovalchuk[1], Abhijeet Kumar[1], Bianca Hofer[1], Oguzhan Yücel[1], Pablo Hernández López[2], Sebastian Heeg[2], Kirill I. Bolotin[1]
[1]Department of Physics, Freie Universitat Berlin, Berlin
[2]Department of Physics, Humboldt-Universität Berlin

Heterostructures (HS) of 2D materials with a slight twist display moire patterns that influence excitons, leading to single photon emission, excitonic insulator transition, and manybody states. However, moire pattern analysis is challenging due to stacking angle sensitivity and lattice relaxation. Our study on $MoSe_2$/WSe_2 utilizes mechanical strain to probe interlayer and intralayer moire excitons. In the intralayer region (>1.5 eV), we identify WSe_2 and $MoSe_2$ excitons with distinct strain dependencies. Unlike monolayer $MoSe_2$, HS with a 1.0° twist angle exhibits up to eight $MoSe_2$-related photoluminescence (PL) peaks, decreasing with stacking angle (four at 2.5° and three at 8°), suggesting moire minibands formation. Interlayer exciton PL shows numerous peaks around 1.35 eV, with two groups exhibiting different strain sensitivities ($\sim$40 meV/% and $\sim$70 meV/%). The latter aligns with bright excitons at the K point of $MoSe_2$ and the K point of WSe_2, while the former corresponds to dark interlayer excitons like K_{WSe2}–Q_{MoSe2} or Γ_{WSe2}–Q_{MoSe2}, supported by lower strain sensitivity and emission energy.

attocube
WITTENSTEIN group

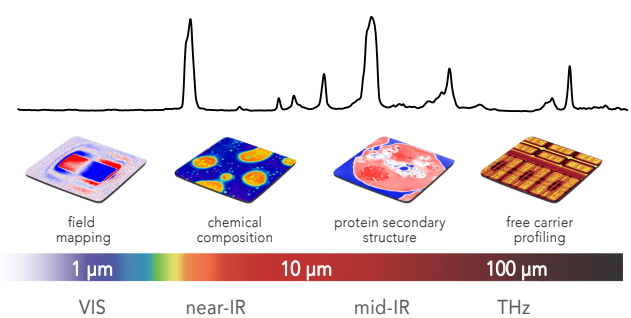
Explore a new dimension.

nano-FTIR

imaging & spectroscopy @10 nm spatial resolution

Product Line
neaspec

- nanoscale chemical ID & compositional mapping
- unmatched spectral coverage (VIS-IR-THz)
- features AFM-IR, s-SNOM, Raman, PL, pump-probe spectroscopy



08:30 – 09:30	TUTORIAL: Hone, New York *2D Materials for Quantum Computing*
09:30 – 10:00	R. Gorbachev, Manchester *Ultraclean Layer Transfer and Atomic Reconstruction in Twisted TMD Lattices*
10:00 – 10:30	Coffee Break
10:30 – 11:00	R. Bratschitsch, Münster *Efficient Light Collection From Single-Photon Emitters in 2D Materials*
11:00 – 11:30	K. Bolotin, Berlin *Nanomechanical Valley Fingerprinting, Hybridization, and Pseudospin Control of Excitons in 2D Materials*
11:30 – 12:00	P. Steeneken, Delft *Magnetic and Thermal Properties of 2D Materials Probed by Nanomechanical Resonance*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	A. Yazdani, Princeton *Visualizing Strongly Correlated Electronic States in 2D Materials*
19:00 – 19:30	S. Forti, Pisa *Probing the Band Structure of Two-Dimensional Materials by Means of Photoemission Spectroscopy*
19:30 – 20:00	M. Morgenstern, Aachen *Photoelectron Spectroscopy of Exfoliated Antiferromagnets*
20:00	Poster II

08:30
2D materials for quantum computing
James Hone[1]
[1]Mechanical Engineering, Columbia University, New York

Superconducting circuits form the basis of the most prominent approach toward quantum computing. Each qubit in such a system is essentially a nonlinear, high-Q resonator, created by combining a Josephson junction with a low-loss capacitor, and typically fashioned out of a metal such as aluminum.
Decades of effort have improved performance by reducing sources of decoherence, enabling qubits to achieve ultra-long coherence times. However, these circuits have large footprint, limiting scaling. Moreover, conventional materials have a limited range of properties that can be exploited for new functionality. Toward this end, we and others have been investigating whether 2D materials and heterostructures can replace conventional materials – and add new functionality – for quantum computing.
This tutorial will first give an overview of the basic aspects of superconducting qubits, and provide understanding of the motivation for current designs. It will then describe recent results and ongoing research toward achieving 2D-based qubits.

09:30
Ultraclean Layer Transfer and Atomic Reconstruction in Twisted TMD Lattices
Roman Gorbachev[1]
[1]National Graphene Institute, University of Manchester, Manchester

Layer-by-layer assembly of van der Waals (vdW) heterostructures underpins new discoveries in solid state physics, material science and chemistry. Despite successes, all current assembly techniques use polymeric supports which limit their cleanliness, ultimate electronic performance, and potential for optoelectronic applications. In the first part of the talk, I will introduce a polymer-free platform for heterostructure assembly using re-usable flexible silicon nitride membranes. This approach enables production of heterostructures with interfaces free from interlayer contamination and correspondingly excellent optoelectronic behaviour. In addition, eliminating polymeric supports allows new possibilities for vdW heterostructure fabrication: assembly at temperatures up to 600℃, and in different environments including ultra-high vacuum and liquid submersion. In the second part, I will review our recent progress on twisted bilayer TMDs bilayers in the reconstruction regime. I will discuss strikingly different behaviour of aligned (R) and anti-aligned (H) TMD monolayer orientations, with ferroelectric domains arising in the former case and piezoelectric texture in the latter.

10:30
Efficient light collection from single-photon emitters in 2D materials
Rudolf Bratschitsch[1]
[1]Institute of Physics, University of Münster, Münster

Single-photon sources are crucial components for quantum networks and communications. Recently, single-photon sources in 2D materials have emerged as robust solid-state light emitters. Commonly, bulky and expensive objective lenses are used for collecting and making use of single photons emitted from 2D materials.
Here, we present polymer microlenses, which are 3D-printed directly on single-photon emitters in commercially available hBN nanocrystals. First, a regular array of hBN nanocrystals is created using capillary assembly [1]. Subsequently, we 3D-print elliptical polymer microlenses onto the nanocrystals. The light emission is efficiently collimated to angles below 5° [2]. The small angle of emission of the new single-photon source allows for using collection lenses with very low numerical apertures, including optical fibers, which renders these single-photon sources highly promising for quantum optics and photonic quantum technologies.
References: [1] J. Preuß et al., 2D Mat. 8, 035005 (2021) [2] J. Preuß et al., Nano Lett. 23, 407 (2023)

11:00

Nanomechanical Valley Fingerprinting, Hybridization, and Pseudospin Control of Excitons in 2D Materials

Kirill I. Bolotin[1]
[1]Department of Physics, Freie University, Berlin, Germnay

Mechanical strain can be used to manipulate material's symmetries. In this talk, we will i) demonstrate an approach to induce mechanical strain with controlled tensorial components in 2D materials at cryogenic temperatures and ii) use the strain response of 2D semiconductors and heterostructures to study their excitons. First, we discuss the approaches toward mechanical strain engineering of high-quality suspended 2D materi- als capable of inducing uniform or uniaxial strain with in-situ tunable magnitude and compatible with cryogenic measurements. Next, show that normally "dark" excitons with vanishing oscillator strength become observable in strained devices. Then, we discuss the approach to detect the valley character of intervalley excitons by examining their strain signatures. Finally, we show that the application of uniaxial strain leads to the behavior of the pseudospin degree of freedom that can be described in the language of the pseudomagnetic field. Such a pseudomagnetic field will be used to establish the many-body character of debated excitonic states.

11:30
Magnetic and thermal properties of 2D materials probed by nanomechanical resonance

Peter G. Steeneken[1,2]
[1]Precision and Microsystems Engineering Department, TU Delft, The Netherlands
[2]Kavli Institute of Nanoscience, TU Delft, The Netherlands

The dynamics of suspended 2D materials have received increasing attention during the last decade. One exciting possibility is the use of nanomechanical resonance as a probe for characterising the magnetic, electronic and thermal properties of 2D materials. This avenue is expecially enticing since it offers the prospect of studying the thickness dependent properties down to the monolayer limit, where concurrent techniques break down.
In this presentation, it will be shown how nanomechanical resonance can be used as a sensitive probe for studying condensed matter physics in ultrathin layers. Examples include investigations into thermal properties[1] and thermodynamics in 2D, the detection of phase transitions in magnetically and electronically ordered materials, and the study of magnetisation via anisotropic magnetostriction[2].

[1] Liu, Hanqing, et al. "Optomechanical methodology for characterizing the thermal properties of 2D materials." arXiv:2312.06070 (2023).
[2] Houmes, Maurits JA, et al. "Magnetic order in 2D antiferromagnets revealed by spontaneous anisotropic magnetostriction." arXiv:2303.11234 (2023).

19:30
Visualizing strongly correlated electronic states in 2D materials
Ali Yazdani[1]
[1]Physics, Princeton University, Princeton

Strong electronic correlation in flat bands created by either strong magnetic field or moire superstructures gives rise to a wide variety of novel quantum states in two-dimensional (2D) materials. I will describe in this talk experiments to visualize variety of novel broken symmetry stated and states with fractionalized quasi-particles with the scanning tunneling microscope that form in strongly correlated 2D materials.

19:00

Probing the band structure of two-dimensional materials by means of photoemission spectroscopy

Stiven Forti[1]

[1]Center for Nanotechnology Innovation, IIT@NEST, Piazza San Silvestro 12, 56127 Pisa, Italy

One of the most impacting ways to characterize a given material, is to map its electronic properties, as it allows to manipulate and control them in targeted applications. Most of the times, the preferential way to probe the electronic properties of a material is to derive them from transport measurements, which in general require several processing steps and could damage the material, especially if two-dimensional (2D). In this lecture, we will introduce the foundations and basic principles of angle-resolved photoemission spectroscopy (ARPES) and will see how it nowadays represents an ever more popular way for mapping the electronic dispersion in 2D crystals. ARPES does not require lithography and it allows for getting insight of the electronic properties at energies not accessible by transport by directly visualizing the band structure of the material. Some examples of real-measurements on materials of interest, like graphene, transition metal dichalcogenides and their hybrid structures will be shown.

19:30
Photoelectron spectroscopy of exfoliated antiferromagnets
Markus Morgenstern[1]
[1]II. Institute of Physics B, RWTH Aachen, Aachen

Exfoliated magnetic 2D materials added magnetism to the toolbox for stacking different types of van-der-Waals materials. Thiophosphates are relatively inert intralayer antiferromagnets with multiple magnetic configurations (Neel, zigzag, in-plane, out-of-plane, canted). I will present micron-scale angle-resolved photoelectron spectroscopy at various photon energies of exfoliated $MnPS_3$, $NiPS_3$, $FePS_3$ and $CrPS_4$ above and below their Neel temperature, partly down to the monolayer. Favorable comparison with density functional theory calculations enables identifying the orbital character of the observed bands. For $MnPS_3$, we find pronounced changes across the Néel temperature for bands consisting of Mn 3d and 3p levels of adjacent S atoms. They can be interpreted as caused by a competition of direct and superexchange. For the other materials the changes are more subtle and will be discussed in detail.

MON 1
AFM imaging of single and multilayered 2D materials using photothermally-actuated cantilevers

Jonathan D. Adams[1], Hans Gunstheimer[1], Paul Markus[1], Ed Nelson[2]
[1]Nanosurf AG, Liestal, Switzerland
[2]Nanosurf USA, Woburn, MA, USA

In multilayered structures of two-dimensional materials, the electronic properties strongly depend on layer-to-layer orientation. The need for measuring this orientation drives a need for imaging methodologies that reveal atomic lattice resolution and moiré superlattice resolution. Towards this aim, atomic force microscopy is a powerful technique, especially when higher eigenmodes or torsional modes of the cantilever are used. Photothermal excitation in particular gives flexible, direct and wide bandwidth actuation of AFM cantilevers, allowing for straightforward extension of standard imaging modes to include cantilever excitation at additional frequencies. In this work, we will describe the principle of photothermal actuation and illustrate examples of its application with regards towards high-resolution imaging of single and multilayered 2D materials.

MON 2
Imaging ellipsometry for layer number identification and optical characterization of 2D-materials

Sebastian Schaper[1], Hossein Ostovar[1], Jakob Henz[1], Pierre-Maurice Piel[1], Hendrik Lambers[1], Ursula Wurstbauer[1]
[1]Institute of Physics, University of Muenster, Muenster

Ellipsometry allows to determine the optical properties and thicknesses of thin films simultaneously. The change to the state of polarization of the reflected light from a sample surface is measured in the ellipsometric angles Δ and Ψ, that describe the phase shift and amplitude ratio of p- to s-polarized light respectively. In combination with a microscopic lens and CCD-camera as detector, spectroscopic imaging ellipsometry (SIE) allows to measure optical properties and thicknesses with a microscopic view on the sample.

Here we utilize the microscopic part of SIE to quickly visualize and identify any 2D-materials flakes of desired thicknesses where we know the optical properties of the material. Therefore, we localize such flakes either by a reference sample or by calculation of the expected contrast for desired flake thickness upon an arbitrary substrate.

If the optical properties are unknown, we utilize the ellipsometric part of SIE, to characterize optical properties. We will evaluate a novel approach to decouple the optical properties from thicknesses of thin layers, allowing to characterize flakes of hBN and other 2D-materials of various thicknesses.

MON 3
Far Field Excitation of Phonon Polaritons in h-BN

Ori Avayu[1]
[1], Tel Aviv

We demonstrate the properties of Phonon Polaritons, by launching confined Phonon polaritons in low dimensional van der Waals (vdW) heterostructure, composed of nanometric-size cubes, on top of h-BN flakes. The cubes act as a mid-IR antenna, launching highly confined electromagnetic modes carrying large momentum

MON 4
Noble metal dichalcogenides: Strain-dependent optoelectronic and non-linear response

Stefan Heiserer[1], Natalie Galfe[1], Maximilian Wagner[1], Simon Schlosser[1], Silke Boche[1], Tanja Stimpel-Lindner[1], George de Coster[1], Georg S. Duesberg[1], Paul Seifert[1]
[1]University of the Bundeswehr Munich, Institute of Physics, Faculty of Electrical Engineering and Information Technology, Neubiberg, Germany

Noble metal dichalcogenides belong to the material class of layered 2D materials. In particular, these materials transition from direct band gap semiconductor to semimetal with increasing layer thickness and were shown to host type-II Dirac semimetallic behavior, as well as topological surface states and superconductivity [1,2]. Moreover, strain-dependent electrical characterization in the compound $PtSe_2$ reveals a piezo-resistivity with giant thickness dependent gauge factor [3]. We fabricate free-standing $PtSe_2$ bridges in order to systematically study their optoelectronic properties under controlled strain. We elucidate mechanisms that can give rise to both negative and positive gauge factor in poly-crystalline $PtSe_2$. Finally, we analyze the low-frequency optoelectronic response of $PdTe_2$ with spectral resolution and identify signatures of non-linear response whose symmetry constrains can give rise to a strong anisotropy in its optoelectronic response to THz radiation [4].

[1] W. Zheng et al., PRB 97, 235154 (2018)
[2] O.J. Clark et al., PRL 120, 156401 (2018)
[3] S. Wagner et al., Nano Lett. 18, 6, 3738 (2018)
[4] C. Guo et al. Sci. Adv. 6, 36 (2020)

MON 5
Dry transfer of Graphene nanoribbons for gate tunable devices

Debopriya Dutta[1], Amogh Kinikar[1], Gabriela Borin Barin[1], Roman Fasel[1]
[1]nanotech@surfaces laboratory, Empa, Dübendorf

Graphene nanoribbons (GNR) have been captivating significant interest with unique electronic, mechanical, and thermal properties. Their precise synthesis and manipulation offer unprecedented opportunities for tailoring material properties at the

nanoscale. Of particular interest is how the tunability of electronic and magnetic properties in GNRs at the single-atom level could potentially be harnessed to host quantum effects. This contribution explores progress in utilizing GNRs as a framework for studying such quantum effects through the development of GNR based gate tunable FETs. Such FETs require a dielectric environment to electrically control the manipulation of charge and spin states. One of the fundamental challenges for fabricating them is the 'transfer' of the GNRs from their growth substrate (Au (111)) onto gateable substrates such as SiO2. Herein, we have tried to address this challenge by using multiple approaches including polymer based and Au assisted transfer to efficiently transfer GNRs. Such transfer methodology could also be potentially used in ultra-high vacuum essentially allowing to study manipulation of the charge and spin states at the single-atom level.

MON 6
Collective Optical Excitations in Thin Films of Alpha-Sexithiophene on Two-Dimensional Materials

Chantal Isabel Mueller[1], Sabrina Juergensen[1], Nikolai Severin[2], Adrián Dewambrechies[1], Niclas S. Mueller[3], Jürgen Rabe[2], Kirill I. Bolotin[1], Stephanie Reich[1]
[1]Physics, Freie Universität Berlin, Berlin, Germany
[2]Physics, Humboldt Universität zu Berlin, Berlin, Germany
[3]Physical Chemistry, Fritz Haber Institute, Berlin, Germany

To study collective optical excitations, thin films of alpha-sexithiophene (α-6T) molecules were grown on 2D materials by physical vapour deposition. Different arrangements of molecules were observed by varying the growth parameters leading to changes in their optical response. Fluorescence spectroscopy and microscopy identified the different lattices and revealed correlations between molecular packing, dipole-substrate interactions and exciton dynamics.
Collective states, characterized by electronic excitation delocalized over multiple molecular units, exhibit unique properties such as giant oscillator strength and superradiance, contributing to their high emissivity. Overall, the study explores the impact of diverse growth parameters on the molecular lattices in thin films of α-6T to learn more about collective states and to improve optoelectronic devices based on organic semiconductors.

MON 7
Strain fingerprinting of exciton valley character in 2D semiconductors

Abhijeet Kumar[1], Denis Yagodkin[1], Roberto Rosati[2], Douglas Bock[1], Christoph Schattauer[3], Sarah Tobisch[3], Joakim Hagel[2], Bianca Höfer[1], Jan N. Kirchhof[1], Pablo Hernández López[4], Sebastian Heeg[4], Cornelius Gahl[1], Florian Libisch[3], Ermin Malic[2], Kirill I. Bolotin[1]
[1]Free University Berlin, Germany
[2]Philipps-Universität Marburg, Germany
[3]TU Wein, Austria

[4]Humboldt-Universität Berlin, Germany

Momentum-indirect intervalley excitons define optoelectronic properties of 2D semiconductors but are challenging to detect due to their weak coupling to light. Complexities associated with momentum-selective probes further limit the identification of exciton's valley content. Here, we show that under mechanical strain, the excitons exhibit valley-specific energy shifts, allowing their valley fingerprinting. To this end, we apply controlled strain up to 2% at cryogenic temperatures in suspended 2D materials. This approach allows us to identify multiple previously inaccessible excitons with wavefunctions localized in K, Γ, and Q valleys, as well as different types of localized excitons. Overall, our powerful optomechanical approach may be used to tune and unravel intervalley excitons in various 2D systems.

MON 8

Large Tunable Kinetic Inductance in twisted trilayer graphene superconductor

Rounak Jha[1,2], Martin Endres[1], Kenji Watanabe[3], Takashi Taniguchi[4], Christian Schoenenberger[1], Mitali Banerjee[2], Paritosh Karnatak[1]
[1]Department of Physics, University of Basel, Basel, Switzerland
[2]Laboratory of Quantum Physics (LQP), École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
[3]Research Center for Functional Materials, National Institute for Material Science, 1-1 Namiki, Tsukuba, Japan
[4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan

Magic angle twisted graphene heterostructures have been shown to host a wide gamut of correlated states such as correlated insulators, ferromagnetism, and superconductivity, owing to the strong electron-electron interactions in these systems. Electrostatic tunability between such phases makes this an ideal platform for investigating various physical phenomena. In this work, we construct superconducting quantum interference devices (SQUIDs) with magic angle twisted trilayer graphene (MATTG) as the weak link and superconducting Molybdenum Rhenium (MoRe) as the superconducting loop. We study the current phase relation (CPR) in various configurations by electrostatically tuning the two MATTG weak links. We show that superconducting MATTG has a large kinetic inductance up to 100 nH per square and is electrostatically tunable. This opens avenues for using MATTG as a tunable element in superconducting circuits.

MON 9

Exciton Transitions in Quasi-2D Perovskites at Cryogenic Temperatures

Patrick Grenzer[1], Klaus H. Eckstein[1], Friedrich Schöppler[1], Tobias Hertel[1]
[1]Julius-Maximilians-Universität Würzburg, Würzburg

Two-dimensional (2D) perovskites exhibit unique optical properties, attracting interest for a range of applications where understanding the origin of photophysical relax-

ation pathways is crucial. Recent studies have investigated the exciton fine structure (EFS) in 2D perovskites at low temperatures [1,2]. However, spectroscopic experiments resolving the EFS in their quasi-2D analogues are still lacking.
Here, we report a series of temperature-dependent photoluminescence (PL) measurements on mechanically exfoliated quasi-2D perovskites $(C_6H_5C_2H_4NH_3)_2(CH_3NH_3)_{n-1}Pb_nI_{3n+1}$ with n = 1, 2, 3 or 4. At temperatures below about 60 K the exciton bands are found to break up into a series of individual transitions. Evidence for the excitonic nature of these transitions is provided by absorption spectroscopy, power-dependent and polarization-dependent PL measurements. Our investigations provide new insights into the EFS of quasi-2D perovskites and shed light on the role of quantum confinement in this class of low-dimensional semiconductors.

[1] Do et al., Nano Lett. 2020, 20, 5141-5148
[2] Posmyk et al., Adv. Optical Mater. 2023, 2300877

MON 10

Impact of competing energy scales on the shell-filling sequence in elliptic bilayer graphene quantum dots

Samuel Möller[1,2], L. Banszerus[1,2], A. Knothe[3], L. Valerius[1], K. Hecker[1,2], E. Icking[1,2], K. Watanabe[4], T. Taniguchi[5], C. Volk[1,2], C. Stampfer[1,2]
[1]2nd Institute of Physics, RWTH Aachen University, Aachen, Germany
[2]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany
[3]Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany
[4]Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan
[5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan

Bilayer graphene quantum dots have the potential to play a vital role in future quantum technologies based on 2D materials, as they can serve as building blocks for quantum sensing, quantum metrology, spintronics, and quantum information devices. It is therefore of great interest to fully understand the quantum states and the shell-filling sequence in few-electron QDs. Here we show that in order to understand the shell-filling of the first three orbital states in elliptic QDs, it is necessary to both include short-range electron-electron interactions on the order of 0.2 to 0.8 meV, and wave function-dependent valley magnetic moments. Furthermore, we analyze data from 31 different BLG QDs, finding that short-range interaction and valley magnetic moment increase for smaller QDs. Interestingly, the electrostatic charging energy shows no simple functional relation with respect to QD size, highlighting that the electrostatics of gate-defined BLG QDs, which have low charge carrier density lead regions, are non-trivial.

MON 11

Photoluminescence enhancement of the 7-armchair graphene nanoribbons deposited onto polystyrene microspheres

Pavel V. Fedotov[1,2], Natalia R. Arutyunyan[1,2], Andrey A. Kozlov[3], Elena D. Obraztsova[1,2]
[1]A.M. Prokhorov General Physics Institute, RAS, Moscow, Russia
[2]Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Russia
[3]Lomonosov Institute of Fine Chemical Technology, Moscow, Russia

Ultra-narrow graphene nanoribbons (with 0.3-1.0 nm width) (GNRs) demonstrate much brighter photoluminescence (PL) than single-wall carbon nanotubes.In this work we demonstrate the PL enhancement of the 7-armchair GNRs deposited on polystyrene microspheres. The observed series of narrow PL peaks of GNRs is associated with whispering gallery modes (WGMs) of microspheres. The GNR films were synthesized from DBBA molecules via a CVD method based on the bottom-up approach [1]. To individualize nanoribbons the 7-AGNR films were partially suspended in toluene via gentle stirring or/and ultrasonication procedure. To deposit GNRs on microspheres a simple drop-casting method was introduced. First, the microspheres were deposited from water suspension on Si/SiO2 substrate followed by drying. Further, the GNR toluene suspension was drop-casted on the substrate with microspheres. After prolonged drying period the optical measurements were carried out.The results obtained open the road for using GNRs as an active material for lasers [2].

1. P.V. Fedotov, et. al., J. Phys. Chem. C 124 (2020) 259.
2. Jia-Shiang Chen et al., ACS Nano 16 (2022) 16776.

MON 12

Imaging the Impact of Interlayer Excitons on TMD Heterostrucutres

Oisin Garrity[1], Annika Bergmann[2], Tobias Korn[2], Patryk Kusch[1]
[1]AG Reich, FU Berlin - Institut für Experimentalphysik, Berlin
[2]Universität Rostock

Heterostructures of transition metal dichalcogenides (H-TMDs) have become a hotbed of research due to their inherent optical properties and tunability. The H-TMDs have tunable bandgaps, exhibit intralayer and interlayer excitons with strong binding energies at room temperature, and their properties can be affected and tuned according to moiré physics. The optical properties in H-TMDs are heavily influenced by inter and intralayer excitons. Investigating the impact of interlayer excitons on optical properties is extremely important for application and fundamental understandings, however challenging to do with diffraction-limited techniques due to the fact that these particles exist often in nanoscaled areas. Here we show that the scattering type-scanning near-field optical microsopce can be used to measure

the impact of interlayer excitons on the dielectric function in a $MoSe_2$/WSe_2 heterostructure. We found an additional resonance induced by the quasi-particles that is missing in the TMDC monolayers. We support our finding by calculation of the dielectric function with the finite dipole model giving acess to the interlayer exciton absorption energies and lifetimes

MON 13

Spatial coherence in 2D systems probed by nano-Raman spectroscopy

Rafael Nadas[1], Andreij C. Gadelha[1,2], Lucas Liberal[1], Tiago C. Barbosa[1,3], Rafael Martins[4], Cassiano Rabelo[5], Vitor Monken[5,6], Thiago L. Vasconcelos[7], Ive Silvestre[4], Leonardo C. Campos[1,3], Riichiro Saito[8], Luiz Gustavo Cancado[1], Ado Jorio[1,6]

[1]Departamento de Fisica, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil
[2]Departamento de Fisica Universidade Federal do Ceara, Campus do Pici, Fortaleza, Brazil
[3]Centro de Tecnologia em Nanomateriais e Grafeno, Belo Horizonte, Brazil
[4]Departamento de Fisica, Universidade Federal de Ouro Preto, Ouro Preto, Brazil
[5]Fabrica de Nanosolucoes - FabNS, Belo Horizonte, Brazil
[6]Programa de Pós-Graduação em Inovação Tecnológica e Propriedade Intelectual, Belo Horizonte, Brazil
[7]Divisao de Metrologia de Materiais, Duque de Caxias, Brazil
[8]Department of Physics, Tohoku University, Sendai, Japan

Raman spectroscopy is known for being a spatially incoherent phenomenon. However, this is only true for micro-Raman, where the spatial resolution provided by visible light is orders of magnitude greater than the Raman coherence length (L_c). In nano-Raman (in particular tip-enhanced Raman spectroscopy - TERS), the spatial resolution is in the order of tens of nm, allowing the Raman scattered photons to interfere with one another. In this work, using TERS, we determine the dependence of L_c with the Fermi level in graphene due to Kohn's anomaly effect, as well as the values for L_c in transition metal dichalcogenides (TMDs) MoS_2, WS_2, $MoSe_2$ and WSe_2 and we show that, not only L_c decreases when approaching the Dirac point in graphene, but also that it differs for different TMDs.

MON 14

SnS_2 thin film with in-situ and controllable Sb doping via atomic layer deposition for optoelectronic applications

Dong-Ho Shin[1,2], Jun Yang[1,3], Samik Mukherjee[4], Amin Bahrami[1], Sebastian Lehmann[1], Noushin Nasiri[5], Fabian Krahl[1], Chi Pang[1], Angelika Wrzensinska-Lashkova[1,6], Yana Vaynzof[1,6], Steve Wohlrab[1], Alexey Popov[1], Kornelius Nielsch[1,2]

[1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany
[2]Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

[3]Institute of Materials Science, Technische Universität Dresden, Dresden, Germany
[4]Jio Institute, Navi Mumbai, Maharashtra, India
[5]School of Engineering, Faculty of Science and Engineering, Macquarie University, Sydney, New South Wales, Australia
[6]Chair for Emerging Electronic Technologies, Technische Universität Dresden, Dresden, Germany

SnS_2 stands out as a highly promising two-dimensional material with significant potential for applications in the field of electronics. Numerous attempts have been undertaken to modulate the physical properties of SnS_2 by doping with various metal ions. Here, we deposited a series of Sb doped SnS_2 via atomic layer deposition (ALD) super-cycle process, and compared its crystallinity, composition, and optical properties to those of pristine SnS_2. We found that the increase in the concentration of Sb is accompanied by a gradual reduction in the Sn and S binding energies. The work function is increased upon Sb doping from 4.32 eV (SnS_2) to 4.75 eV (Sb-doped SnS_2 with 9:1 ratio). When integrated into photodetectors, the Sb-doped SnS_2 showed improved performances, demonstrating increased peak photoresponsivity values from 19.5 A/W to 27.8 A/W at 405 nm, accompanied by an improvement in response speed. These results offer valuable insights into next generation optoelectronic applications based on SnS_2.

MON 15

Quantification of oxygen and aryl quantum defects in single-walled carbon nanotubes by Raman spectroscopy

Finn L. Sebastian[1], Felicitas Becker[1], Simon Settele[1], Yohei Yomogida[2], Yuuya Hosokawa[2], Sebastian Lindenthal[1], Han Li[3], Benjamin S. Flavel[3], Kazuhiro Yanagi[2], Jana Zaumseil[1]
[1]Institute for Physical Chemistry, Heidelberg University, Heidelberg, Germany
[2]Graduate School of Science and Engineering, Tokyo Metropolitan University, Hachioji, Tokyo, Japan
[3]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

The functionalization of semiconducting single-wall carbon nanotubes (SWCNTs) with luminescent quantum defects results in increased photoluminescence (PL) quantum yields and enables single-photon emission in the near-infrared (nIR). For the application of functionalized SWCNTs in nIR biological imaging, metabolite sensing, and light-emitting devices, precise tuning of the structure and density of luminescent defects is essential. While structural control over the type of defect and binding configuration on the SWCNT lattice is possible by variation of reactants and experimental conditions, the quantification of quantum defects commonly relies only on relative measures, e.g., the D/G mode ratio from Raman spectra. Here, we combine PL quantum yield measurements and Raman spectroscopy to derive a universal method for the absolute quantification of aryl and oxygen quantum defects in SWCNTs. This quantification method accounts for the Raman excitation energy and is applicable to a range of small-diameter SWCNTs in aqueous and organic solvent

dispersions.[1,2]

[1] Sebastian et al., J. Phys. Chem. Lett. 2022, 13, 3542.
[2] Sebastian et al., ACS Nano 2023, 17, 21771.

MON 16

Cholic acid tuning the binary surfactant system for the high-efficiency separation of the enantiomers of (5, 4) carbon nanotubes

linhai Li[1], Jiamin Cui[1], Chaojing Shi[1], Dehua Yang[1], Wenke Wang[1], Xiaojun Wei[1,2,3], Yunliang Li[1], Weiya Zhou[1,2,3,4], Huaping Liu[1,2,3,4]
[1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
[2]Center of Materials Science and Optoelectronics Engineering, and School of Physical Sciences, University of Chinese Academy of Sciences, Beijing, China
[3]Beijing Key Laboratory for Advanced Functional Materials and Structure Research, Beijing, China
[4]Songshan Lake Materials Laboratory, Dongguan, Guangdong, China

High-efficiency separation of the enantiomers of (5, 4) single-wall carbon nanotubes (SWCNTs) is of great importance for the study of the properties and applications of SWCNTs in bioimaging, chiral molecule screening and molecule detection due to their high photoluminescence quantum efficiency and emission wavelength that can be detected by silicon detectors. In this work, we discovered a new surfactant cholic acid (HC) with high hydrophobicity that has high resolution selectivity in modulating the selective adsorption of small-diameter SWCNTs in gel columns. With this technique, (5, 4) SWCNTs, which usually have little content in raw mixture materials due to their low growth efficiency, were highly selectively adsorbed in gel columns by tuning HC concentrations. Afterward, high-purity enantiomers of single-chirality (5, 4) SWCNTs were separated by the ternary surfactant system of sodium dodecyl sulfate, sodium cholate, and sodium deoxycholate to selectively desorb their enantiomers from gel columns.

MON 17

Broken symmetries probed by non-linear optoelectronic transport

Christoph Kastl[1], Maanwinder Singh[1], Jonas Kiemle[1], Lukas Powalla[2], Alexander W. Holleitner[1], Marko Burghard[2]
[1]Walter Schottky Institut, Technische Universität München, Garching
[2]Max-Planck-Institut für Festkörperforschung, Stuttgart

I will present examples of (un)intentionally broken symmetries in van der Waal materials and the resulting nonlinear optoelectronic transport. For $MoTe_2$, photocurrent imaging reveals a disordered transition between the monoclinic 1T' phase to low-temperature orthorhombic T_d phase, where ultrafast photocurrents originate from the local breaking of the electronic symmetries (2D Mater. 2022, 9, 011002). In

graphene-based heterostructures, we address gate-tunable, non-linear transport arising from strong spin-orbit coupling, which may be used to efficiently manipulate spin-polarized carriers by both optical and electrical means. In commensurate graphene/Bi_2Te_2Se heterointerfaces, we find an enhanced helicity-dependent photocurrent due to the peculiar spin-orbit proximity of the commensurate alignment (ACS Nano 2022, 16, 12338-12344). In graphene/WTe_2, we demonstrate optical detection of current-induced spin polarisations related to a non-linear anomalous Hall effect in the heterostructure. Even for a nominal in-plane transport, out-of-plane spins are induced by a corresponding out-of-plane current. (Nat. Commun. 2022, 13, 3152).

MON 18

Unconventional spin-orbit-parity coupled superconductivity in the kagome superconductor AV_3Sb_5

Ben-Chuan Lin[1], Shuo Wang[1], Kam Tuen Law[2], Dapeng Yu[1]
[1]International Quantum Academy, Southern University of Science and Technology, Shenzhen
[2]Department of Physics, Hong Kong University of Science and Technology

The recently discovered kagome superconductors offer a promising platform for investigating intertwined orders and novel states, including topology, superconductivity, charge density waves, and more. The interplay among these orders can spontaneously break rotational symmetry, giving rise to exotic phenomena such as nematicity or even nematic superconductivity. Here we present our findings on the two-fold symmetric superconductivity in thin-flake AV_3Sb_5 in response to a direction-dependent in-plane magnetic fields, in contrast to the inherent six-fold structural symmetry of the crystal lattice. The two-fold symmetry was evidenced through a combination of magnetoresistance transport experiments, critical magnetic field measurements, and observations of anisotropic superconducting gaps. Notice that though the normal states have two-fold symmetry due to the charge density wave driven nematicity, it doesn't guarantee the two-fold symmetry observed in the superconducting states, particularly within the inversion-symmetric kagome superconductors. We propose that the unconventional spin-orbit-parity-coupled superconductivity is responsible for the anisotropic superconducting gap.

MON 19

Rhombohedral graphite preparation via crystallographically oriented exfoliation

Krisztian Marity[1], András Pálinkás[1], Zsolt E. Horváth[1], Levente Tapasztó[1], Péter Nemes-Incze[1]
[1]HUN-REN Centre for Energy Research, Budapest, Hungary

The investigation of correlation effects in topological flat bands, such as in Landau levels or 'magic angle' bilayer graphene, is a key area in condensed matter physics.

Rhombohedral Graphite (RG) is particularly notable for hosting a symmetry-protected flat band, without the need for moiré superlattices, facilitating the study of many-body effects, especially in thicker samples. However, RG preparation has been a significant bottleneck in exploring the properties of this simple 2D-crystal. Here we show, that hexagonal graphite transforms to RG, during exfoliation. This transformation can be enhanced, by crystallographically oriented exfoliation. By aligning the exfoliation tape parallel to the armchair direction of large graphite single crystals, the yield can be enhanced to 50%, meaning every second flake examined contains rhombohedral regions. The typical size of RG domains is found to be between 5 to 20 µm. This development not only enhances our ability to produce RG but also broadens the scope of research into correlated electron systems in topological flat bands.

MON 20
Automatic detection of atomic defects in TEM images of single- and three-layer 2D materials and signatures in PL and Raman

Moritz Quincke[1,2], Narine Moses Badlyan[3], Johannes Biskupek[1], Manuel Mundszinger[1], Janina Maultzsch[3], Ute Kaiser[1,2]
[1]Central Facility Materials Science Electron Micros, Ulm University, Ulm
[2]Institute for Quantum Optics, Ulm University, Ulm, Germany
[3]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Two-dimensional (2D) materials have unique optical and electronic properties that can be tuned by atomic defects. [1] Here we use spherical and chromatic aberration-corrected high-resolution transmission electron microscopy [2] to image and introduce atomic defects. However, relating the atomic defects to their signature in ex-situ optical measurements poses significant challenges e.g. how to transfer the imaged flake to the requested substrate. We develop a corresponding preparation technique [3] and present an approach that relates structural results in single-layer MoS_2 and WS_2 with spectroscopic features in photoluminescence and Raman. Moreover, we identify the optimal substrate for the optical measurements as we find that the substrate plays a crucial role.
Our automated defect recognition allows to identify not only the lateral but also the vertical position of the atomic defects in 1-3-layer MoS_2[4]. The latter might be important also for electric tunneling devices[5].

[1] Qin et al., Adv. Opt. Mater. (2016)
[2] Linck et al., Phys. Rev. Lett. (2016)
[3] Quincke et al., ACS A. N. M. (2022)
[4] Quincke et al., in prep.
[5] Keren et al., Nat. Comm. (2020)

MON 21
Identifying perfect rhombohedrally stacked graphite by electronic Raman scattering

András Pálinkás[1], Krisztián Márity[1], Konrád Kandrai[1], Zoltán Tajkov[1,2], Martin Gmitra[2], Péter Vancsó[1], Levente Tapasztó[1], Péter Nemes-Incze[1]
[1]HUN-REN, Centre for Energy Research, Budapest, Hungary
[2]Centre of Low Temperature Physics, Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia

Rhombohedral graphite (RG) shows strong correlations in its topological flat band, with enhanced many-body effects as the layer number (N) increases. A major challenge in preparing RG samples is identifying perfect RG, especially for flakes thicker than 5 layers, where traditional Raman identification methods, such as examining the 2D peak shape, become unreliable. Furthermore, the probability of stacking faults in these thicker crystals increases exponentially with N. We demonstrate that the strong layer dependence of the band structure can be harnessed to identify perfect RG flakes by measuring its electronic Raman scattering signal. This measurement can be performed using a conventional confocal Raman spectrometer at room temperature, using visible excitation wavelengths. This advancement in RG identification is crucial for exploring the rich correlation effects in its flat band. We have resolved the identification challenge using a simple and fast optical measurement technique, thereby helping to establish RG as a platform for studying strong correlations in one of the simplest crystals possible.

MON 22
Lithium-Induced Reorientation of Few-Layer MoS_2 Films

Michaela Sojková[1], Igor Píš[2], Jana Hrdá[1], Tatiana Vojteková[1], Lenka Pribusová Slušná[1], Karol Vegso[3], Miloš Krbal[4], Paul Fons[5], Edmund Dobročka[1], Peter Nádaždy[1], Frans Munnich[6], Martin Hulman[1], Federica Bondino[2]
[1]Institute of Electrical Engineering, Slovak Academ, Bratislava
[2]IOM-CNR, Istituto Officina dei Materiali, Basovizza, Trieste, Italy
[3]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia
[4]Center of Materials and Nanotechnologies (CEMNAT), Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic
[5]Faculty of Science and Technology, Keio University, Department of Electronics and Electrical Engineering, 223-8522 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa 223-8522, Japan
[6]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Few-layer MoS_2 films have garnered significant attention for their potential applications in electronics, optics, and energy conversion/storage. The introduction of alkali metals, particularly Li, presents an opportunity to tailor the electronic properties of MoS_2. Despite this potential, the impact of Li on growth of MoS_2 layers remains underexplored. In this study, we investigate the influence of Li on structural and optical

characteristics of MoS_2 few-layer films.[1] Employing a novel one-zone sulfurization method with Li_2S as the Li source, we enable the integration of lithium into octahedral and tetrahedral sites of pre-existing MoS_2 films or during their formation. Our findings reveal a significant role of Li in promoting epitaxial growth and horizontal alignment of films. Additionally, lithiation induces a vertical-to-horizontal reorientation in vertically aligned MoS_2 films. The measurements demonstrate long-term stability and preserved chemical composition of horizontally aligned Li-doped MoS_2.

[1] M. Sojková et al., Chem. Mater. 35, 6246 (2023).

MON 23
Experimental parameters that allow reliable determination and formation of atomic defects in single layer TMD's by TEM

Sophie Stolte[1,2], Moritz Quincke[1,2], Christopher Leist[1,2], Ute Kaiser[1,2]
[1]Institute for Quantum Optics, Ulm University, Ulm
[2]Central Facility Electron Microscopy, Ulm University, Ulm

Single-layer molybdenum disulfide (MoS2) is a semiconductor, which exhibits unique mechanical, optical and electronical properties promising for applications in integrated flexible electronics [1]. However, its usage strongly depends on the exact knowledge of the atomic defect structure, which can be determined by high-resolution TEM (HRTEM). HRTEM images allow quantifying damage cross-sections and assessing the defect development relative to the applied electron dose. In literature varying values were published [2-4] and the factors influencing the damage cross-section remain widely unclear.
Here, we employ spherical and chromatic aberration-corrected HRTEM to determine the damage cross-section. Diverse defect recognition algorithms are applied and compared. Besides, the impact of preparation techniques and defined external factors on the damage cross sections is evaluated, examining the diverse values for MoS2 published in the literature [2-4].

[1] Li et al., Nat Electron, 3, 711, (2020)
[2] Kretschmer, Lehnert et al., Nano Lett, 4, 2865, (2020)
[3] Speckmann et al., Phys. Rev. B, 107, 094112, (2023)
[4] Komsa et al., Phys. Rev. Lett., 109, 035503, (2012)

MON 24
Stacking 2D chalcogenides utilizing ALD

Sebastian Lehmann[1], Jun Yang[1], Dong-Ho Shin[1], Alejandra Garcia[1], Amin Bahrami[1], Kornelius Nielsch[1]
[1]IFW Dresden, Dresden

Chalcogenides, especially transition metal dichalcogenides (TDMCs, but also some other chalcogenides like SnS_2 and Sb_2Se_3) have a layered structure similar to

graphene, but instead of being a semimetal they offer a wide variety from semiconducting to conducting materials that are interesting for efficient, fast (and possibly flexible) electronics. Their electronic behavior can be strongly influenced by the thickness of the material.
With Atomic Layer Deposition (ALD) the layer stacking and individual layer thickness can be precisely controlled in the nm scale. Unlike other methods for the synthesis of 2D materials e.g. exfoliation, ALD is scalable which is an additional benefit for semiconductor industry and chip manufacturing companies.
We utilize ALD to deposit superlattice stacks of 2D materials with "spacing" materials in between to examine their electrical properties. An example is our fabrication of a superlattice consisting of SnS_2 and SbS_x via ALD but results on other systems including multilayers of SbO_x – Sb_2Te_3, Sb_2Te_3 - Sb_2Se_3 and other chalcogenides will be presented as well.

MON 25
Optical signatures of defects in hBN: comparing different calculation methods

Ludger Wirtz[1], Henry Fried[1], Daniel Barragan[1], Florian Libisch[2]
[1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg
[2]Institute for Theoretical Physics, Vienna University of Technology, Austria

Hexagonal boron nitride, both in its monolayer and bulk form, is recently receiving a lot of attention, not only as a flat and insulating substrate for other 2D materials, but also for its intrinsic optical properties in the UV range. The intrinsic luminescence spectrum of bulk hBN comprises four phonon-assisted peaks around 5.9 eV. However, various peaks at lower energy have been observed as well. These are related to the presence of defects. Besides, hBN is also being discussed as a material for single-photon emission.
We are pursuing different routes towards the calculation of optical signatures of defects in hBN. One route is the use of the GW+Bethe Salpeter approach, using supercells. Another route is the calculation of charge transition levels, which can be done by comparing total energies. We analyze the difference between charge transition levels, optical transition levels and the position of defect related quasi-particle states. For the calculation of the latter, we have developed a machine learning approach where we fit tight-binding parameters on the local density of states. With these parameters, we can then calculate quasi-isolated defects in large supercells.

MON 26
Micro-ARPES of exfoliated 2D antiferromagnets

Jeff Strasdas[1], Benjamin Pestka[1], Miłosz Rybak[2], Adam K. Budniak[3], Niklas Leuth[1], Honey Boban[4], Vitaliy Feyer[4], Iulia Cojocariu[4], Daniel Baranowski[4], José Avila[5], Pavel Dudin[5], Aaron Bostwick[6], Chris Jozwiak[6], Eli Rotenberg[6], Carmine Autieri[7], Yaron Amouyal[8], Lukasz Plucinski[4], Efrat Lifshitz[3], Magdalena Birowska[9], Markus Morgenstern[1]

[1]II. Institute of Physics B and JARA-FIT, RWTH-Aachen University, Aachen, Germany
[2]Department of Semiconductor Materials Engineering Faculty of Fundamental Problems of Technology Wrocław University of Science and Technology, Wrocław, Poland
[3]Schulich Faculty of Chemistry, Solid State Institute, Russell Berrie Nanotechnology Institute and Helen Diller Quantum Center, Technion – Israel Institute of Technology, Haifa, Israel
[4]Forschungszentrum Jülich, Peter Grünberg Institute (PGI-6), Jülich, Germany
[5]Synchrotron-SOLEIL, Université Paris-Saclay, Saint-Aubin, Paris, Gif sur Yvette, France
[6]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA
[7]International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
[8]Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel
[9]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

Exfoliated magnetic 2D materials enable versatile tuning of magnetization, e.g., by gating or providing proximity-induced exchange interaction. However, their electronic band structure after exfoliation has barely been probed, presumably due to their photochemical sensitivity. Here, we provide micron-scale angle-resolved photoelectron spectroscopy of the exfoliated intralayer antiferromagnet $MnPS_3$ above and below the Néel temperature down to one monolayer. Favorable comparison with density functional theory calculations enables identifying the orbital character of the observed bands. Consistently, we find pronounced changes across the Néel temperature for bands consisting of Mn 3d and 3p levels of adjacent S atoms. The deduced orbital mixture indicates that the superexchange is relevant for the magnetic interaction. There are only minor changes between monolayer and thicker films demonstrating the predominant 2D character of $MnPS_3$. The novel access has also been applied to other MPX_3 materials such as FePS3 and NiPS3 providing distinct antiferromagnetic arrangements.

MON 27

Acousto-Optoelectric Spectroscopy on Transition Metal Dichalcogenide Monolayer with Surface Acoustic Waves

Emeline Denise Sophie Nysten[1], Matthias Weiss[1], Benjamin Mayer[1], Tobias Petzak[2], Ursula Wurstbauer[1], Hubert Krenner[1]
[1]Physikalisches Institut, Universität Münster, Münster
[2]Lehrstuhl für Experimentalphysik 1, Universität Augsburg, Augsburg

Surface acoustic waves (SAWs) have proven to be a useful tool for the manipulation, control and probing of the charge carrier dynamics inside semiconductor nanostructures [1,2,3]. In this work, we integrated a monolayer of WSe_2 onto a $LiNbO_3$ SAW

device by an exfoliation process. Then, the impact of the SAW on the photoluminescence of the monolayer was systematically studied in the time domain. We observe a clear increase in the photoluminescence intensity of the monolayer as well as the previously not observed dynamic modulation of the emission by the 150MHz SAW. Both effects strongly depend on the position within the monolayer and prove a sensitivity to localisation and trapping sites, which are not resolved in static PL. This indicates that the SAW induced dynamics provide a powerful and sensitive tool to detect and investigate local variations in the dielectric and strain environment induced by the unavoidable inhomogeneities in 2D TMDCs.

[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 28
Optical dipole orientation of single photon emitters in MoS_2

Katja Barthelmi[1,2], Lukas Sigl[1], Tomer Amit[3], Mirco Troue[1], Thomas Klokkers[1], Anna Herrmann[1], Takashi Taniguchi[4], Kenji Watanabe[5], Sivan Refaely-Abramson[3], Alexander W. Holleitner[1,2]
[1]Walter Schottky Institut and Physik Department, Technical University of Munich, Garching, Germany
[2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany
[3]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Revohot, Israel
[4]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan
[5]Research Center for Electronic and Optical Materials, National Institute for Materials Science, Tsukuba, Japan

Single photon emitters in monolayer MoS_2 can be formed by helium ion irradiation. The irradiation results in defects with an emission energy of 1.75 eV and a high position accuracy [1-3]. To further understand the defects, we study their emission dipole orientation by back focal plane imaging. We find that the optical dipole of the quantum emitters is in-plane orientated. Additionally, we resolve the far-field emission pattern spectrally through back focal plane spectroscopy. The novel method allows us to also study emission lines of lower intensity.

[1] K. Barthelmi et al., in: Applied Physics Letters 117, 070501 (2020).
[2] J. Klein et al., in: Nature Communications 10, 2755 (2019).
[3] J. Klein and L. Sigl., in: ACS Photonics 8, 669-677 (2021).
[4] K. Barthelmi et al. (2024)

MON 29
Reducing disorder in MoS_2 nanotube and -ribbon quantum dots

Robin Schock[1], Jonathan Neuwald[1], Stefan Obloh[1], Konstatin Schneider[1], Matthias Kronseder[1], Matjaž Malok[2], Luka Pirker[2,3], Maja Remškar[2], Andreas K. Hüttel[1]
[1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg
[2]Solid State Physics Department, Jožef Stefan Institute, Ljubljana, Slovenia
[3]J. Heyrovský Institute of Physical Chemistry, v.v.i., Czech Academy of Sciences, Prague, Czech Republic

Extensive research is focused on planar TMDCs due to their exceptional electronic and optical characteristics, arising from their inherent two-dimensional structure. Despite many investigations into their optical behavior, achieving single-level transport in lithographic quantum dots at low temperatures, a crucial step towards quantum electronic devices, has faced challenges. These arise from the need for extremely small confinement potentials and the disorder introduced by dangling bonds at nanoflake edges.
A promising solution is the use of MoS_2 nanotubes, which can naturally confine electrons in the QDs, and avoiding Schottky barriers by utilizing bismuth as a contact material[1]. Our low temperature measurements clearly show that bismuth forms non-destructive and transparent contacts, indicating single level transport at temperatures below 100 mK[2]. To further reduce disorder we employ a novel dry transfer technique, using anthracene crystals as pick-up material[3]; we discuss different fabrication recipes.

[1]P.C. Shen et al., Nature 593, 211 (2021)
[2]R. T. K Schock et al., Adv. Mat. 35, 13 (2023)
[2]K. Otsuka et al., Nat. Commun. 12, 1 (2021)

MON 30
Scanning probe measurements of a MoS_2/hBN/graphene heterostructure

Katharina Nisi[1,2,3], John Thomas[3], Takashi Taniguchi[4], Kenji Watanabe[5], Alexander Weber-Bargioni[3], Christoph Kastl[1,2], Alexander W. Holleitner[1,2]
[1]Walter Schottky Institute and Physics Department, Technical University of Munich, Germany
[2]Munich Center of Quantum Science and Technology (MCQST), Germany
[3]Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, United States
[4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan
[5]Research Center for Functional Materials, National Institute for Materials Science, Japan

High-quality, atomically thin hBN has experienced growing importance as an insulating building block for 2D tunneling device structures, among others due to its

high breakdown field. Theoretical calculations and experimental measurements have demonstrated a large deviation between the measured and predicted hBN bandgap of up to 2 eV, which has been appointed to the large screening effects of the Coulomb interactions. Here, we present scanning probe measurements of a vertical metal-insulator-semiconductor device of monolayer MoS_2 on hBN suspended on epitaxially grown graphene. With scanning tunneling spectroscopy (STS), we demonstrate the impact of underlying graphene on the bandstructure of hBN and measure a huge bandgap renormalization from 6 eV (suspended) to 8 eV (free-standing). We observe the alignment of the CB onset to the CB of MoS_2 and the VB onset to the VB of hBN. Lastly, we compare these measurements to MoS_2 suspended directly onto graphene. There, we measure sulfur defects within MoS_2 in direct proximity to graphene and with an intermediate hBN layer, enabling the assessment of the screening effect of graphene.
1) K. Nisi *et al.*, in preparation

MON 31
Aspects of Raman spectroscopy in the fully quantum regime

Ado Jorio[1], Tiago A. Freitas[1,2], Lucas Valente[1], Diego Sier[1], Raul Corrêa[1], Marcelo F. Santos[3], Carlos H. Monken[1], Paula Machado[1,2], Filomeno S. de Aguiar Júnior[2], Christophe Galland[4], Riichiro Saito[4]
[1]UFMG, Belo Horizonte, Brazil
[2]IDOR, Rio de Janeiro, Brazil
[3]UFRJ, Rio de Janeiro, Brazil
[4]EPFL, Lausanne, Switzerland
[5]NTN University, Taipei, Taiwan

In this presentation the Raman scattering will be explored in the fully quantum regime, which means the Stokes and anti-Stokes scattered lights are analysed at the single photon level [1]. The dependence of correlation in energy, linear momenta, scattering time and polarization are studied, including analysis of entanglement based on state tomography and Bell´s inequality test. Entanglement is shown as a consequence of a priory indefinition between possible microscopic four-wave mixing processes, which can be phonon mediated (Raman) or purely electronic [2]. How this process differs when happening in a crystalline solid versus in liquids is also discussed.

[1] D. N. Klyshko, Sov. J. Quantum Electron 7, 755 (1977); [2] Freitas et al. Phys. Rev A 108, L051501 (2023).

MON 32
Exciton Polaritons vs Plasmons Polaritons: Nonlocal corrections, confinement and loss

Yonatan Gershuni[1,2,3,4], Itai Epstein[1,3,4]
[1]School of Electrical Engineering, Faculty of Engineering, Tel Aviv University, Israel

[2]School of Physics and Astronomy, Tel Aviv University, Israel
[3]Center for Light-Matter Interaction, Tel Aviv University, Israel
[4]QuanTAU, Quantum Science and Technology Center, Tel Aviv University, Israel

Interband-based VIS/NIR in-plane exciton polaritons in two-dimensional materials, such as transition-metal-dichalcogenides (TMDs), provide an excitonic alternative to plasmonic systems. We compare the properties of such in-plane exciton polaritons supported by monolayer TMDs to the equivalent configuration of SPPs supported by thin metallic films, known as the short-range-SPPs (SRSPPs). Taking into account both excitonic and plasmonic nonlocal corrections, which play a major role in large momentum modes, we find that in-plane exciton polaritons provide confinement factors that are an order of magnitude larger than those of SRSPPs, and with six times lower propagation losses. These properties make in-plane exciton polaritons promising candidates for VIS/NIR nanophotonics and strong light-matter interaction. In addition, we show a means of directional excitation of in-plane exciton polaritons thanks to their excitons' coupling with the valley degree of freedom in TMDs. Altogether our investigation provides an in-depth understanding of the physical nonlocal polaritonic properties of these excitonic modes.

MON 33

Explore polyynes properties by synchrotron-based Raman spectroscopy: from anharmonicity to electron-phonon coupling

Pietro Marabotti[1,2], Matteo Tommasini[3], Chiara Castiglioni[3], Sonia Peggiani[2], Barbara Rossi[4], Andrea Li Bassi[2], Valeria Russo[2], Sebastian Heeg[1], Carlo Spartaco Casari[2]
[1]Department of Physics, Humboldt-Universität zu Berlin, Berlin
[2]Micro and Nanostructured Materials Laboratory - NanoLab, Department of Energy, Milano, Italy
[3]Department of Chemistry, Materials and Chem. Eng. "G. Natta", Milano, Italy
[4]Elettra Sincrotrone Trieste, Trieste, Italy

Polyynes represent finite realizations of 1D linear chains with sp-hybridized CC bonds, displaying intriguing optoelectronic properties [1]. Raman spectroscopy is a powerful tool for exploring polyynes, providing insights into their bandgap, structure, electron-phonon coupling, and anharmonicity [2].
Our study delves into polyynes' vibrational and electronic properties using synchrotron-based UV resonance Raman spectroscopy. By analyzing the intensity and frequency modulations of the fundamental vibrational mode and its overtones, we extract the vibrational energy levels' fine structure [3]. Analysis of experimental Raman overtone bands indicates higher anharmonicity with increasing wire length, confirmed by DFT calculations [4]. We observed a length-dependent increase in π-electron conjugation and the Huang-Rhys factor, indicative of electron-phonon coupling, also influenced by specific terminations [3,4].
[1] C. S. Casari et al., Nanoscale, 2016, 8, 4414–4435
[2] A. Milani et al., Beilstein J. Nanotechnol., 2015, 6, 480–491

[3] P. Marabotti et al., Nat. Commun, 2022, 13, 5052
[4] P. Marabotti et al., Carbon, 2024, 216, 118503

MON 34
Morphology matters: The impact of thin film structure on electrical properties of PtSe2

Stefan Heiserer[1], Natalie Galfe[1], Markus Wolff[1], Nikolas Dominik[1], Kango Lee[1], George de Coster[1,2], Cormac Ó Coileáin[1], Paul Seifert[1], Georg S. Duesberg[1]
[1]Institute of Physics, Faculty of Electrical Engineering and Information Technology, University of the Bundeswehr Munich and SENS Research Center, Neubiberg, Germany
[2]DEVCOM Army Research Laboratory, Adelphi, Maryland, United States

Two dimensional materials have received increasing interest for next generation semiconductor applications. Among these materials, $PtSe_2$, a noble metal dichalcogenide, has more recently come to prominence. When thinned from bulk to monolayer, $PtSe_2$ undergoes a semimetal to semiconductor transition, making it a promising material for many applications, such as sensing devices. Numerous techniques can be used to produce $PtSe_2$ thin films, such as bottom-up methods like thermally assisted conversion (TAC) and top-down methods like mechanical exfoliation from bulk crystals. From large-area polycrystalline films to small-scale single crystals, various morphologies can be obtained.
In our study, we fabricate different $PtSe_2$ thin films and investigate their morphology. It is evident that the electrical properties of the devices are largely influenced by the material structure. Understanding these effects is crucial for material application and identifying the optimal synthesis approaches for different device types.

MON 35
Vibrations of liquids in low-dimensional confinement in Nanofluidic Channels

Charlotte Berrezueta Palacios[1], Mathieu Lizée[2], Lyderic Bocquet[2], Stephanie Reich[1]
[1]Physics, Freie Universität Berlin, Berlin, Germany
[2]Laboratoire de Physique de l'École Normale Supérieure, ENS, Université PSL,CNRS, Sorbonne Université, Université Paris Cité, Paris, France

Fluids confined at the manometer scale can drastically change their behavior compared to their bulk counterparts. Novel properties have been shown to emerge when fluids are restricted to dimensions lower than 10 nm. For a further understanding of the molecular dynamics in liquid transport, the vibrational properties must be further studied. In Addition, a tuneable platform where the geometry and environment can be controlled needs to be implemented. This can be achieved by nanofluidic devices formed by 2D channels assembled by van der Waals interactions.
Here we present a Raman study of the nanoconfinement's influence on the vibrational properties of water and selected organic components. We show the vibrational

modes of a two-dimensional bilayer graphene nanofluidic channel sandwiched between two hexagonal boron nitride flakes. We can identify the signal from the liquids inside the channels and analyze their surface interaction. We compare the Raman response of two liquids: glycerol and water inside the channels with respect to their bulk counterparts. Our study explores confinement effects arising when the wall spacing is reduced to 7 Å. These results provide an insight into nanofluidic transport.

MON 36
Magnetic anisotropy in excitonic resonances and exciton-phonon coupling of the 2D magnetic semiconductor CrSBr

Pierre-Maurice Piel[1], Florian Dirnberger[2], Nicolai-Leonid Bathen[1], Julian Klein[3], Zdenek Sofer[4], Ursula Wurstbauer[1]
[1]Institute of Physics, Muenster University, Germany
[2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden University of Technology, Dresden, Germany
[3]Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA
[4]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

The van der Waals material CrSBr comprises several intriguing characteristics: it is an optically active semiconductor and an air-stable 2D magnet with ferromagnetic ordering within each layer and antiferromagnetic coupling between adjacent layers. It has also a highly anisotropic electronic band structure, rendering it a quasi-one-dimensional electronic system [1].

In order to unravel the impact of magnetic order and magnetization direction on various aspects, including exciton-phonon coupling and collective excitations, we employ magnetic field-dependent photoluminescence and resonant Raman experiments around 4 Kelvin, below the Néel temperature.

We observe distinct differences for anti-ferromagnetic and ferromagnetic order in in the excitonic signatures from PL measurements and in resonant Raman spectra, both showing magnetic anisotropy for different crystallographic orientations. While the Raman-allowed first order phonon modes are unaffected by magnetization direction, new and well resolved magnetic-field dependent modes occur in the resonant-Raman spectra indicating strong exciton-phonon coupling.

[1] J. Klein et al. ACS Nano, 17, 5316-5328 (2023)

MON 37

Investigation of the interlayer coupling of twisted bilayer CVD-grown MoS_2 via Raman spectroscopy

Eileen Schneider[1], Narine Moses Badlyan[1], Yuri Koval[1], Janina Maultzsch[1]
[1]Department Physik, Friedrich-Alexander-Universität, Erlangen, Germany

Stacking two monolayers of TMDCs on top of each other with a twist angle introduces several novel phenomena as, e.g., the formation of moiré phonons and modifications of the band structure. In addition, the fabrication process and the twist angle both influence the coupling between the two layers. Here, this interlayer coupling will 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 few-layer systems. This is because the C exciton - in contrast to A and B excitons - expands over both layers and, therefore, couples the layers electronically. Taking well-coupled twisted MoS_2 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. In the next step we will test our results by using other TMDCs, e.g., $MoSe_2$, where the C exciton resonance can be studied using laser energies in the visible spectrum because of the smaller bandgap.

MON 38

Dominant 1/3-filling Correlated Insulator States and Orbital Geometric Frustration in Twisted Bilayer Graphene

Marc Bockrath[1], Haidong Tian[1], Emilio Codecido[1], Dan Mao[2], Kevin Zhang[2], Shi Che[1], Kenji Watanabe[3], Takashi Taniguchi[4], Dmitry Smirnov[5], Eun-Ah Kim[2,6,7,8], Chun Ning Lau[1]
[1]Department of Physics, Ohio State University, Columbus
[2]Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca NY, USA
[3]Research Center for Electronic and Optical Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan
[4]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan
[5]National High Magnetic Field Laboratory, Tallahassee FL, USA
[6]Radcliffe Institute for Advanced Study at Harvard, Harvard University, Cambridge MA, USA
[7]Department of Physics, Harvard University, Cambridge MA, USA
[8]Department of Physics, Ewha Womans University

A canonical example of geometric frustration is a triangular lattice with antiferromagnetic nearest neighbor spin coupling, which can lead to phases such as spin ices and spin liquids. Much less studied is geometric frustration based on orbital coupling. In our recent work, we have shown that incompressible states form at 1/3 fractional filling factors in twisted bilayer graphene at angles larger than the magic

one that are strongly dominant over integer fillings. These states persist in magnetic fields and display magnetic ordering signatures and tripled unit cell reconstruction. These results are in agreement with a strong-coupling theory based on Coulomb interactions between electrons occupying three-lobed Wannier orbitals, leading to symmetry-broken phases with distinct charge, spin, and valley order. Twisted bilayer graphene is therefore an excellent system to study orbitally geometrically frustrated systems.

MON 39

A Mechanosensitive Naphthalenophane as a Platform for Quantum Interference Studies

Sebastiaan van der Poel[1], Juan Hurtado-Gallego[2], Matthias Blaschke[3], Almudena Gallego[4], Migshen Li[1], Rubén López-Nebreda[2], Marcel Mayor[4], Fabian Pauly[3], Nicolás Agraït[2], Herre S. J . van der Zant[1]
[1]Kavli Institute of Nanoscience, Delft University of Technology, Delft
[2]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid
[3]Institute of Physics and Centre for Advanced Analytics and Predictive Sciences, University of Augsburg, Augsburg
[4]Department of Chemistry, University of Basel, Basel

Mechanically induced destructive quantum interference is a feature known to be found in certain paracyclophane structures. When such structures are prone to mechanical deformation, a particular configuration of the molecule can be probed, in which the frontier orbitals of the molecule overlap in such a way that the conductance is significantly suppressed. Using Mechanically Controlled Break-Junction (MCBJ) or Scanning Tunneling Microscopy Break-Junction (STM-BJ) techniques this quantum interference dip can be probed at room temperature and shows up in modulation experiments where the electrode separation distance is periodically increased and decreased (stretching and compressing the molecule), after which those individual dips can be used for statistical analysis. Here, we present the study of a naphthalenophane. Due its rigidity and high conductance it provides a versatile platform to not only study the mechanical dependence of the destructive quantum interference, but also for simultaneous thermoelectric measurements (using STM-BJ) and measurements at low temperatures (using MCBJ).

MON 40

Photo-induced charge and spin transfer in the heterostructure CrSBr/$MoSe_2$

Andreas Beer[1], C. Serati de Brito[1,2], K. Zollner[1], T Taniguchi[3], K. Watanabe[3], H. S. J. van der Zant[4], Y. Galvao Gobato[2], C. Schüller[1,3]
[1]Experimental and applied physics, University of Regensburg, Regensburg
[2]Universidade Federal de São Carlos
[3]National Institute for Materials Science
[4]Delft University of Technology

Van der Waals (vdW) heterostructures composed of two-dimensional (2D) transition metal dichalcogenides (TMD) and vdW magnetic materials offer an intriguing platform to functionalize valley and excitonic properties in non-magnetic TMDs. This Here, we report a two-color pump probe investigation of monolayer (ML) $MoSe_2$ on the layered A-type antiferromagnetic (AFM) semiconductor CrSBr.

The material combination is predicted to feature a type III band alignment (broken bandgap), which leads to an p-doping in $MoSe_2$. By an ultrafast pump pulse, we can create free electrons in CrSBr. They can tunnel to $MoSe_2$ and reduce the background doping. This we detect by enhancement (reduction) of the reflectivity of the exciton (trion).

Remarkably by pumping the heterostructure with circular polarized light we can observe the Kerr effect in $MoSe_2$. We explain our results by tunneling spins from CrSBr to $MoSe_2$ and an out of plane spin component in the first layer of CrSBr.

MON 41
Phonon-assisted Auger recombination in a solid-state quantum emitter

B. Maib[1,2], M. Zöllner[1], H. Mannel[1], F. Rimek[1], A. Ludwig[3], A. D. Wieck[3], M. Geller[1], A. Lorke[1]
[1]Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany
[2]Present address: Chair of Experimental Physics, Friedrich-Alexander-University, Erlangen, Germany
[3]Chair of Applied Solid State Physics, Ruhr University Bochum, Bochum, Germany

The Auger recombination is a scattering effect, where the transition energy can be transferred to a third charge carrier (non-radiative Auger) or to charge carrier and another photon (radiative Auger). Besides spin- and charge noise and the photoeffect, it can be another source of decoherence in a solid-state quantum emitter that should be minimized to realize, for instance, a high-fidelity spin-photon interface. We have observed another electron-electron and phonon scattering effect in a self-assembled quantum dot: Phonon-assisted Auger recombination, where a phonon is absorbed or emitted before the electron emission occurs via the nonradiative Auger recombination of the trion transition. We were able to measure with high-accuracy the electron emission rate by the Auger recombination using time-resolved resonance fluorescence measurements. Near the trion transition we clearly observe the acoustic phonon sideband at a temperature of 4 K in such an absorption experiment. At high laser intensities in pulsed quantum state preparation and measurement schemes, it could have a significant influence on the coherence of the spin and photon state.

MON 42
Valley Polarization of the 5-8-5 graphene line defect

Siyar Duman[1], Christoph Schattauer[1], Florian Libisch[1]
[1]Institute for Theoretical Physics, Vienna University of Technology, Vienna

In recent years many proposals for the manipulation of the valley degree of freedom of graphene have been presented. One candidate, the set of line defects in graphene, has been observed and synthesized in experiment [1] and analytical calculations predict the valley-filtering property [2]. We perform tight binding simulations of the graphene 5-8-5 line defect embedded in a ribbon accurately parametrized from DFT [3]. We find two distinct valley polarization phenomena dependent on the angle of incidence and energy: (i) Sharp and almost perfect valley polarization peaks at energies coincidental with boundstates of the line defect, akin to Fano resonances. (ii) An energy interval within which valley polarization is linear as a function of the angle of incidence. The latter observation was predicted earlier by a nearest-neigbor tight-binding model and symmetry arguments. Our more realistic simulations confirm such behavior for realistic line defects - albeit only for a narrow energy region. Valley filtering properties of line defects could thus be a key step towards valleytronic applications.

[1] Nature Nanotech 5, 326–329
[2] PRL 106.13 136806
[3] npj. Comp. Mat. 8, 116

MON 43
Hyper-gap optical materials

Zhengran Wu[1,2], Xiaolei Hu[1,2], Kun Chen[1,2], Zhilin Li[1], Ling Lu[1]
[1]Institute of Physics, Chinese Academy of Sciences, Beijing
[2]School of Physical Sciences, University of Chinese Academy of Sciences

Optical materials largely refer to transparent insulators and semiconductors for guiding, diffracting, and nonlinearly-generating light at photon energies below the electronic bandgaps. Here we show that a solid can be equally lossless above the fundamental bandgap inside an energy interval dubbed the hyper-gap, in a class of crystals consisting of well-isolated conduction and valence bands. The optics within the hyper-gap can completely defy the conventional rules and limits, including the low-loss negative permittivity unavailable in metals for plasmonic metamaterials, the anomalous-dispersion phase-matching in isotropic bulks without birefringence nor periodic patterns for nonlinear and quantum optics, as well as the negative group-velocity dispersion from the visible to the deep-ultraviolet unattainable in known dielectrics for ultrafast optics. We perform high-throughput searches among all existing inorganic materials and discover over 200 hyper-gap candidates, that could potentially transform optics with unexplored material opportunities.

MON 44
Photoluminescence as a predictive measure for the optical quality of monolayer semiconductors

Matan Meshulam[1]
[1]Electrical Engineering, Tel Aviv University, Tel Aviv

Monolayer semiconductors, such as transition-metal-dichalcogenides (TMDs), support robust excitons in the visible to near-infrared spectrum. One of the most important characteristics of the quality of the optical response of these excitons is reaching their homogeneous linewidth. However, the latter is broadened by various effects that increase with temperature, owing to interaction with phonons. Since monolayer TMDs and their heterostructures are fabricated at room temperatures, the only way to actually know the quality of the exciton's optical response is to perform spectroscopic measurements at low temperature (4-10K). In this work, we have developed a new approach for predicting the optical quality of TMD excitons through the analysis of two-dimensional PL imaging at room temperature, thereby eliminating the need to perform low temperature spectroscopic measurements. The approach provides a valuable tool for the prediction of the physical and optical properties of monolayer TMDs and their heterostructures in a fast and straightforward manner.

MON 45

New interlayer excitons in 2D bilayers revealed under strong electric field

S. Kovalchuk[1], K. Greben[1], A. Kumar[1], S. Pessel[1], J. Soyka[2], Q. Cao[2], K. Watanabe[3], T. Taniguchi[3], D. Christiansen[4], M. Selig[4], A. Knorr[4], S. Eigler[2], K. I. Bolotin[1]
[1]Physics Department, FU Berlin, Berlin
[2]Institute of Chemistry and Biochemistry, FU Berlin, Berlin
[3]National Institute for Materials Science, Tsukuba, Japan
[4]Physics Department, TU Berlin, Berlin

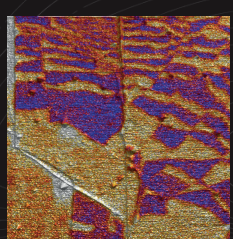
Excitons in bilayer transition metal dichalcogenides (2L-TMDs) are Coulomb-bound electron/hole pairs that can be viewed as broadly tunable analogs of atomic or molecular systems. Here, we study the properties of 2L-TMD excitons under a strong electric field. To overcome the field limit reached in previous experiments, we developed a new organic/inorganic molecular gating technique. This approach allows us to achieve an electric field strength of about 0.35 V/nm, more than a factor of two higher than achieved previously in purely solid-state gated devices. Under this field, inter- and intralayer excitons are brought into an energetic resonance, allowing us to discover new emergent properties of the resulting states. We detect a previously unseen interlayer exciton that only becomes visible at high electric field through hybridization with A exciton. Moreover, the system experiences an ultrastrong Stark splitting of $>$ 380 meV with exciton energies tunable over a large range of the optical spectrum, holding potential for optoelectronics. Our work paves the way for using strong electric fields to study new physical regimes and control exciton hybridization in 2D semiconductors.

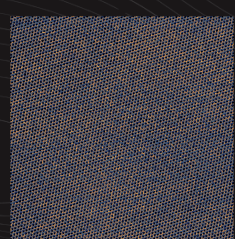
DriveAFM

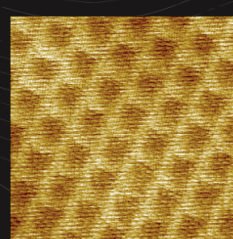
Performance without Compromise

What makes DriveAFM unusual?

- Versatility in all dimensions: Sample, scan size, mode, experience level, software.
- Sample-independent performance with Nanosurf's high performance tip-scanner.
- Python scripting: Freedom to develop and create with low-level coding access.
- The AFM pioneer's choice: A perfect playground for mode development.
- Future proof: Designed to grow with nanotechnology advancements.
- Nanosurf Studio Software: Configurable workspace, new features each quarter.







Nanosurf AG
Gräubernstr. 12-14
4410 Liestal
Switzerland

nanosurf.com/DriveAFM

nanosurf

08:30 – 09:00	U. Wurstbauer, Rome *Moiré Minibands, Twist Disorder and Exciton-Phonon Coupling in van der Waals Stacks*
09:00 – 09:30	L. Baldassarre, Rome *Resonance Raman Spectroscopy with Infrared Excitation Energy on Graphene and TMDs*
09:30 – 10:00	E. Malic, Marburg *Ultrafast Charge Transfer Dynamics in van der Waals*
10:00 – 10:30	Coffee Break
10:30 – 11:00	A. Loiseau, Chatillon *Excitonic Properties in Hexagonal Boron Nitride and BN/BN Homostructures*
11:00 – 11:30	Y. Kato, Japan *Exciton Physics and Cavity Quantum Electrodynamics in Air-Suspended Carbon Nanotubes*
11:30 – 12:00	O. Yaffe, Rehovot *Raman Scattering from Disordered Single Crystal*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	Carlo S. Casari, Milano *Electronic and Vibrational Properties of 2D Carbon Materials Beyond Graphene*
19:00 – 19:30	L. Classen, MPI-FKF/TUM *Field Control of Many-Body Phases in Frustrated Moiré Bilayers*
19:30 – 20:00	G. Schleder, Campinas *Machine Learning for 2D Materials Discovery and Design: Topological Insulators and Multi-System Moiré Assemblies*

08:30

Moiré Minibands, twist disorder and exciton-phonon coupling in van der Waals stacks

Hendrik Lambers[1], Nihit Saigal[1], Nicolai-Leonid Bathen[1], Velko Antic[1], Lennart Klebl[2], Dante M. Kennes[3,4], Tim O. Wehling[2], Ursula Wurstbauer[1]
[1]Institute of Physics, Münster University, Münster, Germany
[2]Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany
[3]Institute for Theory of Statistical Physics, RWTH Aachen University, and JARA Fundamentals of Future Information Technology, Aachen, Germany
[4]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg, Germany

The weak van der Waals coupling between layers of most two-dimensional (2D) materials allows the realization of precisely tailored 2D quantum systems. Heterobilayers of transition-metal dichalcogenides such as MoSe2/WSe2 host dense ensmebles of interlayer excitons potentially forming a coherent many-body state at low temperature [1-2]. Moreover, twisted homobilayers such as tWSe2 are prone to the formation of moiré minibands. Guided by theoretical predication, we study tWSe2 homobilayer encapsulated in hBN by low-temperature resonant inelastic light scattering (RILS). We find resonant modes interpreted as single-particle collective intermoiré-band excitations (IMBE) allowing to quantitatively probe the formation of a series of moiré-bands [3]. Moreover, we find that the resonance profiles particularly of the degenerated WSe2 A1'/E' phonon modes are significantly impacted by the assembly in vdW stacks suggesting a higher order Raman scattering process presumably involving simultaneous excitation and annihilation of phonon-modes with finite momentum. [1] L. Sigl et al. PPRL 2, 042044(R) (2020). [2] M. Troue et al., PRL. 131, 036902 (2023). [3] N. Saigal et al. arXiv:2310.14417.

09:00

Resonance Raman Spectroscopy with infrared excitation energy on graphene and TMDs

Leonetta Baldassarre[1]
[1]Department of Physics, Sapienza University of Rome, Rome Italy

Raman spectroscopy has been a key asset to study the electronic and vibrational properties of graphene and other two-dimensional materials that display Raman spectra composed of first order modes together with narrow second-order double resonant modes arising from intervalley or intravalley scattering. Notably, by changing the excitation laser energy, different regions of the electron and phonon dispersions can be probed. In this presentation I will discuss our experimental approach to study the competing low-energy interactions in these systems by lowering the excitation energy and leveraging on Raman processes resonant with electronic states in the infrared. The development of the experimental setup will be discussed together with results on $MoSe_2$ and $MoTe_2$. At last I will present our results on graphene where, thanks to the excitation energy close to the Dirac point at K, we find a giant increase of the intensity ratio between the double-resonant 2D and 2D' peaks. By comparing to ab-initio calculations, we explain our experimental observation by an enhanced, momentum-dependent electron-phonon coupling between electrons and zone-boundary optical phonons.

09:30
Ultrafast charge transfer dynamics in van der Waals
Ermin Malic[1]
[1]Fachbereich Physik, Philipps-Universität Marburg, Marburg

Transition metal dichalcogenides (TMDs) exhibit a rich exciton landscape. Recent experiments have demonstrated an ultrafast charge transfer in TMD heterostructures. However, the nature of the transfer process has remained elusive. Based on a microscopic theory combined with ARPES measurements, we reveal that phonon-mediated scattering via hybridized dark excitons governs the charge transfer. We track the time- and momentum-resolved relaxation dynamics of optically excited excitons and determine the temperature- and stacking-dependent charge transfer times. Furthermore, we find an unexpected increase of the photoelectron energy in ARPES upon a hole transfer process across the interface. This is surprising, as the electron remains rigid in the conduction band during the hole transfer, and since any relaxation mechanism typically leads to energy dissipation. However, we do not observe a free electron, but the blue-shift is a direct consequence of the correlated nature of the Coulomb-bound electron-hole-pair. The provided insights present an important step forward in microscopic understanding of the technologically important charge transfer process in TMD heterostructures.

10:30
EXCITONIC PROPERTIES IN HEXAGONAL BORON NITRIDE AND BN/BN HOMOSTRUCTURES

A. Loiseau[1], S. Roux[1,2], E. Carré[1,2], L. Ren[3], C. Robert[3], F. Fossard[1], F. Ducastelle[1], X. Marie[3], J. Barjon[2]
[1]Université Paris-Saclay, ONERA-CNRS, LEM, 92320 Châtillon, France
[2]Université Paris-Saclay, UVSQ, CNRS, GEMaC, 78000, Versailles, France
[3]Université de Toulouse, INSA-CNRS-UPS, LPCNO, 31077 Toulouse, France

This talk will review the latest developments we have performed, on the study of excitonic properties in hexagonal boron nitride thanks to a new time-resolved (TRCL) system dedicated to the UV range. First we have provided a first estimate at 27 ns of the radiative life time of free excitons emitting at 215 nm from a single experiment comparing hBN crystals issued from different synthesis routes. This was done by measuring, for each sample, both the internal quantum yield and the exciton life time. The estimate is much shorter than in other indirect bandgap semiconductors, that we will discuss as accounting for the unusual high luminescence efficiency of this material [1]. Second, we have studied the excitonic luminescence arising at 4 eV at the interface between two disoriented BN flakes. The exciton properties are investigated by exploring their luminescence dynamics in TRCL as a function of twist angle and temperature. Analysing the temporal decay of free excitons emitting at 215 nm reveals their trapping and detrapping from the interface, which is shown to be thermally activated [2]. [1] S. Roux et. Al., Phys. Rev. B 104, L161203 (2021) [2] S. Roux et al, submitted (2023)

11:00

Exciton physics and cavity quantum electrodynamics in air-suspended carbon nanotubes

Yuichiro K. Kato[1,2]
[1]Nanoscale Quantum Photonics Laboratory, RIKEN Cluster for Pioneering Research, Japan
[2]Quantum Optoelectronics Research Team, RIKEN Center for Advanced Photonics, Japan

Electron-hole pairs form tightly-bound excitons in carbon nanotubes due to limited screening of the Coulomb interaction, and there exist various dark states with optical transitions forbidden by spin, momentum, and parity selection rules. By studying the dynamics and diffusion properties of the bright excitons and the even-parity dark excitons, we find that more than half of the dark excitons can be transformed into the bright excitons [1]. Silicon photonic crystal nanobeam cavities can be used to induce cavity quantum electrodynamical effects [2], and we take advantage of the Purcell enhanced decay rate to determine the radiative quantum efficiency of bright excitons to be near unity at room temperature [3]. With high-efficiency light emission and single-photon generation capabilities, carbon nanotubes offer new opportunities in nanoscale quantum photonics.

Work supported in part by MIC (SCOPE JP191503001), JSPS (KAKENHI JP20H02558, JP23H00262), and MEXT (JPMXP09F21UT0006).

[1] A. Ishii $et\ al.$, Phys. Rev. X 9, 041048 (2019).
[2] R. Miura $et\ al.$, Nat. Commun. 5, 5580 (2014).
[3] H. Machiya $et\ al.$, Phys. Rev. Research 4, L022011 (2022).

11:30
Raman scattering from disordered single crystals
Omer Yaffe[1]
[1]Weizmann Institute, Rehovot

In recent years, my team and I have studied the structural dynamics of halide, oxide, and sulfide perovskite crystals, employing THz-Range Raman scattering as our primary investigative tool. The study of perovskite crystals is particularly intriguing due to their display of numerous anharmonic phenomena. These include soft modes, phase transitions, and local fluctuations, all of which influence the crystals' electronic characteristics. Such characteristics include dielectric response, carrier lifetimes, and carrier mobilities. One notable aspect of these anharmonic effects is their ability to relax the strict selection rules for Raman scattering, which are based on the symmetry of the crystal's unit cell. This relaxation results in Raman spectra that are challenging to interpret due to their complexity, yet they are simultaneously rich sources of information about the crystal properties.
In this talk, initially, I will highlight a discrepancy between data from x-ray diffraction, which typically indicates perfectly structured single crystals, and the Raman data, which suggests the presence of disorder. Following this, I will detail how we employ generalized scattering.

18:30

Electronic and Vibrational Properties of 2D Carbon Materials Beyond Graphene

Carlo S. Casari[1], P. D'Agosta[1], F. Tumino[1,3], J. Lobo Checa[2], L. Petaccia[4], G. Di Santo[4], V. Russo[1], A. Li Bassi[1], A. Orbelli Biroli[5], S. Achilli[6]
[1]Department of Energy, Politecnico di Milano, Italy
[2]INMA - Instituto de Nanociencia y Materiales de Aragón, Universidad de Zaragoza Spain
[3]Department of Physics, Engineering Physics and Astronomy, Queen's University, Canada
[4]Elettra Sincrotrone Trieste, Italy
[5]Department of Chemistry, Università di Pavia, Italy
[6]Department of Physics, Università di Milano, Italy

Graphdiynes forming a network of sp and sp^2 hybridized carbon atoms represent a class of 2D carbon materials beyond graphene [1]. Different 1D and 2D structures have been produced by on-surface synthesis on Au(111) and Ag (111) [2-5]. Here we investigate the vibrational and electronic properties of graphdiyne nanoribbons [2,5] and 2D graphdiyne-like extended networks [3,4]. By in situ scanning tunneling microscopy and spectroscopy (STM/STS), Raman spectroscopy, and density functional theory (DFT) simulations we show how the properties are affected by the metal substrate. The extended and well-ordered metallorganic graphdiyne-like structure on Ag(111) allowed to investigate the electronic bandstructure by synchrotron-based angle resolved photoemission spectroscopy (ARPES) revealing characteristic valence bands of the network.

[1] P. Serafini et al. J. Phys Chem C 125, 33, 18456-18466 (2021)
[2] A. Rabia et al. Nanoscale, 11, 18191 (2019)
[3] A. Rabia et al. ACS Appl. Nano Mater. 3, 2178 (2020)
[4] S. Achilli et al. 2D Materials 8 044014 (2021)
[5] S. Achilli et al. Phys. Chem. Chem. Phys. 24, 13616 (2022)

19:00
Field control of many-body phases in frustrated moiré bilayers
Lorenzo Del Re[1], Laura Classen[1,2]
[1]Max Planck Institute for Solid State Research
[2]Technical University of Munich

We determine the ground states and excitation spectra of the paradigmatic four-flavour Heisenberg model with nearest- and next-nearest-neighbor exchange couplings on the triangular lattice in a field controlling the flavor-imbalance. Such a system arises in the strongly correlated limit of moiré bilayers of transition metal dichalcogenides in an electric or magnetic field, and can be simulated via ultracold alkaline-earth atoms. We argue that the field tunes between effective SU(4) and SU(2) symmetries in the balanced and fully polarised limits and employ a combination of mean-field calculations, flavour-wave theory, and exact diagonalisation to analyse the imbalanced regime. We find different symmetry-broken phases with simultaneous spin and excitonic order depending on the field and next-nearest-neighbor coupling. Furthermore, we demonstrate that there is a strongly fluctuating regime without long-range order that connects candidate spin liquids in the SU(2) and SU(4) limit. The strong fluctuations are facilitated by an extensive classical degeneracy, and we argue that they are also responsible for a strong polarisability at 1/3 polarisation.

19:30

Machine Learning for 2D Materials Discovery and Design: topological insulators and multi-system moiré assemblies

Gabriel R. Schleder[1,2]
[1]Brazilian Nanotechnology National Laboratory (LNNano/CNPEM), Campinas, Brazil
[2]School of Engineering and Applied Sciences, Harvard University

One of the main goals and challenges of materials discovery is to find the best candidates for each interest property or application. Machine learning rises in this context to efficiently optimize this search, exploring the immense materials space, consisting of simultaneously the atomic, compositional, and structural spaces. For many applications, further development is limited by the scarcity of viable candidates. Here we present and discuss two machine learning–accelerated strategies for searching the materials space for two-dimensional materials. The first employs the power of available databases for creating predictive models capable of determining the electronic topology of materials, with an accuracy of over 90% [1]. The second demonstrates how active learning can greatly accelerate data collection when no data is available a priori, showing electronic tunability of twisted assemblies with different materials and layers [2].

[1] G. R. Schleder, B. Focassio, and A. Fazzio, *Appl. Phys. Rev.* 8, 031409 (2021).
[2] G. A. Tritsaris, S. Carr, and G. R. Schleder, *Appl. Phys. Rev.* 8, 031401 (2021).

HÜBNER Photonics

Coherence Matters.

08:30 – 09:30	TOTORIAL: M. Hersam, Evanston *Boron in the 2D Limit: Borophene, Borophane, and Beyond*
09:30 – 10:00	B. Liu, Shenzhen *Mass-production of two-dimensional h-BN and its liquid crystals for deep UV light modulation*
10:00 – 10:30	Coffee Break
10:30 – 11:00	A. MORPURGO, Geneva *A new generation of ionic liquid gated devices*
11:00 – 11:30	T. Knobloch, Vienna *Gate Insulators for 2D Semiconductor-Based Field Effect Transistors*
11:30 – 12:00	G. Duesberg, Neubiberg *Versatile 2D material surface functionalization with organic adlayers*
12:00 – 17:00	Mini Workshops
17:00 – 18:30	Dinner
18:30 – 19:00	A. Bachtold, Barcelona *The sound of tiny guitars approaching the quantum regime*
19:00 – 19:30	I. Epstein, Tel Aviv *Novel Polaritonic Phenomena in 2D Materials*
19:30 – 20:00	R. Hillenbrand, San Sebastian *THz nanoscopy of ultraconfined in-plane anisotropic plasmon polaritons*
20:00	Poster III

08:30
Boron in the 2D Limit: Borophene, Borophane, and Beyond
Mark C Hersam[1]
[1]Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA

The experimental realization of 2D boron (i.e., 'borophene') has spurred broad interest in its unique material attributes such as in-plane anisotropy, high mechanical strength and flexibility, massless Dirac fermions, and charge density wave phenomena. This presentation will explore the ultrahigh vacuum synthesis and atomic-scale characterization of borophene. In addition to distinct borophene polymorphs, conditions for forming self-assembled intermixed phases, superlattices, bilayers, and nanoribbons will be delineated. By exploiting spatially inhomogeneous surface chemistry, seamless 2D heterointerfaces are realized between borophene and other materials including organic semiconductors, graphene, and graphene nanoribbons, each of which show atomically sharp electronic interfaces as confirmed by scanning tunneling microscopy and spectroscopy. To further control the properties of 2D boron, covalent hydrogenation results in a series of 'borophane' polymorphs with tunable work function and high chemical stability in ambient conditions. Overall, this work establishes a series of design rules for integrating 2D boron into a range of nanoelectronic and quantum technologies.

09:30

Mass-production of two-dimensional h-BN and its liquid crystals for deep UV light modulation

Bilu Liu[1]
[1]Shenzhen International Graduate School, Tsinghua University, Shenzhen

Light modulation is important for optical devices. For example, liquid crystal based display is a typical light modulation technology with a global annual market over 100 billion US dollars. Nevertheless, modulation of light at extreme wavelengths like deep UV (wavelength <300 nm) is challenging despite its importance in many applications. Current technologies cannot do it because the widely-used organic liquid crystal molecules are not stable under deep UV light, and birefringence of inorganic crystals is difficult to be tuned by external fields. In this talk, I will discuss our recent work on the fabrication of a stable and tunable deep UV light modulator by using 2D h-BN. The ultra-wide optical bandgap, high stability in deep UV, and large optical anisotropy factor resultant sensitive magnetic-field response, collectively making 2D h-BN an ideal candidate for stable and continuous deep UV light modulation. Such 2D h-BN can be produced in large quantities by scaled top-down exfoliation technologies, suggesting its clear potential for practical uses.

10:30
A new generation of ionic liquid gated devices
Alberto Morpurgo[1]
[1]University of Geneva, Geneva

I will discuss results on ionic liquid gated devices based on 2D tranistition metal dichalchogenides, to illustrate a number of important recent developments. These include the ability to perform quantitative spectroscopic measurements of the band structure of 2D semiconductors (i.e., the quantiative determination of the band gap and of band offsets) and of their quantum capacacitance (with quantum capacitance effects that dominate the total capacitance, because of the extremely large geometrical capacitance of ionic liquid gates). On the technical side, a key development is the introduction of Li-ion glass substrates solid electrolytes, which allow ionic gating at electron denisties larger than 10^{14} cm^{-2} without covering the top of the 2D material, and allow new types ofexperiments. I will discuss one of them, namely the realization of double ionic gated devices, which allow the indepenent control of electron density and perpendicular electric field. I will show that in these devices perpendicular electric fields as large as 3 V/nm can be applied, sufficient to quenche the 1.65 eV band gap of bilayer WSe_2

11:00
Gate Insulators for 2D Semiconductor-Based Field Effect Transistors
Theresia Knobloch[1]
[1]Institute for Microelectronics, TU Wien, Vienna

Two-dimensional (2D) semiconductors, for example, transition metal dichalcogenides (TMDs), provide in their monolayer form sizable carrier mobilities and enhanced gate control when used as a channel material in ultrascaled field-effect transistors (FETs). In this way, TMD channels could offer performance gains over silicon channels in ultra-scaled technology nodes with gate lengths approaching 10nm in complementary FETs. However, to allow for fast, stable, and reliable transistor operation, scaled gate insulators are required to form high-quality interfaces with small densities of interface traps. Up to now, a variety of potential gate insulators have been suggested, including amorphous oxides, like HfO_2, Al_2O_3 or ZrO_2, layered insulators, like h-BN, layered zipper materials, like mica or Bi_2SeO_5, ionic crystals, like CaF_2, or perovskites, like $SrTiO_3$, but so far none of these candidates can live up to the multitude of requirements. Here, we will analyze the trade-offs in their material properties and discuss the most critical fabrication requirements, highlighting the most promising gate insulators for ultrascaled FETs.

11:30
Versatile 2D Material Surface Functionalization with Organic Adlayers
Georg S. Duesberg[1]
[1]Institute of Physics & FZ SENS, University of the Bundeswehr Munich, Neubiberg

The surface chemistry of 2D materials an intriguing field, as it goes hand in hand with the modification of the entire 2D layer. However, strategies for the reliable functionalization are still in infancy, in particular because of detrimental polymeric residues on 2D material surfaces. We have identified ubiquitously hydrocarbon adlayers on 2D materials form storage conditions besides residues from transfer processes. [1] This has been revealed by a comprehensive TOF-SIMS investigation of various TMD materials. On the other hand we have developed a robust method for non-covalent functionalization of 2D materials. The functional layer is applied to pristine as-grown 2D materials layers, avoiding detrimental effect due to contaminations. Examples for the modification MoS2 mono and double layers with these self-assembled monolayers will be shown. As for graphene these well define adlayers allow the attachment of antibodies for the specific sensing of small bio-active molecules. [2] These selective layers are highly attractive selective sensor arrays based on graphene.

[1] Tilman et al. ACS Nano 2023, 17, 11, 10617–10627
[2] von Lüders et al. Angew. Chemie 62, 22, 2023

18:30
The Sound of Tiny Guitars Approaching the Quantum Regime
Adrian Bachtold[1]
[1]ICFO, Barcelona

Mechanics has historically played a pivotal role in science by providing the basis for classical physics. Today, with the advent of nanoscale mechanical devices combined with quantum electronic devices, we are witnessing a renaissance in the field of mechanics. Here, I will discuss our recent advances on mechanical resonators based on carbon nanotubes. The nanotube in these devices vibrates as a guitar string. Single-electron tunneling enables coupling the mechanical vibrations to electrons by a large amount. I will show how to use this coupling to create a nonlinear mechanical oscillator approaching the quantum regime, where the resulting quantum energy levels of the mechanical oscillator are no longer evenly spaced [1]. I will also discuss our effort towards the first realization of a mechanical qubit, following the proposal in [2].

[1] C Samanta, SL De Bonis, CB Møller, R Tormo-Queralt, W Yang, C Urgell, B Stamenic, B Thibeault, Y Jin, DA Czaplewski, F Pistolesi, A Bachtold, Nature Physics 19, 1340 (2023).
[2] F. Pistolesi, A.N. Cleland, and A. Bachtold, Phys. Rev. X 11, 031027 (2021).

19:00
Novel Polaritonic Phenomena in 2D Materials
Itai Epstein[1]
[1]School of Electrical Engineering, Tel Aviv University, Tel Aviv, Israel

Polaritons, i.e. coupled light-matter quasi-particles in the form of optical excitations, play a major role in nanophotonics owing to their ability to control, confine and enhance light at the nanoscale. In 2D materials, polaritonic phenomena are abundant and unique owing to their low dimensionality and the extraordinary properties of the supported quasi-particles. In this talk, I will discuss basic aspects of polaritons, their manifestation in 2D materials, and our prediction of novel polaritons based on excitonic response.

19:30

THz nanoscopy of ultraconfined in-plane anisotropic plasmon polaritons

Rainer Hillenbrand[1]
[1]CIC nanoGUNE BRTA, San Sebastian

We discuss ultraconfined in-plane anisotropic THz plasmon polaritons on monoclinic Ag2Te platelets, observed by polariton interferometry with a scattering-type scanning near-field optical microscope (s-SNOM) [1]. Ag2Te is a narrow-bandgap semiconductor, where the effective masses of the charge carriers exhibit strong anisotropy. By placing the platelets above a Au layer, we achieve hybridization of the plasmon polaritons with their mirror image, yielding acoustic plasmon polaritons (APPs), which increases the direction-dependent relative polariton propagation length and the directional polariton confinement. Importantly, the in-plane anisotropy of the polariton propagation is qualitatively retained and the increased APP propagation lengths reveal an elliptical isofrequency contour in the wavevector space. By crystal structure analysis using STEM, we can explain the rather symmetric (elliptical) polariton propagation along the monoclinic (thus low-symetry) Ag2Te crystal. We finally demonstrate how the elliptical APPs can be exploited for measuring in-plane anisotropic effective carrier masses.

[1] S. Chen et al, Nat. Mater. 22, 860 (2023)

WED 1
Mechanically Stable Kondo Resonance in an all-Organic Radical Single Molecule Junction

Tristan Bras[1], Thomas Y. Baum[1], Chunwei Hsu[1], David Vogel[2], Marcel Mayor[2], Herre S. J. van der Zant[1]
[1]Quantum Nanoscience, Delft University of Technology, Delft
[2]Department of Chemistry, University of Basel, Basel, Switzerland

We studied electronic transport in all-organic neutral mono-radicals. These molecules are promising candidates for applications in molecular spintronics due to their intrinsic magnetic moment, their low spin-orbit coupling and their weak hyperfine interactions. We analyse the difference in charge transport between two Nitronyl-Nitroxide Radicals (NNR); one with a backbone in the para configuration and the other with a backbone in the meta configuration. We find that the para-NNR displays a Kondo resonance at 6 K, while the meta-NNR does not. Additionally, the observed Kondo peak width in the differential conductance is roughly constant, independent of the conductance through the molecule, consistent with a scenario where the molecule is coupled asymmetrically to the electrodes. This asymmetric configuration is stabilized by the nitronyl nitroxide group, which for the meta configuration is less likely to occur. These results provide us with a better understanding of the effect the molecular structure has on electron pathways and the presence of magnetic fingerprints in it.

WED 2
Towards tunable graphene phononic crystals

Yuefeng Yu[1], Jan N Kirchhof[1], Aleksei Tsarapkin[2], Victor Deinhart[2,3], Oguzhan Yücel[1], Bianca Höfer[1], Katja Höflich[2], Kirill I Bolotin[1]
[1]Department of physics, FU-berlin, Berlin
[2]Ferdinand-Braun-Institut gGmbH Leibniz-Institut für Höchstfrequenztechnik, Berlin
[3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin

Phononic crystals (PnCs) are artificially patterned media exhibiting bands of allowed and forbidden zones for phonons-in analogy to the electronic band structure of crystalline solids arising from the periodic arrangement of atoms. Many emerging applications of PnCs from solid-state simulators to quantum memories could benefit from the on-demand tunability of the phononic band structure. Here, we demonstrate the fabrication of suspended graphene PnCs in which the phononic band structure is controlled by mechanical tension applied electrostatically. We show signatures of a mechanically tunable phononic band gap. The experimental data supported by simulation suggests a phononic band gap at 28–33 MHz in equilibrium, which upshifts by 9 MHz under a mechanical tension of 3.1 N m$-$1. This is an essential step towards tunable phononics paving the way for more experiments on phononic systems based on 2D materials.

WED 3
Low-Temperature ALD of SbOx/Sb2Te3 Multilayers with Boosted Thermoelectric Performance

Jun Yang[1,2], Sebastian Lehmann[1], Axel Lubk[2], Tobias Ritschel[3], Jochen Geck[4], Kornelius Nielsch[1,2]
[1]Institute for Metallic Materials, Leibniz Institute for Solid State and Materials Research, Dresden, Germany
[2]Institute of Materials Science, Technische Universität Dresden, Dresden, Germany
[3]Institute for Solid State Research, Leibniz Institute for Solid State and Materials Research, Dresden, Germany
[4]Institute of Solid State and Materials Physics, Technische Universität Dresden, Dresden, Germany

Nanoscale superlattice (SL) structures enhance thermoelectric (TE) properties in thin films. In this study, a $\mathrm{Sb_2Te_3}$ thin film with sub-nanometer layers of $\mathrm{SbO_x}$ was synthesized via ALD at 80 °C. The SL structure, tailored by adjusting cycle numbers of $\mathrm{Sb_2Te_3}$ and $\mathrm{SbO_x}$, achieved a remarkable power factor of $520.8\,\mu\mathrm{Wm^{-1}K^{-2}}$ at room temperature with a $\mathrm{SO:ST}$ cycle ratio of $1:1000$. Findings suggest that at max thickness (ten ALD cycles), $\mathrm{SbO_x}$ layers act as potential barriers, filtering out low-energy charge carriers. The $\mathrm{SbO_x}$ sub-layer enhances scattering of mid-to-long-wavelength phonons at the $\mathrm{SbO_x/Sb_2Te_3}$ interface, inducing confinement effects and strain forces in the $\mathrm{Sb_2Te_3}$ thin film. These effects enhance the Seebeck coefficient while reducing thermal conductivity, providing insights into SL-structured TE materials and devices.

WED 4
Lattice dynamics and complete polarization analysis of Raman-active modes: from mode differentiation to Raman-tensor elements

Hans Tornatzky[1], Benjamin Janzen[2], Zbigniew Galazka[3], Manfred E. Ramsteiner[1], Markus R. Wagner[1,2]
[1]Paul-Drude-Institut, Berlin, Germany
[2]Technische Universität Berlin, Berlin, Germany
[3]Institut für Kristallzüchtung, Berlin, Germany

Raman spectroscopy has been very popular to study for example the composition in alloys or the layer number in few layered materials. This technique, however, can provide much deeper insight into the physics of the studied material.
In our poster, we will present the in-depth analysis of angle-resolved polarized Raman scattering (ARPRS), yielding the best chances to observe and differentiate phonon modes in a given crystal, as well as allowing to determine the relative Raman tensor elements. These are of great interest to be able to understand and model the phonon's scattering intensity and many other phonon related effects, such as thermal transport, charge-carrier dynamics, etc.
This study will be exemplary shown on $LaInO_3$ and the β-polymorph of Ga_2O_3, both

wide band gap semiconductors, while the latter provides a further challenge by being birefringent.

WED 5
Optical Helicity Sensing Using Graphene-Templated Achiral Hybrid Perovskite

Oleksandr Volochanskyi[1,2], Golam Haider[1], Essa A. Alharbi[3,4], George Kakavelakis[4,5], Martin Mergl[1], Mukesh Kumar Thakur[1], Anurag Krishna[4], Michael Graetzel[4], Martin Kalbáč[1]
[1]J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Department of Low-Dimensional Systems, Prague, Czech Republic
[2]University of Chemistry and Technology in Prague, Faculty of Chemical Engineering, Department of Physical Chemistry, Prague, Czech Republic
[3]Microelectronics and Semiconductors Institute, King Abdulaziz City for Science and Technology (KACST), Riyadh, Saudi Arabia
[4]École Polytechnique Fedérale du Lausanne, Laboratory of Photonics and Interfaces, Lausanne, Switzerland
[5]Hellenic Mediterranean University, School of Engineering, Department of Electronic Engineering, Chania, Crete, Greece

The manipulation and detection of optical polarization have emerged as a prominent area of fundamental and applied research in optoelectronics. This work investigates the templating effect of graphene on solution-processed hybrid perovskite growth, allowing for the creation of structural anisotropy at the heterojunction. Employing polarized photoluminescence, we studied perovskite film grown on SiO_2 and graphene substrates and observed spin-split bands and signs of enhanced Rashba coupling within a perovskite/graphene heterostructure. This intriguing effect is subsequently transferred to the electrical read-out, supported by the spin-photoconductive effect, yielding a polarized photocurrent asymmetry factor of 0.32. Furthermore, under these conditions, our device boasts an impressive photoresponsivity of 10^5 A/W at 500 nm excitation. Later, we emphasize the significance of the inversion symmetry effect within the heterojunction by reducing the quantity of bulk perovskite, leading to an exceptional photocurrent asymmetry factor of 0.51. Our study underscores the potential of graphene/achiral hybrid perovskite for thin film polarization-sensitive photodetection.

WED 6
Raman Spectroscopy of 2D MoS2 Interacting with Metals

Valeria Russo[1]
[1]Department of Energy, Politecnico di Milano, Milano

The research on MoS2 has progressed significantly, prompted by its remarkable optoelectronic properties. Raman spectroscopy is extensively used to characterize the structure and thickness of MoS2 films [1]. Recent works on MoS2-metal interfaces and metal-assisted synthesis methods have shown that Raman spectra are

significantly affected by the interaction with metals, especially for MoS2 grown by vapor phase techniques [2,3], however, a clear understanding of how such interaction modifies the MoS2 vibrational properties is still lacking. Here we discuss how the Raman response of single- or few-layer MoS2 and MoS2/WS2 heterostructures, deposited in UHV by Pulsed Laser Deposition on Ag(111), Au(111) and Ag(110) surfaces, is affected by interaction with the metal and how it modifies upon exposure to ambient conditions or after transfer of MoS2 on different substrates, such as silicon oxide [4,5].
[1] X. Zhang et al., Chem. Soc. Rev. 44, 2757 (2015) [2] F. Tumino et al., Nanoscale Adv. 1, 643 (2019) [3] P. D'Agosta et al., Nanoscale 15, 7493 (2023) [4] F. Tumino et al., J. Phys. Chem. C 125, 9479 (2021) [5] F. Tumino et al., Crystals 13, 1271 (2023)

WED 7
Probing Polaronic Effects via Optical Pump - Terahertz Range Raman Probe

Guy Reuveni[1], Selina Nöcker[1,2], Omer Yaffe[1]
[1]Department of Chemical and Biological Physics, Weizmann Institute of Science, Rehovot, Israel
[2]Institute of Condensed Matter Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Understanding the impact of excited electrons on structural dynamics is essential for comprehending various macroscopic phenomena, for example, carrier mobility. The investigation of polarons has predominantly relied on indirect probing techniques such as temperature-dependent photoluminescence and carrier mobility measurements. Alternatively, time-dependent X-ray diffraction methods have been employed, but they often involve complex instrumentation.
In this study, I present a cutting-edge optical setup that directly probes lattice distortions induced by excited electrons. Our state-of-the-art approach involves a visible pulsed pump and continuous off-resonance Raman probe, enabling a direct detection and differentiation of polaronic effects. I will demonstrate the effectiveness of this table-top optical setup mainly on $BiVO_4$ single crystal and 2D perovskites, showing clear signatures of small polarons.

WED 8
Reducing thermal conductivity of layered MoS2 by nanopatterning

Peng Xiao[1,2], Alexandros El Sachat[1,3], Emigdio Chávez Angel[1], Ryan C. Ng[1], Giorgos Nikoulis[4], Joseph Kioseoglou[4], Konstantinos Termentzidis[5], Clivia M. Sotomayor Torres[1,6], Marianna Sledzinska[1]
[1]Phononic and Photonic Nanostructures Group, ICN2, Barcelona
[2]Departamento de Física, Universidad Autónoma de Barcelona, Bellaterra, Barcelona, Spain
[3]National Center for Scientific Research "Demokritos", Athens, Greece
[4]Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece

[5]Univ Lyon, CNRS, INSA Lyon, CETHIL, Villeurbanne, France
[6]ICREA, Passeig Lluis Companys 23, Barcelona, Spain

Efficient thermal management of electronic devices poses significant challenges due to the high power densities involved. Here we report how layered MoS2 phononic crystals (PnCs) effectively allow the control of the thermal conductivity (k) with minimum impact on the electrical conductivity. With suspended MoS2 PnCs an extraordinarily low k of approximately 0.1 W/mK can be reached, beyond the amorphous limit while maintaining the crystalline structure. Molecular dynamic simulations, including film thickness, porosity and temperature, support these findings. We find that the layered PnCs surpass the performance of Si and SiC PnCs with comparable periodicity by approximately 100-fold, owing to the high anisotropic k of layered materials. To demonstrate the practical efficiency of this methodology, we construct suspended heat-routing structures designed to confine and direct heat flow along predetermined pathways in the PnCs. This study highlights the considerable potential of layered materials as directional heat spreaders, thermal insulators, and active components for thermoelectric devices offering a potential solution for thermal management in nanoelectronics.

WED 9
Probing type-II Ising pairing using the spin-mixing parameter b^2

P. Jureczko[1], J. Hanis[2], P. E. Faria Junior[3], M. Gmitra[2,4], M. Kurpas[1]
[1]Insitute of Physics, University of Silesia in Katowice, Katowice, Poland
[2]Institute of Physics, Pavol Jozef Safarik University in Kosice, Kosice, Slovakia
[3]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany
[4]Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia

We present an efficient approach to identify type-II Ising pairing in centrosymmetric superconductors from first principles calculations [1]. The method is based on the anisotropy of spin-mixing parameter b^2, which indicates the out-of-plane direction of intrinsic spin-orbit fields indispensable in the Ising pairing mechanism [2,3]. We test our approach on superconducting $PdTe_2$ for which the measured in-plane critical field exceeds the Pauli limit B_P more than seven times [3]. Using a simple theoretical model, we estimate the upper critical field for monolayer $PdTe_2$ as large as 12 B_P, depending on temperature and doping. We also discuss the origin of spin-mixing in bands of interest and show that not all of the 4-fold degenerate bands of $PdTe_2$ contributed by p_{xy} orbitals can participate in Ising pairing.

[1] P. Jureczko et al. arXiv:2302.02699

[2] Y. Liu et al. Nano Lett. 20, 5728 (2020)

[3] J.Falson et al. Science 367, 1454 (2020)

WED 10
Semiconductor moiré superlattices based on 2D Janus heterobilayers

Wenjin Zhang[1], Zheng Liu[2], Hiroshi Nakajo[3], Soma Aoki[3], Haonan Wan[4], Yanlin Wang[4], Yanlin Gao[5], Mina Maruyama[5], Takuto Kawakami[6], Yasuyuki Makino[1], Masahiko Kaneda[1], Tongmin Chen[7], Kohei Aso[7], Tomoya Ogawa[1], Takahiko Endo[1], Yusuke Nakanishi[1], Kenji Watanabe[8], Takashi Taniguchi[8], Yoshifumi Oshima[7], Yukiko Yamada-Takamura[7], Mikito Koshino[6], Susumu Okada[5], Kazunari Matsuda[4], Toshiaki Kato[3], Yasumitsu Miyata[1]
[1]Department of Physics,Tokyo Metropolitan University
[2]Innovative Functional Materials Research Institute, National Institute of Advanced Industrial Science and Technology
[3]Graduate School of Engineering, Tohoku University
[4]Institute of Advanced Energy, Kyoto University
[5]Department of Physics, University of Tsukuba
[6]Department of Physics, Osaka University
[7]School of Materials Science, Japan Advanced Institute of Science and Technology
[8]National Institute for Materials Science

Moiré superlattices based on van der Waals layered materials have attracted considerable attention because of their rich quantum phenomena and potential applications in optoelectronics. Janus monolayers of transition metal dichalcogenides (TMDCs) are promising building blocks for moiré superlattices due to their built-in electric field and clean fabrication process. However, the moiré superlattices of Janus heterobilayers have not been studied experimentally.Herein, this work reports the fabrication and characterization of semiconductor moiré superlattices in chemically-tailored Janus heterobilayers. MoSSe/MoSe2 Janus heterobilayers were prepared by replacing the top layer Se atoms with S atoms in MoSe2 bilayer using H2 plasma treatment. Scanning transmission electron microscopy (STEM) revealed that an average moiré period of about 14 nm formed due to lattice mismatch resulting from the chalcogen substitutions. The cryogenic photoluminescence spectra showed sharp, near-infrared emissions, which were attributed to excitons trapped by moiré potentials based on comparison with theoretical calculations.

WED 11
Spin-flip excitons in SmFeO3 probed by resonant Raman spectroscopy

Georgy Gordeev[1], Aseem Rajan Kshirsagar[1], Sven Reichardt[1], Stephanie Reich[2], Ludger Wirtz[1], Matthieu J. Verstraete[3], Mael Guennou[1]
[1]Department of Physics and Materials Science, University of Luxembourg, Belvaux
[2]Department of Physics, Freie Universit"at Berlin, Berlin
[3]Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Belvaux, Luxembourg

We predict spin-flip excitons to form in the iron-based perovskite oxides. They originate from the unbound d electrons from the Fe sublattice hybridized with bound

oxygen electrons. The major exciton energies are separated by the crystal field with additional splitting provided by spin-orbit coupling (SOC). Localization of excitons within the Fe-O octahedron leads to unusually high binding energies up to 1 eV placing these states deep inside the band gap. The 'forbidden' optical transitions are enabled by the SOC with finite but moderate oscillator strength. To visualize these excitonic states we leverage resonant Raman excitation and high exciton-phonon coupling secured by the exciton's spatial localization. The modes involving motion of oxygen and iron atoms experience an enhancement when the laser energy matches the energy of the excitonic states. The exciton selection rules shape the scattering cross-section of the symmetric Ag phonons for a particular orientation of the EM field. Moreover, the exciton-phonon coupling depends on the phonon symmetry. By comparing the Raman cross-sections of the different modes we recover the crystal field splitting and SOC.

WED 12
Theory of Piezoelectric Resonator in 2D and in Layered Crystals

Karl H. Michel[1], Cem Sevik[1], Milorad Milosevic[1]
[1]Physics, Universiteit Antwerpen, Antwerpen

Starting from an anharmonic Hamiltonian for ionic displacements in a 2D crystal with point group symmetry D3h a coupled system of optic and acoustic dynamic response functions is derived.The dynamic susceptibilities for the direct and the converse piezoelectric effects are found to be equal and symmetric in the optic and acoustic displacements propagators.The latter satisfy Dyson equations where the anharmonicities account for temperature and size dependent optic and acoustic phonon shifts and dampings.The opto-acoustic coupling consists of a harmonic static and an anharmonic frequency dependent term ,the latter with reactive and absorptive parts.The longitudinal and transverse susceptibilities driven by an altrnating electric field are studied near acoustic fundamental frequencies and overtones depending on sample sizes and temprature.Due to the large in-plane rigidity and small sample sizes a large spectrum of resonance frequencies is obtained.In layered crystals with layer number N ,piezoelectricity occurs only at N uneven and decreases as 1/N .In dynamic theory this decrease might be compensated by susceptibilities increase near resonances.

WED 13
Impact of He Irradiation on Micro- and Nano-Scale Properties in MoS_2 and $PtSe_2$

Luka Pirker[1], Adeel Bukhari[1], Magdalena Scheibe[1], Gregor Hlawacek[2], Matěj Velický[1], Otakar Frank[1]
[1]Department of Electrochemical Materials, J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic
[2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Research on 2D materials is flourishing, impacting physics, chemistry, and practical applications. The atomically-thin nature makes them highly sensitive to their environment, offering vast tuning opportunities—from thickness and deformation to chemical doping and deliberate introduction of defects. To comprehend defects' impact on the materials properties, controlled defect creation and the use of micro- and nano-scaled spectroscopic and microscopy techniques is crucial.
In this work, we investigate the electrical, optical, and vibrational properties of MoS_2 and $PtSe_2$ with induced defects via He irradiation. Samples prepared by large-area exfoliation on gold and direct exfoliation on SiO_2 had defects introduced by varying He ion doses. They were studied using AFM, Kelvin probe force microscopy, and micro- and tip-enhanced Raman and PL spectroscopy (TERS, TEPL), revealing micro- and nano-scale influences of defects. Understanding the effects of defects on 2D materials is crucial for any future application involving defect engineering.

WED 14
Properties of higher order Raman modes of confined carbyne

Johannes Lechner[1], Pietro Marabotti[1], Getulio S Souza Jr[1], Charlotte Berrezueta Palacios[2], Lei Shi[3], Thomas Pichler[4], Sebastian Heeg[1]
[1]Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin
[2]Freie Universität Berlin, Berlin
[3]School of Materials Science and Engineering, Sun Yat-sen University, Guangzhou
[4]Fakultät für Physik, Universität Wien, Wien

Confined carbyne consists of long linear carbon chains ($>$100 atoms) inside carbon nanotubes and is considered a close, stable analogue to the truly 1-dimensional carbon allotrope carbyne. Here we investigate the higher order modes of the Raman active C-mode of single confined carbyne chains by confocal resonant Raman spectroscopy. We observe large frequency shifts which imply strongly anharmonic properties. Analyzing the relative intensities of Raman peaks of different order, we unravel major fluctuations depending on the excitation wavelength, particularly for the second order. Unexpectedly, the relative intensities of different Raman mode orders also change with the frequency of the C-mode. These new discoveries enable further insight into the structural and electronic properties of confined carbyne as a material system.

WED 15
Correlation measurements for carbon nanotubes with quantum defects

Ralph Krupke[1,2,3]
[1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany
[2]Institute of Quantum Materials and Technologies, Karlsruhe Institute of Technology, Germany
[3]Institute of Materials Science, Technical University Darmstadt, Germany

Single-photon sources are one of the essential building blocks for the develop-

ment of photonic quantum technology. In terms of potential practical application, an on-demand electrically driven quantum-light emitter on a chip is notably crucial for integrating photonic integrated circuits. Here, we propose functionalized single-walled carbon nanotube field-effect transistors as a promising solid-state quantum-light source by demonstrating photon antibunching behavior via electrical excitation. The sp^3 quantum defects were formed on the surface of (7, 5) carbon nanotubes by 3,5-dichlorophenyl functionalization, and individual carbon nanotubes were wired to graphene electrode pairs. Filtered electroluminescent defect-state emission at 77 K was coupled into a Hanbury Brown and Twiss experiment setup, and single-photon emission was observed by performing second-order correlation function measurements. We discuss the dependence of the intensity correlation measurement on excitation power and emission wavelength highlighting the challenges of performing such measurements while simultaneously analyzing acquired data.

WED 16
Strain activation of quantum dots in monolayer WSe_2 using AFM indentation

Oğuzhan Yücel[1], Jan Kirschoff[1], Denis Yagodkin[1], Yufeng Yu[1], Abhijeet Kumar[1], Adrian Dewambrechies[1], Douglas J. Bock[1], Kirill I. Bolotin[1]
[1]Physics Department, Freie Universitaet Berlin, Berlin

Semiconductor quantum dots are key contenders for achieving an optimal quantum interface between light and matter in quantum technologies. Despite significant progress, challenges persist in realizing quantum light sources that are bright, pure, indistinguishable, polarizable, and spatially compatible. In this study, we explore quantum dots in monolayer WSe_2 on a polymer substrate, formed through AFM indentation and activated via strain. We present sharp emission peaks at varied spectral positions and controllable locations on the sample surface. Under moderate annealing conditions, the strained WSe_2 regions experience slight relaxation, leading to the disappearance or reappearance of emission peaks at different spectral positions with varying polarization orientations. Furthermore, we detail the strain activation of defect states at cryogenic temperatures, offering statistics on strain values, peak spectral positions and brightness. Our findings contribute to improving quantum dots created through AFM indentation and deepen the understanding of the physical dynamics involved in strain-defect state activation.

WED 17
Carbon Based 2D Materials from Aromatic Precursors

Kati G.-Hubmann[1], T. Lehnert[2], Ute Kaiser[2], N. Severin[3], J. Rabe[3], F. G. Fabozzi[4], S. Hecht[4], Stephanie Reich[1]
[1]Department of Physics, Freie Universität Berlin, Berlin, Germany
[2]Ulm University, Electron Microscopy Group of Materials Science, Ulm, Germany
[3]Department of Physics, IRIS & Centre for the Science of Materials Berlin Adlershof, Physics of Macromolecules Humboldt-Universität zu Berlin, Germany
[4]Laboratory of Organic Chemistry and Functional Materials, Department of Chem-

istry, Humboldt-Universität zu Berlin, Berlin, Germany

We investigate the growth of monolayer materials from the molecular precursors at moderate temperatures, whereby the starting monomers polymerizes, while their aromatic sp^2 skeleton structure is retained. By selecting of the proper starting molecules, and varying of growth condition, films of amorphous carbon, defective and defect-free graphene and graphene antidot superlattices were produced. Different precursor molecules were tested. Amorphous and crystalline domains are grown from Terphenyl molecules. The larger precursor molecules Di(naphthylen)anthracen lead to the growth of polycrystalline graphene. Confocal micro Raman spectra confirm the coexistence of both domains. This was also confirmed by high-resolution transmission electron microscope. The disk-shaped hexabromo-triphenylenes merge in a layer with a hexagonal crystal structure with a lattice constant of 0.95 nm, which was characterized using high-resolution atomic force microscope.

WED 18
Electronic Properties and Interlayer Interactions in Antimony Oxide Homo- and Heterobilayers

Stefan Wolff[1]
[1]Physik, Friedrich-Alexander-Universität, Erlangen

Antimony shows promise as a two-dimensional (2D) mono-elemental crystal, referred to as antimonene. When exposed to ambient conditions, antimonene layers react with oxygen, forming new crystal structures, leading significant changes in electronic properties. These changes are influenced by the degree of oxidation. Utilizing Density Functional Theory (DFT) calculations, stable configurations of bilayer antimony oxide and their corresponding electronic properties are studied. Additionally, different stacking arrangements and their effects on the physical properties of the materials are investigated. Furthermore, the analysis encompasses strain-free hetero-bilayers containing both pristine and oxidized antimonene layers, aiming to understand the interplay between these materials and their collective impact on the bilayer properties. Our results provide insight into how the properties of antimony-based bilayer structures can be modified by adjusting stoichiometry and stacking configurations.

WED 19
BaZrS3, an unconventional perovskite and a conventional semiconductor

Matan Menahem[1], Kevin Ye[2], Tommaso Salzillo[1], Sigalit Aharon[1], Rafael Jaramillo[2], Omer Yaffe[1]
[1]Weizmann Institute of Science, Rehovot
[2]Massachusetts Institute of Technology, MA, USA

Extensive research has been dedicated to lead-halide perovskites, driven by their optoelectronic properties intricately tied to their anharmonic structural dynamics.

Chalcogenide perovskites have emerged as promising contenders in pursuing sustainable alternatives, distinguished by their lead-free composition and heightened chemical stability. Despite these favorable attributes, the optoelectronic characteristics of chalcogenide perovskites still trail those exhibited by their halide analogs. Therefore, we correlate between structural dynamics and optical traits in BaZrS3 compared to CsPbBr3. Temperature-dependent Raman scattering measurements on BaZrS3 unveil sharp, weakly temperature-dependent peaks, indicating a more harmonic structural behavior than CsPbBr3. The evolution of photoluminescence spectra with temperature suggests a similar recombination mechanism with comparable activation energy for both materials. However, substantial differences in luminescence efficiency underscore the crucial role of anharmonic structural dynamics in mitigating optically active defects. This study provides insights into the interplay between properties in this promising class of materials.

WED 20

Solving the mystery of the missing phonon gap in scanning tunnelling spectroscopy measurements of graphene

György Kálvin[1], Pálinkás András[1], Konrád Kandrai[1], Péter Vancsó[1], Levente Tapasztó[1], Péter Nemes-Incze[1]
[1]Nanostructures, HUN-REN EK, Budapest

Recently, our group showed that the common contamination from ambient air on the surface of van der Waals materials (e.g., graphene, hBN, etc.) is composed of a self-organized molecular layer of normal alkanes [1]. This layer significantly influences the interaction of the 2D materials in question with their environment and with measuring probes. Here we show that this alkane layer has a major influence on the tunnelling conductance (dI/dV) measurements and on the measured decay of the tunnelling current with tip-sample distance (Iz spectroscopy). We found that the well-known exponential decay of the Iz spectrum flattens by a factor of 1.5 if the tip is above the molecular layer. This is due to the changes in the decay of the sample wavefunctions into the vacuum, as confirmed by ab initio calculations. In addition, the tunnelling conductance spectrum of contaminated graphite samples does not show the phonon-induced gap near the Fermi energy, solving the long-standing mystery of most STM measurements not reporting this well-known feature of the graphene/graphite tunnelling conductance.

[1] Nat. Commun. 13, 6770 (2022)

WED 21

Optical Models of Excitons in High-quality TMD van der Waals Heterostructures: A Comparative Study

Anabel Atash[1], Itai Epstein[1]
[1]School of Electrical Engineering, Department of Physical Electronics, Tel Aviv University

Excitons in monolayer semiconductor transition metal dichalcogenide (TMD) exhibit strong interaction with light and dominate the optical response of these material. Monolayer TMDs encapsulated in hexagonal boron nitride (h-BN) at cryogenic temperatures exhibit highly improved electrical, optical and excitonic properties. In this study, four different models are used to identify the most accurate model for describing the optical response of TMD excitons. Measurements of reflectance at different temperatures are used to extract the optical parameters of the different modelling approaches, which are then compared for determining the most accurate one.

WED 22
Electron beam induced vacancy-adatom complexes in mono- and bilayer phosphorene

Carsten Speckmann[1,2], David Lamprecht[1,3], Felix Herterich[1], Clemens Mangler[1], Jani Kotakoski[1]
[1]University of Vienna, Faculty of Physics, Vienna, Austria
[2]University of Vienna, Vienna Doctoral School in Physics, Vienna, Austria
[3]TU Wien, Institute for Microelectronics, Vienna, Austria

Phosphorene has peaked a lot of interest in recent years due to its promissing potential in electronics and especially optoelectronics [1]. However, detailed experimental characterizations of its intrinsic defects as well as the creation of additional defects and their diffusion barriers are scarce [2,3]. Here, we report on the creation and stability of a variety of defect configurations under 60 kV electron irradiation in mono- and bilayer phosphorene including the first experimental reports of stable vacancy-adatom complexes which have previously only been discussed in theory [4]. Additionally, we give an estimate on the displacement cross section of phosphorene as well as the recombination rate of adatoms with vacancies. These results will help to improve the understanding of the wide variety of defects in phosphorene, their creation and their stability which might open up new possibilities for defect engineered phosphorene devices.

[1] Ling et al., PNAS 112, 15 (2015)
[2] Yao et al., 2D Mater. 8, 025004 (2020)
[3] Harsh et al., J. Phys. Chem. Lett. 13, 27, 6276-6282 (2022)
[4] Vierimaa et al., Nanoscale 8, 7949-7957 (2016)

WED 23
Light-matter coupling in plasmonic platforms

Gabriela Luna Amador[1], Niclas S. Müller[2], Florian Schulz[3], Holger Lange[3], Stephanie Reich[1]
[1]Freie Universität Berlin, Berlin
[2]Fritz Haber Institute, Max Planck Society, Berlin
[3]Universität Hamburg, Hamburg

Plasmonic supercrystals are novel materials formed by metallic nanoparticles arranged in a face-centered cubic lattice (Schulz 2020). In these crystals, light is confined into hotspots between nanoparticles, which enhances light matter interaction and leads to plasmon-polaritons in the deep-strong light-matter coupling regime (M¨uller 2020). This makes this material the first system to exhibit coupling between light and a continuum of states in the deep-strong regime at ambient conditions. By treating the crystal as an open cavity, we further study light-matter coupling, this time in crystals made of nanoparticles with a diameter larger than 100 nm. Additionally, we investigate the energy losses mechanisms and the plasmon-polariton lifetime.

WED 24
Non-epitaxial Growth of Wafer-scale Single-crystal 2D Materials on Insulating Substrates

Junzhu Li[1], Bo Tian[1], Xixiang Zhang[1]
[1]Division od Physical Science and Engineering, King Abdullah University of Science and Technology, Thuwal

In this study, we report a universal non-epitaxial synthesis (UNS) strategy for fabricating wafer-scale single-crystal 2D materials on diverse insulating substrates. High-quality 2D-material layers were grown on both surfaces of our single-crystal metal foil, which was pre-placed on an insulating substrate. A brief high-temperature treatment was applied, bringing the foil to an extremely soft near-molten state, which facilitated the adhesion of the metal foil–2D layer onto the insulator surface underneath. Eventually, the 2D material remained on the insulating substrate after cooling and removing the foil. This UNS strategy has been utilized to synthesize large-area single-crystal monolayer hBN and graphene on various insulators, as well as bi- and trilayer graphene after replacing the Cu(111) foil with the CuNi(111) alloy. This approach is expected to be extended to the future synthesis of other metal-substrate CVD-grown 2D materials and wafer-scale multilayer 2D van der Waals heterostructures on insulating substrates.

WED 25
Nanoscale Charge Transport Characterization of Novel Type 2D MOFs and COFs

Jonas F. Pöhls[1], Zhiyong Wang[2], Laura Frey[3], Renhao Dong[2], Dana D. Medina[3], Xinliang Feng[2], R. Thomas Weitz[1]
[1]I. Institute of Physics, Georg-August-University Goettingen, Göttingen
[2]Technical University Dresden, Dresden
[3]Ludwig-Maximilians-University Munich, Munich

In recent years, Metal Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs) have emerged as fascinating and promising materials classes, owing to their exceptional structural versatility and tunable properties, which make them interesting for a wide range of technological applications. At the same time, the

study of 2D van der Waals materials has become the probably most relevant and dynamic area in solid state research at present, offering numerous opportunities to uncover novel physical phenomena and engineer advanced nanoscale devices. With recent advances in the synthesis of two-dimensional MOFs and COFs, these material classes have also entered the field of van der Waals materials. We will characterize the charge transport in novel type 2D coordination network materials like Cu-BHT, considering also the influence of properties like structure or defects. By that, we will demonstrate why they are promising candidates for implementation into van der Waals heterostructures.

WED 26
Light-matter interaction with bound states in the continuum in monolithic van der Waals metasurfaces

Luca Sortino[1], Stefan A. Maier[2,3], Andreas Tittl[1]
[1]Chair in Hybrid Nanosystems, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany
[2]School of Physics and Astronomy, Monash University, Clayton VIC, Australia
[3]The Blackett Laboratory, Department of Physics, Imperial College London, London, United Kingdom

Van der Waals (vdW) materials, like hexagonal boron nitride (hBN) and Transition Metal Dichalcogenides (TMDCs), show extraordinary optical properties, from strongly bound excitons and optically addressable spin defects, to significant optical anisotropy and high refractive index values, making them attractive for innovative nanophotonic devices. Here, we leverage the physics of quasi-bound states in the continuum (qBIC) to generate sharp optical resonances in dielectric metasurfaces composed solely of hBN or TMDCs. This entirely monolithic method achieves optical resonances with quality factors surpassing 10^2. In hBN metasurfaces, we demonstrate spectral tuning across the entire visible spectrum and enhanced emission from implanted native spin defects. Furthermore, our platform presents intriguing possibilities for strong light-matter coupling, exemplified by the anti-crossing between qBIC resonances and intrinsic excitons in TMDC metasurfaces, resulting in Rabi splitting of 116 meV at ambient conditions. Our results highlight the potential of combining qBIC metasurfaces with vdW material, paving the way for novel nanophotonic platforms and room temperature polaritonic devices.

WED 27
Moiré-induced phonon coupling in twisted bilayers

Nina Girotto[2], Lukas Linhart[1], Florian Libisch[1]
[1]Institute for Theoretical Physics, Vienna University of Technology, Vienna
[2]Centre for Advanced Laser Techniques, Institute of Physics, Zagreb, Croatia

Twisting two stacked layers of two-dimensional materials relative to each other significantly alters the physical properties of the resulting bilayer. For magic angle

graphene the electronic band structure features a flat band at the Fermi level giving rise to interesting many-body physics such as correlated insulators or superconductivity. Likewise, a finite twist angle modifies the phonon band structure. We investigate the continuous evolution of the phonon band structure with twist angle using a continuous momentum-space model [1,2]. At intermediate angles, we find a complicated structure of the phonon density of states around the frequency of the layer breathing mode, that is substantially broadened by the moiré-induced interaction with the acoustic phonon branches. We infer optical activities and suggest Raman experiments to validate our predictions. Our results suggest that suitably twisting structures may manipulate both phonon and electron properties of such a system, and thus set the stage to test electron-phonon contributions to the observed correlated states.

[1] N. Girotto et al., PRB 108, 155415 (2023)
[2] J. Quan et al., Nature Materials 20, 1100 (2021)

WED 28
Growth of continued rods based on MWCNT (Multi-Wall Carbon Nanotubes) and the possibility of their metallic doping during arc discharge in higher alkanes.

Krzysztof Jankowski[1]
[1]Institute of Nanotechnology and Nanobiology , Jacob of Paradies University, Gorzów Wielkopolski

The possibility of controlled carbon rods based on MWCNT (Multiwall Carbon Nanotubes) growth between graphite electrodes (electrode deposits) during an AC arc discharge (60 Hz) in liquid paraffin and the doping of iron powder with a gradation of > 10 μm as a medium were discussed. The surface morphology of the obtained carbon nanomaterials was determined using the following techniques: reflected light optical microscopy, scanning electron microscopy (SEM) with an EDX detector, X-ray microtomography (uCT), and atomic force microscopy (AFM). Qualitative analysis studies were carried out using Raman spectroscopy, FTIR, and X-ray powder diffraction (XRD). Using AFM techniques in SThM and CP modes, the temperature and electrical conductivity of the obtained nanostructures were determined. The use of high-voltage alternating current (HVAC) arc discharge for the controlled growing of doped electrode deposit rods may be a new network for obtaining cheap porous carbon nanomaterials based on MWCNT used in various branches of science.

WED 29
Out-of-plane band structure of graphite under applied electric field

Amit Singh[1], Artem Mishchenko[1,2]
[1]Department of Physics and Astronomy, University of Manchester, Manchester, UK
[2]National Graphene Institute, University of Manchester, Manchester, UK

Using density functional theory, we calculated the out-of-plane (along H-K-H high symmetry points) band structure of bulk AA, AB, and ABC stacked graphite under various electric field orientations. In the absence of E-field, AA stacked graphite has strongly dispersing bands touching at H-point, in AB stacking it shows degenerate weakly dispersing bands with band overlap of 23 meV, while ABC stacked graphite is gapped (0.55-0.57 eV band gap). Application of an in-plane E-field does not alter the out-of-plane band structure of graphite allotropes. When a vertical E-field of 0.5 V/nm is applied to the AA stacked graphite, band gap of 1 eV opens and bell-shaped out-of-plane bands flatten. In AB stacked graphite, E-field opens 40 meV band gap, while in ABC stacked graphite, the band splits into three discrete bands reducing the out-of-plane band gap by 30 meV. Our work offers a perspective for electric field driven band structure engineering in graphitic materials.

WED 30
GRAPHENE QUANTUM DOTS IN A MOLECULAR CRYSTAL

Trung Thanh Huynh[1], Suman Sarkar[1], Hugo Levy-Falk[1], Daniel Medina-Lopez[1], Elsa Cassette[1], Loic Rondin[1], Stephane Campidelli[1], Jean-Sebastien Lauret[1]
[1]Paris-Saclay University, Orsay
[2]CEA Paris-Saclay, Gif-sur-Yvette

Graphene quantum dots (GQDs) synthesized by bottom-up chemistry are a tunable bandgap-material and promise applications in optoelectronic[1]. The recent investigations on the intrinsic properties of these GQDs classify them as a stable and bright single photon source[2,4]. Moreover, temperature dependent PL study of GQDs' embedded in a polymer matrix shows the reduction of the spectral linewidth down to 2.3 meV at low temperature[3]. Despite this reduction, the linewidth is still few orders of magnitude higher than the estimated radiative limit of 1µeV due to coupling of the electronic states of GQD with the vibration modes of the host matrix [3]. Therefore, changing the matrix to molecular crytal is mandatory to reach this theoretical limit. In this poster, I will report on a study of the photophysics of the C114-tBu10 GQD embedded in a molecular crystal made of C78 dendrimers. The PL of GQDs are studied down to the single crystal.

[1]X.Yan,X.Cui,and L.-s.Li,J.Am.Chem.Soc.132,5944 (2010)
[2]S.Zhao et al,Nature Communications,9,3470 (2018)
[3]T.Liu et al,Journal of Chemical Physics 156,104302 (2022)
[4]D. Medina-Lopez et al, Nature Communications 14, 4728 (2023)

WED 31
Spintronics with Black Phosphorus

Hao Wei[1], M. Galbiati[1], J. Peiro[1], S.M.M. Dubois[3], F. Brunnett[1], V. Zatko[1], R.Galceran[1], P.Brus[2], F.Godel[1], D.Perconte[1], F.Bouamrane[1], E. Gaufrès[4], A. Loiseau[4], F.Petroff[1], JC Charlier[3], M.-B.Martin[1], B.Dlubak[1], P.Seneor[1]
[1]Laboratoire Albert Fert (UMR137),CNRS, Thales, Université Paris-Saclay, Palaiseau,

France
[2]Thales Research and Technology, Palaiseau, France
[3]Institute of Condensed Matter and Nanosciences (IMCN), Université Catholique de Louvain, Louvain-la-Neuve, Belgium
[4]Laboratoire d'Étude des Microstructures (LEM), CNRS, ONERA, Université Paris-Saclay, Châtillon, France

Spintronics targets beyond-CMOS technologies, from data storage to quantum info. To this aim graphene[1,2] has been highlighted to provide efficient spin transport and filtering, but lacks a bandgap. Interestingly Black Phosphorus (BP) provides both high mobilities and low spin-orbit coupling that could enable efficient spin transport like graphene, but with a bandgap. This is key for spin manipulation and developing spin gates, positioning BP as a potentially pivotal material for spintronics. However, its exploration for spintronics has remained scarce.[3]
Here we report on the first demonstration of BP integration showing spin signals as large as 90% in hybrid Co/BP/MgO/Co and 500% in Co/BP/Co vertical devices. Those findings unveil a novel spin selective transport mechanism, spin-splitted in the reciprocal-space as shown by first-principle investigation. Our results illustrate the potential of BP for spin injection/detection, strongly supporting BP's vision as an outstanding platform for spintronics.

[1]Zatko ACS Nano 16,(2022) 14007;Piquemal Nat Comm 11,(2020) 5670
[2]Dlubak Nat Phys 8,(2012) 557;Seneor MRS Bulletin 37,(2012) 1245
[3]Kern APL 114,(2019) 053107

WED 32
Vertical Electronic Transport in 2D materials investigated in the nanoscale

Eduardo Bede Barros[1]
[1]Physics, Universidade Federal do Ceara, Fortaleza, Brazil

The study of the electronic transport through 2D nanomaterials and their stacked heterostructures have undergone great advances in the recent years. This is due to the fact that these are ultra-thin, highly flexible materials which form atomically defined interfaces and present interesting optical properties. One of the open issues about these 2D vertical heterostructures is the electronic transport mechanism between their composite atomic planes. In this sense, SPM techniques, in special the CAFM measurements have been applied to deepen the knowledge of the electronic behavior of these systems.

In this work we discuss the latest developments in the vertical transport through the layers for thin samples of 2D materials using the CAFM technique. In these experiments a conducting AFM tip is contacted to a the 2D material flake which has been deposited on a conductive substrate. The electric current between the substrate and the AFM tip is measured as a function of the applied bias and the loading force.

WED 33

Gate-controlled suppression of light-driven proton transport through graphene

Eoin Griffin[1], Shiqi Huang[1], Marcelo Lozada-Hidalgo[1]
[1]Physics and Astronomy, University of Manchester, Manchester

Recent experiments demonstrated that proton transport through graphene electrodes can be accelerated by over an order of magnitude with low intensity illumination. Here we show that this photo-effect can be suppressed for a tuneable fraction of the infrared spectrum by applying a voltage bias. Using photocurrent measurements and Raman spectroscopy, we show that such fraction can be selected by tuning the Fermi energy of electrons in graphene with a bias, a phenomenon controlled by Pauli blocking of photo-excited electrons. These findings demonstrate a dependence between graphene's electronic and proton transport properties and provide fundamental insights into molecularly thin electrode-electrolyte interfaces and their interaction with light.

WED 34

Exploring the Growth and Optical Properties of $MoTe_2$ and WTe_2 Thin Layers

Martin Hulman[1], Lenka Pribusová-Slušná[1], Tatiana Vojteková[1], Michaela Sojková[1], Jana Hrdá[1]
[1]Institute of Electrical Engineering SAS, Bratislava

This presentation explores the growth and optical properties of $MoTe_2$ and WTe_2 polycrystalline thin layers developed through the tellurisation of metallic films. We focus on the WTe_2 and $MoTe_2$ phases, potentially hosting Weyl fermions characteristic of Weyl topological semimetals (WSMs) with unique band structures. Our work advances the growth process, enhancing crystallinity and phase purity. Our presentation will include findings from Raman spectroscopy and optical measurements in the far- and mid-infrared regions conducted across varying sample temperatures and thicknesses. The primary objective is to elucidate the impact of these variables on fundamental optical properties, such as refractive indices and optical conductivity. Our findings may have implications for the understanding and application of WSMs in advanced optical and electronic devices.

WED 35

Preparation of two-dimensional transition metal thiophosphates for SP-STM and ARPES

Niklas Leuth[1], Wendong Wang[3], Jeff Strasdas[1], Benjamin Pestka[1], Adi Harchol[2], Efrat Lifshitz[2], Roman Gorbachev[3], Markus Morgenstern[1]
[1]2nd Institute of Physics B, RWTH Aachen, Aachen, Germany
[2]Department of Solid-State, Technion Institute, Haifa, Israel
[3]National Graphene Institute, University of Manchester, Manchester, UK

Transition metal thiophosphates are a class of antiferromagnetic Van-der-Waals (VdW) materials which allow detailed studying of 2D magnetism since they pos-

sess different magnetic structures but similar crystal structures. In comparison to other VdW crystals they are air-stable, simplifying preparation. To study their magnetism in 2D, they are needed in their 2D form. Here, a preparation technique which allows exfoliation of mono-/few-layers of these materials with sizes of $\sim (100)^2$ µm is presented. To achieve this, a scotch-tape technique with exfoliation to a gold substrate is used. The gold provides good bonding to the sulphur atoms of the thiophosphates. Prior to the exfoliation, an oxygen plasma is used to treat the substrate surface which enhances the yield of the exfoliation. The produced samples were already successfully characterised by angular resolved photoelectron spectroscopy and are intended for spin-polarized scanning tunnelling microscopy measurements. Currently, a very clean inorganic transfer method developed by the University of Manchester is adapted in cooperation with them to create heterostructures with clean surfaces to further investigate 2D magnetism.

WED 36
Optical properties of PtSe2 twisted structures

Paulina Jureczko[1], Marcin Kurpas[1]
[1]Institute of Physics, University of Silesia, Katowice

Monolayer of $PtSe_2$ is a transition metal dichalcogenide semiconductor with an indirect gap and 1T-type crystal structure. Besides promising electrical and optical properties, $PtSe_2$ exhibits good air stability with high room-temperature carrier mobility (1) and indicates excellent tunability of electronic properties by controlling the number of layers (2).
We study the twist-angle dependence of electronic and optical properties of bilayer $PtSe_2$. Using first-principles calculations based on the density functional theory, we calculate the electronic band structure and imaginary part of the dielectric function. We find that the most significant changes in the dielectric function are observed between 0° and 180° twist angles, while for twist angles between 13° and 32°, optical properties do not differ much.
We also study the effects of vertical strain on the electronic and optical properties. Our numerical results show that for experimentally accessible strain values, an additional peak in the dielectric function appears at the photon energy of 1eV due to the band gap reduction.

(1) Y. Wang et al. 10.1021/acs.nanolett.5b00964
(2) Li et al. 10.1021/acsnano.1c02971

WED 37
Unravelling interactions between TMDCs and metals

Michaela Hanušová[1,2], Matěj Velický[1], Luka Pirker[1], Otakar Frank[1], Casey Cheung[3,4]
[1]J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic
[2]Department of Physical Chemistry, University of Chemistry and Technology, Prague,

Czech Republic
[3]Department of Physics and Astronomy, University of Manchester, UK
[4]National Graphene Institute, University of Manchester, UK

Various approaches for obtaining TMDCs monolayers have been explored. However, a suitable route for producing large areas of high-quality monolayers remains challenging. Gold-assisted exfoliation has attracted interest due to the high yields and large lateral size of monolayer flakes. The use of other noble metals might also lead to successful exfoliation, but their use is somewhat limited due to their susceptibility to oxidation in air-prepared samples.[1,2]
We use mechanical exfoliation of TMDCs onto metallic surfaces under controlled atmosphere conditions. That allow us to prevent the substrate surface from oxidation. Herein, we investigate the fundamentals of the interaction between MoS_2 and various metals. Using Raman spectroscopy, TERS, AFM and KPFM, we explore the influence of the exfoliation method on interfacial strain and charge doping.
Our findings shed light on the nature of the TMDC-metal interactions, which could lead to an improvement of the exfoliation mechanism and the possibility of using non-Au substrates for large-area exfoliation.

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

[2] Velický et al., Adv. Mater. Interfaces 7, 2020, 20013

WED 38
Raman spectroscopy of edge-extended graphene nanoribbons

Jeong Ha Hwang[1], Amogh Kinikar[1], Mickael L. Perrin[2], Roman Fasel[1], Gabriela Borin Barin[1]
[1]nanotech@surfaces Laboratory, Empa, Dübendorf, Switzerland
[2]Transport at Nanoscale Interfaces Laboratory, Empa, Dübendorf, Switzerland

Raman spectroscopy has been widely used to characterize sp2-hybridized carbon nanomaterials including atomically precise graphene nanoribbons (GNRs). Through Raman spectroscopy, it is possible to probe the distinct vibrational modes of GNRs, which provides valuable insights into their structural parameters, such as width, edge structure, and length. However, such investigations so far are concentrated only on GNRs that are robust under ambient conditions and can easily be exposed to air after their growth in ultra-high-vacuum (UHV) conditions. Here, we propose the implementation of Raman spectroscopy to identify structural changes in graphene nanoribbons that are reactive under ambient conditions, such as GNRs with zigzag edges and GNRs with topological edge extensions. For that, we built a UHV chamber that allows Raman spectroscopy characterization on samples without exposing them to air. We study the effect of controlled oxygen dosing on edge-extended GNRs, which show clear signs of degradation. Further, we will also discuss the possibility of in-situ Raman characterization during GNR growth and the effect of temperature on the characteristic GNR Raman vibrations.

WED 39
Delocalized Spin states at Zigzag Termini of Graphene Nanoribbon

Abdou Hassanien[1]
[1]Condensed Matter Physics, Jozef Stefan Institute, Ljubljana

Using scanning tunneling microscopy and spectroscopy we demonstrate a revival of magnetism in 7-armchair nanoribbon by unpassivated atoms at the termini. Namely, a pair of intense Kondo resonances emerges at the peripheries of zigzag terminus revealing the many-body screening effects of local magnetic moments. Although Kondo resonance originates from a missing local orbital, it extends to a distance of 2.5 nm along the edge of the ribbon. The results are complemented by density functional theory calculations which suggest a possible coupling between Kondo states despite screening effects of substrate electrons. These findings indicate a possibility to restore intrinsic magnetic ordering in graphene nanoribbon without major structural modifications.

WED 40
Imaging Propagating Polaritons in Ångstrom Thick WS_2 in Real Space

Mira Kreßler[1], Denis Iagodkin[1], Bianca Höfer[1], Niclas S. Mueller[2], Kirill I. Bolotin[1], Patryk Kusch[1]
[1]Department of Physics, Freie Universität Berlin, Germany
[2]Fritz Haber Institute of the Max Planck Society, Germany

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 down to 10 nm in thickness have been shown [1], 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 WS_2 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 shows pronounced backbending around the binding energies of the A and B exciton, alluding to strong light-matter coupling between excitons and polaritons. This is further supported by modelling the dispersion of a TE_0 mode in monolayer WS_2.

[1] F. Hu et al., Phys. Rev. B 100, 121301 (2019)

WED 41
Optical properties of perovskite/carbon nanotubes hybrid material

Valentina Eremina[1], Petr Obraztsov[1]
[1]Department of Physics and Mathematics, Center for Photonics Sciences, University of Eastern Finland, Joensuu, Finland

The distinctive qualities of perovskite materials, including a high absorption coefficient, superior quantum efficiency, and excellent charge carrier mobilities with large diffusion lengths, make them highly sought after for a wide range of applications. However, a significant drawback of hybrid perovskites is their susceptibility to instability, leading to the loss of properties under ambient conditions. To address this challenge, single-walled carbon nanotubes (SWCNTs) emerge as a promising solution due to their inherent stability, allowing them to effectively host molecules. In this study, we utilized the gas-phase technique to fill large-diameter single-walled carbon nanotubes with $MAPbBr_3$ perovskite. Our investigation reveals notable changes in the optical properties of both perovskites and SWCNTs. We conducted a thorough examination employing photoluminescence, Raman spectroscopy, UV-vis-NIR spectroscopy, and ultrafast transient absorption spectroscopy to characterize the hybrid material.

WED 42
Probing the impact of the substrate on the electron-phonon coupling in graphene

Taoufiq Ouaj[1], Navjot Bamrah[1], Mrityunjay Pandey[1], Patricia Pesch[1], Corinne Steiner[1], Simone Sotgiu[2], Tommaso Venanzi[2], Elena Stellino[3], Claudia Fasolato[4], Marvin Metzelaars[1,5], Paul Kögerler[5,6], Leonetta Baldassarre[2], Bernd Beschoten[1,7], Lutz Waldecker[1], Christoph Stampfer[1,8]
[1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany
[2]Department of Physics, Sapienza University of Rome, Rome, Italy
[3]Sapienza University of Rome, Department of Basic and Applied Science for Engineering, Rome, Italy
[4]Institute for Complex System, National Research Council (ISC-CNR), Rome, Italy
[5]Institute of Inorganic Chemistry, RWTH Aachen University, Aachen, Germany
[6]Peter Grünberg Institute, Electronic Properties (PGI-6) Forschungszentrum Jülich, Jülich, Germany
[7]JARA-FIT Institute for Quantum Information, Forschungszentrum Jülich GmbH and RWTH Aachen University, Aachen, Germany
[8]Peter Grünberg Institute (PGI-9) Forschungszentrum Jülich, Jülich, Germany

Graphene exhibits the highest charge carrier mobility at room temperature on various substrates, limited mainly by electron-phonon scattering. The microscopic details of the electron-phonon coupling (EPC), and how the substrate affects the maximum achievable carrier mobility, are not yet fully understood. Here, we study the electronic properties as well as the EPC in graphene with different environments using Raman spectroscopy. We focus on two 30° twisted graphene layers to study the influence of screening for two graphene layers in proximity to each other. A 2D linewidth of $12.5\,cm^{-1}$ confirms the presence of two electronically decoupled layers and indicates a high electronic quality, comparable to graphene encapsulated in hBN. We further observe a blue shift of the 2D Raman peak position, which we link to a softening of the Kohn anomaly at the K-point. Magneto-Raman measure-

ments reveal a reduced Fermi velocity which may be linked to efficient screening of electron-electron interactions, suppressing the renormalization of the Fermi velocity. Importantly, separation by a monolayer hBN is already sufficient to lift this impact of the two graphene layers on each other.

WED 43

Terahertz time domain spectroscopy used on 2D heterostructures including Graphene. Applications

David Arcos[1,3], Joan Esteve[2], Núria Ferrer-Anglada[3]
[1]Universitat de Vic, Vic (Barcelona)
[2]Department of Applied Physics, Universitat de Barcelona, Barcelona
[3]Department of Physics, Universitat Politècnica de Catalunya, Barcelona

We present here a review of the Terahertz time domain spectroscopy methode used to characterize 2D heterostructures with graphene, including graphene with Transition-Metal-Dichalcogenides (TMD). THz time domain spectroscopy is a non destructive, contactless methode allowing to obtain the electrical conductivity of materials in a range of THz frequencies, including 2D materials and heterostructures [1]. Also we analize the applications of those materials on different fields: new optoelectronic devices and sensors, photoconductivity switches, polarized light photodetectors,THz amplification and modulation, THz lasers, picosecond ultrafast pulses, thermoelectric or piezoelectric devices, energy harvesting and storage, batteries, supercapacitors, spintronic devices [2].

[1] Optoelectronic characterization of 2D heterostructures. Gr/MoS2 and Gr/WS2. D. Arcos, D. Nuño, M. Farook Khan, J. Eom, L. Ametller, N. Ferrer-Anglada, 2023, 2300202.DOI: 10.1002/pssb.202300202.
[2] Optoelectronic Properties of Heterostructures.The Most Recent Developments Based on Graphene and Transition Metal Dichalcogenides. N. Pradhan et al, 2017, DOI: 10.1109/MNANO.2017.2676185.

08:30 – 09:00	U. Kaiser, Ulm *From functionalizing inorganic two-dimensional materials on the level of single atoms towards molecular imaging of organic two-dimensional materials*
09:00 – 09:30	D. Akinwande, Austin *Atomristors: Single-Atom Memristors*
09:30 – 10:00	X. Chen, Berlin *Engineering the Chemistry of 2D Transition Metal Dichalcogenides*
10:00 – 10:30	Coffee Break
10:30 – 11:00	F. Fischer, Berkeley *The Road from Semiconductors to Metals: Engineering Topological States in Nanographenes*
11:00 – 11:30	R. Gillen, Swansea *Family Behavior and Dirac Bands in Armchair Nanoribbons with 4-8 Defect Lines*
11:30 – 12:00	I. Stará, Prague 6 *Helicenes as Fascinating Screwed Molecules with Unique Electronic Properties*
12:00 – 17:00	Mini Workshops
17:00 – 17:30	A. Kurzmann, Cologne *Electrostatically defined graphene quantum dots*
17:30 – 18:00	C. Backes, Kassel *Measuring and controlling the dimensions of liquid-exfoliated nanosheets*
18:00 – 18:30	A. Jorio, Belo Horizonte *Summary*
19:00 – 20:30	Farewell Dinner (Bauernbuffet)

08:30
From functionalizing inorganic two-dimensional materials on the level of single atoms towards molecular imaging of organic two-dimensional materials
Ute Kaiser[1]
[1]Ulm University, Ulm

We derive the requirements that must be met to successfully functionalize and image low-dimensional inorganic materials with the electron beam insinde the low-voltage Cc/Cs corrected TEM. Then application on inorganic quantum materials are presented, including TMDs, TMPTs, vertical van der Waals heterostructures and functionalized CNTs. Topics discussed are in situ functionalization of single and multilayer materials, representation of their diverse structural phase polymorphs and transformations with different physical properties, and collective electronic phenomena in the form of excitons and charge density waves. The knowledge gained for the study of inorganic low-D materials is applied to the study of 2D polymers and 2D metal-organic frameworks (MOFs). Key strategies for characterizing defects with sub-2 nm resolution in HRTEM images of imine-based 2D polymer films are presented. These include the choice of a surprisingly low electron acceleration voltage of 120 kV instead of the 300 kV normally used. The talk may be summarized by one sentence that 2D materials and lower-voltage atomic (molecular) resolution TEM are just made for each other.

09:00
Atomristors: Single-Atom Memristors
Deji Akinwande[1]
[1]Electrical and Computer Engineering, The University of Texas at Austin

This presentation focuses on the discovery of memory effect in 2D atomically-thin nanomaterials towards greater scientific understanding and advanced engineering applications. Non-volatile memory devices based on 2D materials are an application of defects and is a rapidly advancing field with rich physics that can be attributed to vacancies combined with metal adsorption. In particular the talk will highlight our pioneering work on monolayer memory (atomristors) that has expanded to over a dozen 2D sheets and can enable various applications including zero-power devices, non-volatile RF switches, and memristors for neuromorphic computing.

09:30
Engineering the Chemistry of 2D Transition Metal Dichalcogenides
Xin Chen[1]
[1]Institute of Chemistry and Biochemistry, Freie Universität Berlin

Since 2004, the rapid gains in graphene-based research and technology have helped propel a resurgence in 2D semiconductors and stimulated the development of 2D materials such as transition metal dichalcogenides (TMDs). From the single-layer transistor to valleytronics, from the TMDs-based heterostructures to the recent twistronics, 2D TMDs have provided unprecedented opportunities in both fundamental research and practical applications. In this talk, I would like to share a few examples of how to engineer the chemistry at the surface and interface of 2D TMDs in order to shape their structures, tailor their optical and electronic properties, and enhance their functions with molecular-level precision.

10:30

The Road from Semiconductors to Metals: Engineering Topological States in Nanographenes

Felix Fischer[1,2,3,4]

[1]Department of Chemistry, University of California, Berkeley, CA 94720, U.S.A.
[2]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, U.S.A.
[3]Kavli Energy NanoSciences Institute at the University of California Berkeley and the Lawrence Berkeley National Laboratory, Berkeley, California 94720, U.S.A.
[4]Bakar Institute of Digital Materials for the Planet, Division of Computing, Data Science, and Society, University of California, Berkeley, CA 94720, U.S.A.

We demonstrated the rational design and experimental realization of a graphene nanoribbon (GNR) superlattices that hosts a 1D array of symmetry-protected topological states, thus generating otherwise inaccessible electronic structure. This new class of materials can be thought of as an extended form of poly-acetylene wherein highly localized half-filled topological states replace the familiar single occupied p-orbitals along a conjugated π-system. Experimental results and first-principles calculations reveal that the frontier band structure of these GNR superlattices is defined purely by the coupling between adjacent topological interface states and can be tuned all the way from a semiconductor and a metal. This novel manifestation of 1D topological phases presents an entirely new route to band engineering in 1D materials based on precise control of their electronic topology and is a promising new platform for future studies of 1D quantum spin physics and metallicity in low dimensional carbon nanomaterials.

11:00

Family Behavior and Dirac Bands in Armchair Nanoribbons with 4-8 Defect Lines

Roland Gillen[1,2], Janina Maultzsch[1]
[1]Department fuer Physik, FAU Erlangen, Erlangen, Germany
[2]College of Engineering, Swansea University, Swansea, UK

Bottom-up synthesis from molecular precursors is a powerful route for the creation of novel synthetic carbon-based low-dimensional materials. The wealth of conceivable precursor molecules introduces a significant number of degrees-of-freedom for the design of materials with defined physical properties. In this context, a priori knowledge of the physical properties provided by modern ab initio simulation methods can act as a valuable guide for the design of novel synthetic carbon-based building blocks.
We performed density functional theory on a family of armchair-edged graphene nanoribbons (AGNR) featuring a bisecting 4-8 ring defect line, which should be accessible through bottom-up synthesis. We show that the electronic structures of defective nanoribbons of increasing width can be classified into three distinct families of semiconductors, similar to the case of pristine AGNR. In contrast to the latter, we find that every third nanoribbon is a zero-gap semiconductor with Dirac-type crossing of linear bands at the Fermi energy. The family behavior arises from the electronic properties of the individual nanoribbon halves on either side of the defect line.

11:30

Helicenes as Fascinating Screwed Molecules with Unique Electronic Properties

Irena G. Stará[1], Ivo Starý[1], Jindřich Nejedlý[1], Jaroslav Vacek[1], Jiří Rybáček[1], Michal Šámal[1], Václav Houska[1]
[1]IOCB Prague, 166 10 Prague 6, Czech Republic

Inherently chiral helicenes[1] have gained significant attention in recent years due to their unique electronic structure, properties and potential applications in various fields such as enantioselective catalysis, molecular recognition, self-assembly, surface science, or as chiral materials.
Here we present the preparation of a series of helicenes with sulfur anchoring groups[2] that were synthesised by intramolecular [2+2+2] cycloisomerisation of corresponding aromatic triynes. Their single-molecule electrical conductance was measured by the STM break-junction method to understand charge transport through helical polyaromatic systems. We also focused on inherently chiral pi-electron macrocycles and their self-assembly into well-ordered 2D molecular crystals on HOPG, which were investigated by ambient AFM and computational methods including MD simulations.[3]

1 Acc. Chem. Res. 2020, 53, 144.
2 J. Org. Chem. 2020, 85, 248.
3 Nanoscale 2023, 15, 1542.

17:00
Electrostatically defined graphene quantum dots
Annika Kurzmann[1], Chuyao Tong[2], Rebekka Garreis[2], Wister Wei Huang[2], Lisa Maria Gächter[2], Jonas Daniel Gerber[2], Max Josef Ruckriegel[2], Folkert Kornelis de Vries[2], Kenji Watanabe[3], Takashi Taniguchi[4], Thomas Ihn[2], Klaus Ensslin[2]
[1]Institute of Physics II, University of Cologne, Cologne
[2]Solid State Physics Laboratory, ETH Zurich, Zurich
[3]National Institute for Materials Science, Research Center for Functional Materials, Tsukuba
[4]National Institute for Materials Science, International Center for Materials Nanoarchitectonics, Tsukuba

Graphene is a promising candidate for future nano-electronic devices including building blocks for quantum information processing. Reasons are the expected long spin lifetimes and high carrier mobility. The improvements in fabrication technologies for graphene nanostructures have leveraged the quality of quantum dots to such an extent, that few-electron or -hole quantum dots have been realized that are comparable to the best devices in gallium arsenide.
Our experimental findings yield a notably clear level scheme for two-particle spectra. Intriguingly, the single-dot two-carrier ground state of bilayer graphene quantum dots is not a paired spin-singlet, but a spin-triplet. This discovery holds significant implications for the design of typical two-carrier singlet-triplet qubits. Through the implementation of charge detection, we have successfully performed Elzerman read-out and measured single-spin relaxation times (T_1) up to 50ms. Recent observations indicate extended valley T_1 relaxation times, approaching 1s, between the spin (valley) (1,1) triplet and (0,2) singlet states in a double quantum dot.

17:30

Measuring and controlling the dimensions of liquid-exfoliated nanosheets

Claudia Backes[1], Stuart Goldie[1], Jonathan N. Coleman[2]
[1]Institute of Chemistry, University of Kassel, Kassel, Germany
[2]CRANN and AMBER, Trinity College Dublin, Ireland

Liquid phase exfoliation (LPE) has become an important production technique for colloidal dispersions and solution-processeable inks of a range of materials. While mass production is possible, samples are inherently polydisperse and size selection, typically by centrifugation, is required to narrow size and thickness distributions. In this talk, I will first discuss our state-of-the-art in measuring nanosheet dimensions through atomic force microscopy, highlighting the challenges associated with this measurement. Then, I will demonstrate that it is possible to derive and validate an accurate equation of motion of nanosheets in the centrifugal field accounting for nanosheet dimensionality. To date, only models exist for spheres. This equation can for example be used to derive expressions for the most probable nanosheet size found in a sediment or supernatant after centrifugation. These describe experimental data for a range of materials in different solvents well. We expect that this equation will allow us to design centrifugation sequences for any nanomaterial beyond size selection by mass, e.g. to change length/thickness aspect ratios in size-selected fractions of 2D materials.

18:00
Summary
Ado Jorio[1]
[1]UFMG, Belo Horizonte, Brazil

Author index