

Name

XXXIIIrd
International Winterschool
on Electronic Properties
of Novel Materials

Molecular Nanostructures

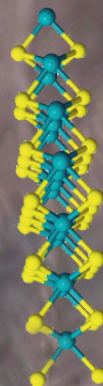
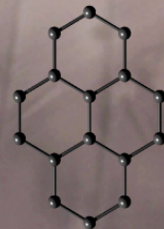
Program

Hotel Sonnalp
Kirchberg/Tirol
Austria



9 - 16 March, 2019

IWEPNM 2019



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Logo designed by Felix Kampmann.

This year's Logo of the IWEPMN shows the surface of a MaPbBr_3 crystal below 145 K and above 150 K, at each of these temperatures a phase-transition occurs. Images were taken by Sebastian Lotter and Felix Kampmann at FAU Erlangen.

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Financial assistance from the sponsors and supporters is greatly acknowledged.

Dear Friend:

Welcome to the 33rd International Winterschool on:

Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of thirty-two 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:

Janina Maultzsch	program
Narine Moses Badlyan	accommodation
Antonio Setaro	finances
Roland Gillen	website, sponsoring
Sören Wasserroth	abstract booklet
Georgy Gordeev	technical assistance, video transfer
Felix Kampmann	announcements, website assistance
Dirk Heinrich	technical assistance, accommodation
Harald Scheel	website
Kati Gharagozloo-Hubmann	technical assistance
Sabrina Jürgensen	technical assistance
Patryk Kusch	sponsoring
Gudrun May-Nasseri	visa applications, general assistance

Also the managers of the hotel, the Mayer family, and their staff promised to help us wherever they can. We want to acknowledge their help.

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

Sincerely yours,
Janina, Stephanie, Andreas, Christoph, and Christian

Chairpersons

J. Maultzsch (Erlangen)

S. Reich (Berlin)

C. Stampfer (Aachen)

A. Hirsch (Erlangen)

C. Thomsen (Berlin)

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J. Robertson (UK)

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 2019 starts on Saturday, 9 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, 16 March, breakfast. There will be a reception party on Saturday, 9 March, after dinner, and a farewell party including dinner on Friday, 15 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 2019 Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria

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

All questions concerning the IWEPNM 2019 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-info@physik.tu-berlin.de, web: www.iwepnm.org

Participation

Participation at the IWEPNM 2019 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 and her team (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 Monday, Tuesday, and Thursday. Poster awards are kindly provided by Wiley VCH.

Conference Publication

Invited and contributed presentations from IWEPM 2019 are scheduled for publication as a special issue in *physica status solidi (pss) (b)*. **Manuscript submission is due on April 30th**. In selected cases articles are highlighted in *pss (RRL)* (Reviews@RRL, Rapid Research Letters) or *Advanced Electronic Materials*. A hard-cover edition will be distributed to the participants.

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

Manuscript preparation and submission

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

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

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

IWEPNM 2019
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 morning, after coffee break evening	Stephanie Reich Nedjma Bendiab Siegmar Roth
Monday, 11.03.	morning morning, after coffee break evening	Janina Maultzsch Hannah Nerl John Robertson
Tuesday, 12.03.	morning morning, after coffee break evening	Otakar Frank Aurélie Pierret Andreas Hirsch
Wednesday, 13.03.	morning morning, after coffee break evening	Christoph Stampfer Francesco Mauri Viera Skakalova
Thursday, 14.03.	morning morning, after coffee break evening	Hans Kuzmany Liv Hornekaer Giusy Scalia
Friday, 15.03.	morning morning, after coffee break evening	Balazs Dora Elena Obratsova Shigeo Maruyama

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

Chairpersons please remember:

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

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

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

We acknowledge your support.

The Organizers

PROGRAM

AND

ABSTRACTS

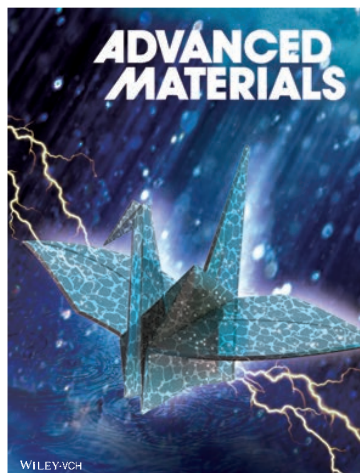
Final program

Sunday, March 10		Monday, March 11		Tuesday, March 12		Wednesday, March 13		Thursday, March 14		Friday, March 15	
Topics	CNT, nanomechanics, TEM	Heterostructures, nanooptics, perovskites	2D materials, excitons, synthesis	Graphene, new materials	Carbon nanostructures, chemistry	Topological properties, applications					
08:30	Wafer-Scale Crystalline Carbon Nanotube Films KONO	TUTORIAL Approaching the Intrinsic Limit in Transition Metal Dichalcogenide van der Waals Heterostructures HONE	Exciton Manipulation in 2D TMDC Heterostructures KIS	TUTORIAL Strategies for band structure engineering in 2D materials ANDREI	Light Emission from Graphene Nanoribbons: Insights from Ab Initio Simulations PREZZI	TUTORIAL Non-hermitian topological photonics SZAMEIT					
09:00	High temperature light emission properties of intrinsic single-walled carbon nanotubes MIYAUCHI		Proximity spin phenomena in 2D materials FABIAN		Bottom-up fabrication of graphene nanoribbons: From molecules to devices BORIN BARIN						
09:30	Thermodynamics at the nanoscale: interfaces, reactive wetting and selective Carbon Nanotubes growth BICHARA	Some theoretical results for twisted bilayer graphene near magic angle ADAM	Redox-Governed Charge Doping in Two-Dimensional Materials Revealed by Optical Spectromicroscopy RYU	Transport in Twisted Bilayer Graphene at Extreme Angles RICKHAUS	Tailoring structural and electronic properties of graphene nanostructures with atomic precision MUGARZA	Photogalvanic effects in Weyl semimetals GOLUB					
10:00 Coffee Break											
10:30	Exploring confined carbyne by Raman spectroscopy HEEG	Phonon Polariton Nanophotonics based on 2D Materials HILLENBRAND	Interlayer excitons in TMDC heterostructures KORN	Dirac electrons in a dodecagonal graphene quasicrystal AHN	Dynamics of Advanced Low-Dimensional Materials by Low-Voltage Atomic-Scale TEM experiments KAISER	Design of Majorana Bound States in Engineered Atomic-Scale Superconductor-Magnet Hybrid systems KIM					
11:00	Nanotube Electro-Mechanical Resonators BACHTOLD	Nonlinear optics and nano-optics with layered and 2D materials DE MATOS	Exciton Linewidth Approaching the Homogeneous Limit in MoS ₂ based Van der Waals Heterostructures MARIE	Ultrafast coherent electron physics in graphene and in a graphene-SiC Schottky junction HOMMELHOFF	Effects of encapsulation on molecular damage under electron irradiation BESLEY	Electroluminescence from carbon nanotubes: low temperature, tailored defects and short channels KRUPKE					
11:30	A graphene-based broadband displacement detector with pm resolution and its applications VERBIEST	Patternable non-polar epigraphene for nano-electronics and Dirac point physics DE HEER	Strained bubbles in van der Waals heterostructures as local emitters of photoluminescence with adjustable wavelength KOPERSKI	Photonic Cooper Pairs and TERS in 2D systems JORIO	Majorana fermions in carbon nanotubes GRIFONI	The photonics of semiconductor nanostructures for new solar energy conversion concepts ALARCON LLADO					

12:00 - 17:00	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops
17:00 - 18:30	Dinner					17:00 Simulation of Raman spectra based on first principles methods KUKUCSKA
18:30	Optics of strained 2D materials HARATS	Double perovskites as p-type conducting transparent semiconductors: A high-throughput search WANG	1-D transition-metal-trichalcogenides in the single-chain limit ZETTL	Oxo-functionalization of graphene and functionalization EIGLER	Chemistry of 2D-Pnictogen Nanomaterials ABELLAN	17:30 Energy transfer in carbon nanotube-based hybrid systems SETARO
19:00	Mapping optical properties of 2D materials in the electron microscope NERL	The many expression of anharmonic nuclear displacements in semiconductors YAFFE	Direct solution-phase synthesis of 1T' WSe ₂ nanosheets MATTEVI	Controlling the Electronic and Chemical Properties of Graphene via Functionalization and Intercalation HORNEKAER	Water-based and bio-compatible inks made of 2D materials for fully printed electronics CASIRAGHI	18:00 Conference Summary JORIO
19:30	First-principles theory of momentum-resolved vibrational spectroscopy in the electron microscope BARONE	A critical review on non-fullerene acceptors - are NFAs the panacea for organic photovoltaics? BRABEC	Polymer Synthesis Enabled by Interfaces: Towards a world of organic 2D materials FENG	Magnetism in the Ultrathin Chromium Trihalides KLEIN	Where did the missing atoms go? From local bandgap tinkering and antidots to nanoporous medley DRNDIC	18:30 - 20:00 Break
20:00	Position and Momentum Mapping of Phonons in the Electron Microscope PICHLER	Poster I Monday	Poster II Tuesday	Two-Dimensional Topological Polymers HEINE	Poster III Thursday	Bauernbuffet Farewell
20:30						
Topics	CNT, nanomechanics, TEM	Heterostructures, nanooptics, perovskites	2D materials, excitons, synthesis	Graphene, new materials	Carbon nanostructures, chemistry	Topological properties, applications
	Sunday, March 10	Monday, March 11	Tuesday, March 12	Wednesday, March 13	Thursday, March 14	Friday, March 15

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**ADVANCED
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WILEY

- 08:30 – 09:00 J. Kono, Houston
Wafer-Scale Crystalline Carbon Nanotube Films
- 09:00 – 09:30 Y. Miyauchi, Kyoto
High temperature light emission properties of intrinsic single-walled carbon nanotubes
- 09:30 – 10:00 C. Bichara, Marseille
Thermodynamics at the nanoscale: interfaces, reactive wetting and selective Carbon Nanotubes growth
- 10:00 – 10:30 Coffee Break
- 10:30 – 11:00 S. Heeg, Zurich
Exploring confined carbyne by Raman spectroscopy
- 11:00 – 11:30 A. Bachtold, Barcelona
Nanotube Electro-Mechanical Resonators
- 11:30 – 12:00 G. J. Verbiest, Delft
A graphene-based broadband displacement detector with pm resolution and its applications
- 12:00 – 17:00 Mini Workshops
- 17:00 – 18:30 Dinner
- 18:30 – 19:00 M. Harats, Berlin
Optics of strained 2D materials
- 19:00 – 19:30 H. C. Nerl, Berlin
Mapping optical properties of 2D materials in the electron microscope
- 19:30 – 20:00 P. Barone, Chieti
First-principles theory of momentum-resolved vibrational spectroscopy in the electron microscope
- 20:00 – 20:30 T. Pichler, Vienna
Position and Momentum Mapping of Phonons in the Electron Microscope

Sunday, March 10th

CNT, nanomechanics, TEM

08:30**Wafer-Scale Crystalline Carbon Nanotube Films**Junichiro Kono¹

¹Department of Electrical and Computer Engineering, Department of Physics and Astronomy, and Department of Materials Science and NanoEngineering, Rice University, Houston

We have recently developed a controlled vacuum filtration method for the preparation of wafer-scale films of crystalline chirality-enriched single-wall carbon nanotubes [1,2]. Here, we will first discuss the controlled vacuum filtration technique, and summarize our recent discoveries in optical spectroscopy studies and optoelectronic device applications using films prepared by this technique. These include the observation of intersubband plasmons [3], microcavity exciton polaritons with polarization-dependent ultrastrong coupling [4], isotropic Seebeck coefficient with anisotropic electrical conductivity [5], and the direct observation of cross-polarized excitons [6].

1. W. Gao and J. Kono, arXiv:1810.02928.
2. X. He *et al.*, *Nature Nanotechnology* **11**, 633 (2016).
3. K. Yanagi *et al.*, *Nature Communications* **9**, 1121 (2018).
4. W. Gao *et al.*, *Nature Photonics* **12**, 362 (2018).
5. K. Fukuhara *et al.*, *Applied Physics Letters* **113**, 243105 (2018).
6. F. Katsutani *et al.*, *Physical Review B* **99**, 035426 (2019).

09:00**High temperature light emission properties of intrinsic single-walled carbon nanotubes**Yuhei Miyauchi^{1,2}¹Institute of Advanced Energy, Kyoto University, Kyoto, Japan²Graduate School of Science, Nagoya University, Nagoya, Japan

In semiconducting single-walled carbon nanotubes (SWNTs), it is expected that excitons are thermally stable even at high temperature more than 1000 K because of their large binding energy [1,2]. Pioneering studies reported high-temperature light emission from heavily carrier-doped SWNTs heated by current injection [3,4]. However, such conditions could considerably modify the system [5], and the fundamental role of excitons in the high temperature radiation still remains to be understood. Recently, we reported thermal radiation from intrinsic (undoped) semiconducting SWNTs individually suspended in vacuum [6]. Emission with very narrow spectral bandwidth was observed even at 1000-2000 K, and the feature was clearly attributed to excitons. Our recent progress in the study on the light emission properties of high temperature SWNTs will be discussed.

[1] F. Wang, et al., *Science* 308, 838 (2005).

[2] J. Maultzsch, et al., *Phys. Rev. B* 72, 241402(R) (2005).

[3] D. Mann, et al., *Nat. Nanotechnol.* 2, 33 (2007).

[4] Z. Liu, et al., *ACS Nano* 5, 4634 (2011).

[5] Y. Miyauchi, et al., *Phys. Rev. B* 92, 205407 (2015).

[6] T. Nishihara, et al., *Nat. Commun.* 9, 3144 (2018).

09:30**Thermodynamics at the nanoscale: interfaces, reactive wetting and selective Carbon Nanotubes growth**Christophe Bichara¹¹Centre Interdisciplinaire de Nanoscience, CNRS and Aix-Marseille Univ, Marseille

Recent progress towards an efficient and selective synthesis of carbon nanotubes [1, 2] should be complemented with an improved understanding of their growth mechanisms. We show here how the structure of the nanotubes can be controlled by the properties of the tube/catalyst interface.

Using tight binding Monte Carlo simulations, we could derive metal-carbon nanoparticle's phase diagrams [3], and understand how to control the nanotube's growth mode [4]. We now develop a thermodynamic modeling of the interface [5] to show that, at low temperature, only zigzag or armchair tubes are stable. Chiral tubes become stable at higher temperature because of the configurational entropy of the tube edge in contact with the catalyst, that is a key element of the model. This enables us to link the catalyst interfacial properties and the temperature with the resulting equilibrium chiral distribution, thus accounting for a number of experimental observations and suggesting ways to design new, selective catalysts.

[1] Nature 510, 522–524 (2014)

[2] Nat. Catal. 1, 326–331 (2018)

[3] PRL 115, 205502 (2015)

[4] Nanoscale 10, 6744, (2018)

[5] Science 362, 212–215 (2018)

10:30

Exploring confined carbyne by Raman spectroscopy

Sebastian Heeg¹

¹Photonics Lab, D-ITET, ETH Zürich, Zürich

Long linear carbon chains encapsulated inside carbon nanotubes are the finite realization of carbyne, the truly one-dimensional allotrope of carbon. In this talk I will present our recent studies of individual pairs of double-walled carbon nanotubes and encapsulated linear carbon chains by wavelength-dependent and tip-enhanced Raman scattering. We observe that the nanotube chirality determines the vibronic and electronic properties of the encapsulated carbon chain and provide a first insight into the dynamics of the chain's excited electronic states. Finally, I will present our most recent result on single, isolated carbon chains inside carbon nanotubes and provide an outlook into future directions.

11:00**Nanotube Electro-Mechanical Resonators**Adrian Bachtold¹¹ICFO - The Barcelona Institute of Science and Technology, Barcelona

Mechanical resonators based on carbon nanotubes feature a series of truly exceptional properties. Carbon nanotubes are so small that they make the lightest resonators fabricated thus far. The mechanical vibrations are enormously sensitive to the dynamics of the electrons through the nanotube, and vice versa. Taking advantage of this coupling, we developed a novel detection method that allows us to measure the mechanical vibrations of nanotube resonators with an unprecedented sensitivity. The detection consists in measuring the electrical noise with a RLC resonator and a high electron mobility transistor (HEMT) amplifier cooled at liquid-helium temperature. This allows us to measure the thermal vibrations of a 91 MHz frequency nanotube resonator with 7 million quality factor down to about 15 quanta of vibrations in a dilution fridge. In this talk, I will discuss our efforts to increase the electro-mechanical coupling, the effect of the vibrations on the quantum electron transport, and how the current through the nanotube amplify and cool the amplitude of the thermal vibrations.

11:30**A graphene-based broadband displacement detector with pm resolution and its applications**G.J. Verbiest¹¹Precision and Microsystems Engineering, Delft University of Technology, TU Delft

Graphene is a single atomic layer of carbon with a low mass density and a high Young's modulus. These properties make mechanical resonators of graphene very sensitive to external perturbations. Graphene resonators allow for electrical read-out which makes them an ideal candidate for microelectromechanical systems (MEMS). The key element is an electrostatic gate underneath the graphene to (i) tune the carrier density and (ii) deflect the graphene resonator. Even a low carrier mobility of $1.500 \text{ cm}^2/\text{Vs}$ translates a change of 20-25 pm in graphene-gate distance into a measurable current of 50 pA. This sensitivity of 400 pm/nA outperforms state-of-the-art read-out schemes for MEMS with force and displacement output. Remarkably, the sensitivity is independent of the mechanical resonance frequencies and therefore puts forward a graphene-based broadband displacement detector.

Here I show that such a graphene-based broadband displacement detector detects ultrasound up to at least 100 MHz as well as the static displacements of a miniaturized comb-drive actuator with pm resolution. Our work paves the way for miniaturized gyroscopes, accelerometers, and high-frequency ultrasound detector.

18:30**Optics of strained 2D materials**Moshe Harats¹, Sviatoslav Kovalchuk¹, Mengxiang Qiao¹, Kirill Bolotin¹¹Fachbereich Physik, Freie Universität Berlin, Berlin

2D materials have attracted a lot of attention from the research community for their unique physical properties. One of their most celebrated features is their stiffness as well as their breaking strength. As an example, Graphene is one of the strongest materials in the world with a Young's modulus of 1TPa. A special class of 2D materials, transition metals dichalcogenides (TMDC) is optically active and hosts excitons even at room temperature. As all TMDC can be deformed easily as any other 2D material, it is crucial to understand the role of strain on their optical properties. In this talk I will present the different approaches in the field of mechanics of 2D materials and how to approach the elastic deformations of 2D materials from the optics side. I will show how by engineering a local strain profile in 2D materials we can achieve two different phenomena – funneling of excitons in WS_2 and creation and annihilation of narrow line emitters in hBN.

19:00

Mapping optical properties of 2D materials in the electron microscope

Hannah Catherine Nerl¹

¹Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin

Macroscopic properties of 2D materials are influenced, even dominated by structural variations occurring at the scale of individual atoms. To date, these macroscopic properties are mostly studied using bulk techniques which average out signals over length scales of microns or more and therefore cannot provide the localised information needed to study 2D materials at the relevant scale.

Recent technical improvements in scanning transmission electron microscopy (STEM) electron energy-loss spectroscopy (EELS) [1, 2] have led to a resolution revolution resulting in a simultaneous and unprecedented improvement in spatial and energy resolution. I will show how using high resolution low loss (LL) STEM EELS techniques, it has now become possible to reliably access new information such as the near-infrared/visible/ultraviolet spectral range to study optical properties at the level of individual atoms. This opens up possibilities to map excitons and plasmons in nanosheets and to study the effects of edges, steps and surface impurities.[3]

1. Krivanek, O.L. et al. *J Microsc*, 2015.
2. Ramasse, Q.M. et al. *Ultramicrosc.*, 2017.
3. Nerl, H.C., et al. *npj 2D Materials and Applications*, 2017.

19:30**First-principles theory of momentum-resolved vibrational spectroscopy in the electron microscope**Paolo Barone¹, Francesco Mauri², Ryosuke Senga³, Thomas Pichler⁴, Kazu Suenaga³¹CNR-SPIN, Chieti, Italy²Dipartimento di Fisica, Università di Roma La Sapienza, Rome, Italy³AIST, Tsukuba, Japan⁴Faculty of Physics, University of Vienna, Vienna, Austria

Recent developments in electron microscopy, aiming at improving momentum and energy resolutions of electron energy loss spectroscopy in transmission (EELS-TEM), allow to measure phonon dispersions of nanosized materials. However, experiments have been limited so far to polar insulating materials, based on the infrared selection rule that applies in the long wavelength limit. Here I will discuss our recently developed first-principle description of EEL vibrational spectra. The EEL intensity can be expressed in a form that reminds the standard expression of the infrared oscillator strengths, in terms of a momentum-dependent effective charge which fully takes into account the effect of valence-electron screening beyond the spherical rigid-ion approximation. Remarkably, our theory shows that sizeable EEL intensities can be expected at large momenta in metals and insulators alike, irrespectively of their infrared polarizability. The simulated spectra are in excellent agreement with those recently measured in boron nitride, graphite and graphene (see also talk by T. Pichler), allowing for a comprehensive interpretation of experimental results.

20:00**Position and Momentum Mapping of Phonons in the Electron Microscope**Thomas Pichler¹, Ryosuke Senga², Kazu Suenaga², Francesco Mauri³, Paolo Barone⁴¹Faculty of physics, University of Vienna, Vienna²aist, Tsukuba, Japan³la sapienza university, Rome, Italy⁴spin-cnr, Rome, Italy

Improving the energy resolution in electron energy loss spectroscopy inside a transmission electron microscope enables the application in phonon spectroscopy. However, these experiments have been still limited regarding their momentum resolution and to polar materials. Here, first examples on position and momentum mapping of phonons in apolar graphene nanostructures will be given [1]. This provides a new pathway to determine the phonon dispersions down to the scale of an individual free-standing graphene monolayer with nanometer size lateral resolution by mapping the distinct vibrational modes for a large momentum transfer. The measured scattering intensities are accurately reproduced and interpreted with density functional perturbation theory (see also talk by P. Barone). Additionally, a nanometre-scale mapping of selected momentum resolved phonon modes using graphene nanoribbon structures allows to spatially disentangle bulk, edge and surface vibrations.

[1] R. Senga et al. arxiv.org/abs/1812.08294

- 08:30 – 09:30 **TUTORIAL: J. Hone, New York**
Approaching the Intrinsic Limit in Transition Metal Dichalcogenide van der Waals Heterostructures
- 09:30 – 10:00 **S. Adam, Singapore**
Some theoretical results for twisted bilayer graphene near magic angle
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **R. Hillenbrand, San Sebastian**
Phonon Polariton Nanophotonics based on 2D Materials
- 11:00 – 11:30 **C. J. S. de Matos, Sao Paulo**
Nonlinear optics and nano-optics with layered and 2D materials
- 11:30 – 12:00 **W. A. de Heer, Atlanta**
Patternable non-polar epigraphene for nanoelectronics and Dirac point physics
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **H. Wang, Halle**
Double perovskites as p-type conducting transparent semiconductors: A high-throughput search
- 19:00 – 19:30 **O. Yaffe, Rehovot**
The many expression of anharmonic nuclear displacements in semiconductors
- 19:30 – 20:00 **C. J. Brabec, Erlangen**
A critical review on non-fullerene acceptors – are NFAs the panacea for organic photovoltaics?
- 20:00 **Poster Session I**

Monday, March 11th

Heterostructures, nanooptics, perovskites

08:30**Approaching the Intrinsic Limit in Transition Metal Dichalcogenide van der Waals Heterostructures**James Hone¹¹Mechanical Engineering, Columbia University, New York

Studying the intrinsic behavior 2D materials requires attention to both external and internal sources of disorder. This talk will first review the techniques used to create clean heterostructures with hBN to reduce environmental disorder. In graphene, ten years of progress has led to device performance now rivaling the highest-quality GaAs-based heterostructures. Semiconducting transition metal dichalcogenides (TMDs) also benefit from hBN encapsulation but are limited by atomic defects. The types and density of atomic defects in TMDs will be reviewed, as well as progress in synthesis of TMDs with dramatically lower defect density. Combining higher crystal quality and clean encapsulation allows observation of greatly enhanced optical properties, including near-unity photoluminescence quantum yield, and long excited-state lifetime in TMD heterostructures. In addition, electronic transport measurements show improved carrier mobility and reveal many new details of the Landau spectra, including observation of fractional quantum Hall states in monolayer TMDs.

09:30**Some theoretical results for twisted bilayer graphene near magic angle[†]**Shaffique Adam¹¹Yale-NUS College, Singapore

When the relative rotation between two sheets of graphene is set to be close to special angles (referred to as “magic angles”), the low-energy effective theory features Dirac fermions with very flat bands. While the role of disorder [Rev. Mod. Phys. 83, 407 (2011)] and electron-electron interactions [Science 361 570 (2018)] for the Dirac fermions in monolayer graphene is now well-established, the properties of the Dirac fermions in twisted bilayer graphene can be very different. In this talk we discuss three recent results showcasing these differences: First, we show using a Boltzmann-RPA theory that for most of the experimental regime, gauge phonons that are irrelevant for monolayer graphene now dominate the transport [arXiv:1902.01405]; Second, we propose a strong-coupling t-J-D model where fluctuations of the anti-ferromagnetic order in the conducting phase mediates superconducting pairing [arXiv:1902.00029]. Finally, we show that in the presence of long-range Coulomb interactions, there is a universal square-root renormalization [arXiv:1809.07775] of the band anisotropy.

[†]Support from the Singapore Ministry of Education (MOE2017-T2-1-130, MOE2017-T2-2-140).

10:30

Phonon Polariton Nanophotonics based on 2D Materials

Rainer Hillenbrand¹

¹CIC nanoGUNE, San Sebastian

Phonon polaritons in 2D materials exhibit ultra-short wavelengths, long lifetimes and strong field confinement, which allows for manipulating infrared light at the nanometer scale. Here, we discuss real-space nanoimaging studies of infrared phonon polaritons in boron nitride and molybdenum trioxide nanostructures and metasurfaces, revealing intriguing aspects such as polariton propagation with anomalous wavefronts or with ultra-long lifetimes of several 10 picoseconds.

11:00

Nonlinear optics and nano-optics with layered and 2D materials

Christiano J. S. de Matos¹

¹MackGraphe, Mackenzie Presbyterian University, Sao Paulo, Brazil

Two-dimensional (2D) materials, as well as bulk crystals composed of layered structures, present a multitude of interesting and unusual optical properties. Despite linear and far-field phenomena being the most widely reported, nonlinear optical effects as well as near-field, nano-optical, phenomena are perhaps between the most promising for novel applications. In this research lecture I will review our recent work on nonlinear optical frequency conversion in 2D materials, such as phosphorene, MoS₂ and graphene, as well as in layered van der Waals materials. Mechanism behind the observed high nonlinearities will be discussed. In the field of nano-optics, I will discuss the investigation of the oxidation process in black phosphorus using infrared nanospectroscopy with a scattering-type near-field optical microscope, as well as the ability to modify the near-field response of optical surfaces with layered materials. The reported work is funded by the Sao Paulo Research Foundation (FAPESP).

11:30**Patternable non-polar epigraphene for nanoelectronics and Dirac point physics**Vladimir Prudkovskiy^{1,3}, Yiran Hu¹, Hue Yu¹, Lei Ma², Claire Berger^{1,3}, Walt A. de Heer^{1,3}¹Georgia Institute of Technology, Atlanta GA USA²Tianjin International Center for Nanoparticles and Nanostructures, Tianjin China³Neel Institute, CNRS, Grenoble, France

Exceptional ballistic conduction with mean free paths that can exceed 100 microns at room, and involve a single ballistic channel ($G = G_0 = e^2/h$) was recently reported. The transport occurs in graphene that grows on the sidewalls of trenches etched into the 0001 face of electronic grade hexagonal silicon carbide using vacuum sublimation techniques (epigraphene). The single channel transport is at odds with the expectation that ballistic transport should involve an even number of channels and therefore indicates that both spin and valley degeneracy are lifted. A permanent electric dipole moment at the sidewall surface was originally expected to cause the symmetry breaking. SiC wafers that were cut at an angle to 0001 face were prepared at the Tianjin International Center for Nanoparticles and Nanostructures. The wafers were graphitized and micron scale top gated Hall bar structures were patterned using standard lithography methods. Magnetotransport measurements revealed striking transport properties. Ballistic transport involving a $1 G_0$ channel is observed even at the Dirac point. A quantum Hall plateau with $G_H = 4G_0$ is observed that involves a graphene monolayer (for which $G_H = 4(n + 1/2)G_0$ is expected). The anomalous value is caused by a quantized current in the Hall bar that does not have a Hall effect. This current is in parallel with an equal current that passes through the Hall bar. These properties are suspected to be caused by edges that are pinned at the Dirac point. The effects appear to be temperature independent and are consistent with those observed in sidewall ribbons. These results indicate that nonpolar epigraphene is not only a promising candidate for epigraphene nanoelectronics but also for Dirac point physics.

Exceptional ballistic transport in epitaxial graphene nanoribbons Jens Baringhaus, Ming Ruan, Claire Berger, Christoph Tegenkamp, Walt A. de Heer, et al. Nature, 506, 349, (2014)

18:30

Double perovskites as p-type conducting transparent semiconductors: A high-throughput search

Haichen Wang¹, Paul Pistor¹, Miguel A. L. Marques¹, Silvana Botti²

¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale)

²Institut für Festkörpertheorie und -Optik, Friedrich-Schiller-Universität

We perform a systematic study of the family of quaternary halide perovskites in order to find good candidates for transparent p-type conduction. This is achieved by using high-throughput techniques based on density-functional theory, and by screening the materials with regard to their stability, electronic band gap, and hole effective masses. We find a total of 17 double perovskites with promising properties, 10 of which not including toxic or rare chemical elements. Furthermore, in most of these systems, doping might be achieved by adjusting the chemical potential of the two cations during the growth process. Due to chemical similarity, we expect that these materials are compatible with current photovoltaic technology based on organic halide perovskites.

19:00

The many expression of anharmonic nuclear displacements in semiconductors

Omer Yaffe¹

¹Weizmann Institute, Rehovot

The dielectric response, charge carrier mobility and lifetimes, and many other physical properties of semiconductors are typically modeled and analyzed in terms of harmonic motion of the relevant nuclei. While this approach captures the main physical properties of tetrahedrally bonded semiconductors such as silicon and GaAs, we find that the harmonic approximation fails for semiconductors that have more complex structural dynamics.

I will present experimental studies on two types of such semiconductors: halide perovskites and organic crystals. Both types exhibit strong anharmonic displacements, but their anharmonic nature is expressed differently. I will discuss the sources of anharmonicity in these semiconductors, how it affects their dielectric response, charge carrier mobility, lifetimes and defects.

19:30

A critical review on non-fullerene acceptors – are NFAs the panacea for organic photovoltaics?

Christoph J. Brabec^{1,2}

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²ZAE Bayern e.V., Division Renewable Energies, Solar Factory of the Future @ EnCN, Immerwahrstrasse 2, 91058 Erlangen

The performance of organic photovoltaics has been continuously increasing over the last years. Interestingly, with the emergence of the perovskite technology, the development speed of organics rather increased than decreased. Efficiencies of 15 % have been certified recently with further reports claiming over 17 %, organic solar cells with a lifetime of over 100.000 hours under 1 sun illumination were reported, selected composites showed a radiative recombination efficiency above 0.01 % and novel concepts allowed the successful deposition of nanoparticulate organic solar cells from water or alcohols.

Interestingly, many of these record performance values were reported when fullerenes were replaced by so called non-fullerene acceptors (NFAs). This led to the impression that NFAs are the panacea for organic photovoltaics which can resolve all the long time challenges of the OPV technology.

This talk will discuss the more fundamental differences between fullerene based and non-fullerene based acceptors, analyzes the gain and loss mechanisms of the single molecules and tries to give insight whether long time problems indeed can be overcome by NFAs.

MON 1**Rational Fabrication of Carbon-Nanostuctures by HF-Nanozipping on Metal Oxide Surfaces**Konstantin Amsharov¹¹Institute of OrganicChemisry II, Universität Erlangen-Nuremberg, Erlangen

The rational on-surface synthesis of nanographenes and carbon nanoribbons directly on nonmetallic surfaces has been an elusive goal for a long time. We report that activation of the C-F bond is a reliable and remarkably versatile tool enabling the intramolecular aryl-aryl coupling directly on metal oxide surfaces. A challenging multistep transformation enabled by C-F bond activation led to a domino-like coupling that yielded tailored nanographenes.[1,2] We show that fluorine positions in the precursor structure unambiguously dictated the running of the “zipping-program” resulting in rolling-up of oligophenylene chains to the preprogrammen nanostructuer. The high efficiency of the HF-zipping makes our approach attractive for the rational synthesis of nanographenes and nanoribbons directly on insulating and semiconducting surfaces.

[1] A.K. Steiner, K. Amsharov, *Angew.Chem.Int.Ed.* 56, 14732–14736 (2018)[2] K. Amsharov et al., *Science* 363,57-60 (2019)**MON 2****Graphene Trampolines: Soft clamping and strain engineering**Jan N. Kirchhof¹, Katja Höflich², Sviatoslav Kovalchuk¹, Kirill Bolotin¹¹Department of Physics, Freie Universität Berlin, Germany²Department Nanoscale structures and microscopic analysis, Helmholtz-Zentrum Berlin, Germany

The unique mechanical properties of graphene make it an ideal candidate for the implementation into nanomechanical resonators. Yet many potential applications of graphene resonators are hindered by their rather low quality factors at room temperature. Here we introduce the approach of soft clamping and strain engineering, which has previously been applied to Silicon Nitride resonators, to 2D-materials. By patterning drum resonators into trampolines of various geometries using a Helium Ion beam lithography, we force a redistribution of the built-in strain away from the clamping points and thereby greatly enhance the quality factors. Overall, this approach forms a promising playground for studying non-linear effects, enhanced side band cooling and amplification and allows to unlock applications such as improved force and mass sensing at room temperature.

MON 3**Towards Tuneable IR Emission by Liquid-Phase Exfoliated Nanosheets**Kevin Synnatschke¹, Sabrina Steffens¹, Zdenek Sofer², Claudia Backes¹¹Applied Physical Chemistry, University of Heidelberg, Heidelberg²Department of Inorganic Chemistry, University of Chemistry and Technology, Prague

Liquid-phase exfoliation (LPE) techniques coupled with centrifugation methods have become popular to prepare dispersions of a versatile class of materials in bulk quantities of variable nanosheet sizes and thicknesses. The properties of these materials are drastically changing from bulk to few- and monolayer sheets due to quantum confinement.

This makes the control over sheet size and thickness by post-exfoliation treatments extremely important. In this regard, liquid-phase cascade centrifugation has been established as promising methodology to obtain narrower sheet size and thickness distributions.

In this contribution, we show recent results on tuneable nIR emission of liquid-phase exfoliated indium selenide nanosheets. The production of dispersions with well-defined size and thickness by centrifugation techniques allows to tailor the band gap and thus the emission energy of the nanomaterial. Statistical TEM calibrated AFM measurements allow to determine the size and thickness distributions precisely and allocate valuable metrics by correlation with optical spectroscopy. These can be used to prepare dispersions of the desired size and thickness on demand.

MON 4

Impact of temperature and excitation laser power on the Raman spectra of chemically functionalized MoS₂

Narine Moses Badlyan¹, Wanzheng Zhang², Kathrin Knirsch², Andreas Hirsch², Janina Maultzsch¹

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In the past few years, transition metal dichalcogenides (TMDCs), such as molybdenum disulfide (MoS₂), have attracted particular attention due to their unique properties, which make them promising for applications in optoelectronics, photonics, and biotechnology.

Due to their large surface, they offer the opportunity to tune their electronic and optical properties as well as the nature of their interaction with the environment by covalent or non-covalent functionalization.

Here we present a spectroscopic study of MoS₂, functionalized with organic molecules and compare it with a chemically exfoliated and reference sample. We discuss the effect of excitation laser power as well as of temperature on the Raman spectra. Our results suggest that the covalent functionalization is removed under certain conditions. In addition, we analyze the differences between mechanically exfoliated MoS₂ and MoS₂ powder used as starting material.

MON 5**Zeeman splitting and inverted polarization of biexciton emission in monolayer WS₂**

Philipp Nagler¹, Mariana V. Ballottin², Anatolie A. Mitioglu², Mikhail V. Durnev³, Takashi Taniguchi⁴, Kenji Watanabe⁴, Alexey Chernikov¹, Christian Schüller¹, Mikhail M. Glazov³, Peter C. M. Christianen², Tobias Korn¹

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²High Field Magnet Laboratory (HFML), Nijmegen, The Netherlands

³Ioffe Institute, St. Petersburg, Russia

⁴National Institute for Materials Science, Japan

Monolayer TMDCs are an ideal testbed to study the physics of quasiparticles in the two-dimensional limit. Besides excitons, more complex many-body states such as trions and biexcitons can emerge due to the strong Coulomb interaction in these materials. Here, we shed light on the intricate many-body physics of biexcitons in monolayer WS₂ [1]. The encapsulation of the monolayer between two sheets of hBN significantly reduces the overall spectral broadening and allows us to observe biexciton emission with linewidths below 5 meV at 4 K. In magneto-PL experiments, we observe an inverted field-induced polarization, implying a preferential population of the high-energy peak in emission. We explain this unusual phenomenon by considering the evolution of the total energy of the biexciton complex in a magnetic field. Based on the experimental results and the developed model, we are able to identify the momentum space configuration of the optically dominant biexciton state of monolayer WS₂.

[1] P. Nagler et al., Phys. Rev. Lett. 121, 057402 (2018)

MON 6**High temperature PIN diodes based on amorphous hydrogenated silicon carbide and boron-doped diamond thin films**

Ha The Stuchlikova¹, Zdenek Remes¹, Vincent Mortet¹, Petr Ashcheulov¹, Grigoriy Krivyakin^{2,3}, Vladimír Volodin^{2,3}, Jiri Stuchlik¹

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The novel a-SiC:H diode structures on transparent conductive boron-doped diamond (BDD), have been deposited by the PECVD. The future of in-situ integration of nanoparticles and quantum dots in thin film structures for optoelectronic applications requires deposition temperatures above 400 °C. On the boron-doped diamond were deposited thin film PIN structure on the base of a-SiC:H. The layers have been studied by the SEM, temperature resolved electrical conductivity, optical absorbance, photocurrent and PL spectroscopy. The BDD/a-SiC:H diodes have been characterized by I-V measurement and by EL spectroscopy. This work was supported by the

CSF project 19-02858J, the MEYS project LTC17029 INTER-COST Action MP1406 and by the Operational Programme Research, Development and Education financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. SOLID21 - CZ.02.1.01/0.0/0.0/16 019/0000760).

MON 7

Excitation-Tunable Tip-Enhanced Raman Spectroscopy

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Tip-enhanced Raman spectroscopy (TERS) is a powerful technique for nanoimaging. TERS provides optical images together with topography information and chemical composition. Conventional TERS is limited to one excitation energy, guaranteeing maximum enhancement. With such a setup, it is impossible to perform excitation-dependent TERS. Varying the excitation energy during TERS will allow performing spatial resolved resonant Raman scattering with nanometer resolution. We present here excitation-tunable TERS (e-TERS). The setup records tip-enhanced Raman spectra as a function of excitation wavelength and tip position. To demonstrate the full potential of the e-TERS setup, we investigate a densely packed film consisting of carbon nanotubes. We nanoimage and identify nine tube chiralities inside a 100 nm x 100 nm sample area inside the film by using the unique assignment via the radial breathing mode. We envision manifold applications of e-TERS as it allows identifying and imaging optical transitions, which opens new possibilities to study electronic and vibronic properties of molecules, macromolecules and different 1D and 2D samples with nanometer spatial resolution.

MON 8

Anisotropic strain effects in small-twist-angle graphene on graphite

Márton Szendrő¹, András Pálinkás¹, Péter Süle¹, Zoltán Osváth¹

¹Hungarian Academy of Sciences, Centre for Energy Research, Institute of Technical Physics and Materials Science, Nanostructures Department

Moiré-patterns are commonly found superstructures in 2D heterostructures. In ideal circumstances the patterns are regular and periodically repeating by a constant Moiré-wavelength. However, when the constituent lattices have atomic scale deformations due to a strain field, the strain can be observed on a much larger scale through the Moiré-pattern, which become irregular and anisotropic. With small twist angle and lattice mismatch the effect is more pronounced. Here we present a new numerical/graphical method which is capable of reconstructing the underlying strain field deduced only from the distortion of the Moiré-pattern measured by STM on a small-twist-angle (0.6°) graphene on HOPG. We observe distorted Moiré-patterns

with a spatially varying period in annealed gr/HOPG, which reflects a locally strained graphene. STS measurements show electronic states at the Dirac point, localized on Moiré-hills. DFT calculations confirm that AAB stacked regions contribute electronic states near the Fermi-level.

A. Pálincás et al. (2016) Carbon, 107, 792–799.

P. Süle, M. Szendrő et al. Nano Letters, 15(12), 8295–8299.

P. Süle, M. Szendrő et al. (2014). Carbon, 77(111), 1082–1089.

MON 9

Passivation Mechanism of the Sulphur Vacancy in MoS₂

John Robertson¹, Haichang Li¹

¹Cambridge University, , Cambridge

Vacancies are common defects in semiconductors and cause carrier recombination, charge trapping and a Fermi level pinning at their contacts. In Si and other 3D semiconductors, it is essential to passivate such defects. Hydrogen is very effective for this in Si, but it is apparently not effective in MoS₂. On the other hand, the superacid TFSI causes a recovery of the photoluminescence efficiency in MoS₂ [1]. This could be linked to passivation by a strong proton donating effect. But what is the mechanism? We show that MoS₂ differs from Si because it has resonant, multi-centered bonding so that three hydrogens are needed in the correct charge state to form a symmetric closed-shell configuration to passivate the vacancy properly [2]. Otherwise, an asymmetric configuration occurs, which does not remove all states from the gap.

[1] M Amani, A Javey, Science 350 1065 (2015)

[2] H Li, J Robertson, APL Mater 6 066104 (2018)

MON 10

MoS₂ thin films fabricated by sulfurization of high quality MoO₃ films

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Two-dimensional materials attract a high research interest and MoS₂ is likely the most explored compound from this group. Sulfurization of a molybdenum oxide (MoO₃) offers a simple method for fabrication of MoS₂ thin films, but the improvement of quality is still a challenge. MoS₂ thin films were fabricated by using one zone sulfurization of the MoO₃ layers. MoO₃ thin layers were fabricated by RF magnetron sputtering under different conditions (temperature, pressure etc.). Structure and thickness of MoO₃ and MoS₂ layers were characterized by x-ray diffraction (XRD) and x-ray reflectometry (XRR), respectively. Thin films were also characterized by

Raman and optical spectroscopy. Surface morphology was studied by atomic force microscopy (AFM). We have studied the properties of the oxide layers prepared under different conditions as well as the influence of MoO_3 on the structure and properties of the final MoS_2 films.

MON 11

Density Functional Theory studies of the Nature of Phase-Transition in Vanadium Dioxide alloys

Haichang Lu¹, John Robertson¹

¹Engineering, University of Cambridge, Cambridge

VO_2 is of great interest on both the physics and applied side because it has a metal-insulator transition involving a change in structure and electronic structure which are related but separate features. For certain applications (non-volatile memories, steep-slope, RF or optical switches, window coatings), it is often desired to vary the band gap and to increase or decrease the transition temperature. This can be done by strain if the VO_2 is grown epitaxially on say TiO_2 . It can also be done by alloying with oxides such as GeO_2 or MgO . Here, we carry out density functional supercell calculations on these alloys. The band gap of the alloys roughly changes because the band edges of both M1 and M2 phases are made of V 3d bands. All MgO alloyed structures have a spin-paired V-V chain and anti-ferromagnetic order as in the M2 phase, indicating that they are phase-switchable. When doped with Ge, the structure relaxes to the rutile phase, because GeO_2 is in the rutile form. The result is consistent with experimental observation and it gives an important view to explain the mechanism of alloys.

MON 12

Resonant, plasmonic Raman enhancement of alpha-6T molecules encapsulated in carbon nanotubes

Sören Wasserroth¹, Sebastian Heeg^{2,3}, Niclas S. Mueller¹, Patryk Kusch¹, Uwe Hübner⁴, Etienne Gaufres⁵, Nathalie Y.-W. Tang⁵, Richard Martel⁵, Aravind Vijayaraghavan², Stephanie Reich¹

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Surface-enhanced and resonant Raman scattering are widely used techniques to enhance the Raman intensity by several orders of magnitude. SERS uses plasmonic near-fields to enhance the Raman scattering process, whereas electronic transitions are the origin of the enhancement in resonant Raman scattering. Typical Raman reporters in SERS are molecules; in the discussion of plasmonic en-

hancement, the intrinsic resonance of the molecules is often ignored. We present a wavelength dependent Raman study of sexithiophenes encapsulated in carbon nanotubes. To distinguish between the intrinsic resonance and plasmonic enhancement we investigate different tube bundles with and without plasmonic near field. The filled nanotubes are placed precisely in a gold dimer gap by dielectrophoretic deposition. Polarization dependent Raman measurements confirmed the alignment of the molecules within the nanotubes and the influence of the plasmonic near-field. By tuning the excitation wavelength, we were able to determine the intrinsic molecular resonance and observed a strong redshift towards the plasmon resonance of maximum Raman intensity under plasmonic enhancement.

MON 13

Phonon dispersion relation and resonances of valley depolarization in in single-layer TMDCs

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We present the first experimental, full basal plane phonon dispersion, determined by inelastic X-Ray scattering with accompanying van-der-Waals corrected DFT-D3 simulations [1]. The implementation of the vdW-correction, allows the simulation of both the dispersion and structural properties, not given in commonly used LDA / PBE calculations. From our calculations, we show the displacement patterns of phonons at the K and M points, allowing further considerations regarding, e.g., scattering selection rules.

Further, we present the resonance behavior of the conservation of circular polarization in single-layer MoS_2 and MoSe_2 [2]. We find that the circular polarization (ρ) of the emitted light is conserved to 100% in MoS_2 and 84% / 79% (A/A^- peaks) in MoSe_2 close to resonance. The values for MoSe_2 surpass any previously reported value. While our measured excitation dependent values of ρ are in good agreement with the previous reported values, the trend of ρ within the resonance of the two materials are distinctively different indicating at least two competing depolarizing processes. We will discuss popular depolarization mechanisms, taking the knowledge of the phonon dispersion into account.

[1]: H. Tornatzky, et al., arXiv:1809.03381.

[2]: H. Tornatzky, et al., Phys. Rev. Lett. 121, 167401 (2018).

MON 14

Statistics and dynamics of the center of mass coordinate in a quantum liquid

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We investigate the properties of the center of mass coordinate of an interacting one dimensional Fermi gas, displaying several distinct phases. While the variance of the center of mass vanishes in insulating phases such as phase separated and charge density wave phases, it remains finite in the metallic phase, which realizes a Luttinger liquid. By combining numerics with bosonization, we demonstrate that the autocorrelation function of the center of mass coordinate is universal throughout the metallic phase. It exhibits persistent oscillations and its short time dynamics reveal important features of the quantum liquid, such as the Luttinger liquid parameter and the renormalized velocity. The full counting statistics of the center of mass follows a normal distribution. Our results are within experimental reach for e.g. carbon nanotubes and cold atomic gases.

MON 15

Excess resistivity in graphene superlattices caused by umklapp electron-electron scattering

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Umklapp processes allow electrons to transfer momentum to the crystal lattice and, therefore, provide a finite electrical resistance in pure metals. Experimental observation of these mechanisms is challenging as they are easily obscured by other dissipation mechanisms. Our recent electron transport studies of graphene-hBN superlattices reveal that umklapp processes dominate the transport characteristics. As the twist angle is reduced, a giant excess resistivity increases degrading the intrinsic carrier mobility over a wide range of temperatures. Aside from fundamental interest, our results have direct implications for the design of possible electronic devices based on heterostructures featuring superlattices.

MON 16

High-density SWCNT thin films towards electric power generation by electrolyte solution flow

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In the Internet of Things (IoT) era, trillions of sensors and devices need power sources, and the new technology collecting small energies from the environment are required. Now we are developing new power generation device, where elec-

trolyte solution flow on atomically thin film generates electric power. In this study, we report the power generation device using high-density single-wall carbon nanotube (SWCNTs) thin films, because of the high mobility and nano-size of SWCNT. Firstly, SWCNTs were separated into semiconducting and metallic SWCNTs by gel column chromatography [1]. To obtain high-density SWCNT thin film, vacuum filtration method was used to make aligned-SWCNTs film. Important point to obtain well-aligned SWCNT film is that the speed of filtration should be slow. Although overall alignment is not good, densely aligned SWCNT films were obtained which confirmed by atomic force microscopy. We fabricated electric power generation device using the SWCNT film and confirmed electric power generation. Details will be discussed in the presentation.

This work was supported by JST CREST Grant Number JPMJCR16Q2, Japan.

1. Y. Yomogida, et al., Nature Commun. 7, 12056

MON 17

Probing the optical properties of a large scale SERS substrate directly by Raman scattering

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We realized and characterized a novel large-scale SERS substrate based on colloidal gold nanoparticles. Drop casting the nanoparticles onto a graphene monolayer, they self-organize nanoparticle layers. The energy of the localized surface plasmon resonance is independent of the number of gold layers, as proven by analyzing the 2D-mode of graphene with energy dependent Raman measurements. We determined the enhancement factor of the SERS substrate through the reporter molecule p-NTP which we studied prior in detail for the SERS measurement without plasmonic enhancement. Position and polarization dependent Raman measurements of the reporter molecule show the high quality and homogeneity of the SERS substrate.

MON 18

Reviving Interlayer Excitons with Suspended MoS₂/WS₂ van der Waals Heterostructures

Kana Kojima¹, Hong En Lim¹, Zheng Liu², Yusuke Nakanishi¹, Takahiko Endo¹, Yu Kobayashi¹, Yutaka Maniwa¹, Yasumitsu Miyata¹

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Recently, large-area van der Waals (vdW) heterostructures with clean interface have been successfully prepared by growing them on the SiO₂/Si substrates using chemical vapor deposition (CVD) method. However, the lattice strain introduced has disrupted the interlayer coupling, while the greater non-radiative relaxation encountered has substantially decreased the PL intensity in such SiO₂/Si supported CVD-grown samples [1]. To better comprehend these phenomena, we prepared suspended monolayer MoS₂ and MoS₂/WS₂ vdW heterostructures by removing them off from the SiO₂/Si surface and investigated the optical responses of the excitons formed.

As compared to the supported ones, the suspended samples show brighter emissions with blue-shifted PL peaks. In addition, the interlayer excitons PL peaks can also be observed in the MoS₂/WS₂ heterostructures after suspension. These results highlight the significance of reducing both the lattice strain and non-radiative relaxation in the interlayer excitons formation, which is crucial for understanding the intrinsic physical properties of vdW heterostructures.

[1] Y. Kobayashi et al. ACS Nano, 9, 4056-4063 (2015).

MON 19

Covalent Diamond–Graphite Bonding: Mechanism of Catalytic Transformation

Semir Tulić¹, Viera Skákalová¹, Thomas Waitz¹, Maria Caplovicova², Gerlinde Habler³, Marian Varga⁴, Mario Kotlar², Viliam Vretenár², Oleksandr Romanyuk⁴, Alexander Kromka⁴, Bohuslav Rezek^{4,5}

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We study the mechanism of converting carbon from a *sp*³-bound to a *sp*²-bound structure via a catalytically driven phase transformation. Using aberration-corrected transmission electron microscopy applied to specimens in cross-sectional geometry, our atom-by-atom observation provides new insights into the interaction between two carbon lattices with extremely different electronic properties; it explains the process of a nanocrystalline diamond to graphite transformation mediated by Ni while drilling channels along grain boundaries. The hemispherical morphology of protruding Ni nanoparticles as well as the crystal orientation and lattice defects of the graphite are explained in terms of a high uniaxial stress that builds up in the channels due to the volume expansion caused by the allotropic transformation. As a highlight, the experimental results provide strong evidence of a covalent bonding between graphite and diamond. Electrical transport through the graphitized surface

of diamond is interpreted by a modified fluctuation-assisted tunneling mechanism, which shows a possible way for novel graphene-diamond devices.

MON 20

Electronic properties of single layer tantalum disulfide on Cu (111)

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We use scanning tunneling microscopy and spectroscopy to characterize monolayer tantalum disulfide grown on single-crystal copper in ultra-high vacuum. We are able to determine the orientation angle between tantalum disulfide and underlying copper lattices using the periodicity of the Moire patterns generated by the interfacial interaction. Furthermore, we show that the interaction also suppresses charge density wave and imparts new electronic properties. We also reveal the atomic scale variations of electronic structure of tantalum disulfide using spatially-dependent spectroscopy. We will discuss the comparison of our experimental results with density functional theory calculations.

MON 21

Continuous Heteroepitaxy of Two-Dimensional Heterostructures Based on Layered Chalcogenides

Yu Kobayashi¹, Shoji Yoshida², Mina Maruyama², Hiroyuki Mogi², Kota Murase², Yutaka Maniwa¹, Osamu Takeuchi², Susumu Okada², Hidemi Shigekawa², Yasumitsu Miyata¹

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²Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba

The in-plane connection and layer-by-layer stacking of atomically-thin layered materials are expected to allow the fabrication of two-dimensional (2D) heterostructures with exotic physical properties and novel engineering applications. However, it is currently necessary to develop a continuous growth process without interface degradation, contamination and/or alloying. Herein, we report the continuous heteroepitaxial growth of 2D multi-heterostructures and nanoribbons based on layered transition metal dichalcogenide (TMDC) monolayers, employing metal organic liquid precursors with high supply controllability. This versatile process enables the formation of in-plane heterostructures with ultra-clean atomically sharp and zigzag-edge straight junctions without defects or alloying around the interface. For the samples grown directly on graphite, we have investigated the local electronic density of states of atomically sharp heterointerface by scanning tunneling microscopy and spectroscopy, together with first principle calculations. These results demonstrate an approach to realizing diverse nanostructures such as atomic layer-based quantum wires and superlattices.

MON 22**Bottom-up graphene growth using non-halogenated precursors**

Kati Gharagozloo-Hubmann¹, Niclas Sven Mueller¹, Christian Lotze¹, Katharina J. Franke¹, Stephanie Reich¹

¹Department of Physics, FU Berlin, Berlin

We present the surface assisted production of graphene in a bottom up approach using a series of non-halogenated organic precursors. The high quality of grown layers are verified by Raman spectroscopy. The high crystall quality of the grown graphene is further verified through transfer onto a TEM-grid and images of the microstructure. The chosen precursor imposes constrictions on the skeleton formula for the low-temperature polymerization to extended sp^2 structures. The polymerization of different CH_3 substituted precursors results in monolayers; their Raman spectra show the characteristic G and 2D bands, but also D band. The measured spectra correlate with the precursor structure and give suggest an uncompleted dehydrogenation of lateral substituted precursors. An excess of precursor molecules causes the growth of fractal structures. Micro Raman spectra of crystal fringes shows narrow lines between the frequency range of the D and G band, reminiscent of graphene nanoribbons.

MON 23**Momentum conserved ultrafast charge transfer dynamics of interlayer excitons in vdW heterostructure**

Pranjal Kumar Gogoi¹, Yung-Chang Lin¹, Ryosuke Senga¹, Kazu Suenaga¹

¹National Institute of Advanced Industrial Science and Technology (AIST), AIST Central 5, Tsukuba 305 - 8565, Japan

Heterostructures of vdW stacked transition metal dichalcogenide monolayers are a fascinating class of 2D materials. Presence of interlayer exciton, where the electron and the hole remain spatially separated in the two layers due to ultrafast charge transfer, is an intriguing feature of these heterostructures. Inevitably, the efficiency of devices with 2D heterostructures is critically dependent on the charge transfer dynamics. However, the role of the relative orientation of the constituent layers on this charge transfer dynamics is not known yet. Investigating MoS_2/WSe_2 vdW heterostructures with aberration-corrected monochromated low-loss electron energy loss (EEL) spectroscopy combined with scanning transmission electron microscopy, we report that momentum conservation is a critical factor in the charge transfer dynamics. The rotation angle dependent EEL spectra reveal that - in the aligned (or anti-aligned) case, the charge transfer rate can be about one order-of-magnitude faster than in the misaligned cases. Our results provide a deeper insight into the role of the fundamental principle of momentum conservation in the 2D vdW heterostructure charge transfer dynamics.

MON 24**Interlayer excitons in stacked TMDC heterostructures**Roland Gillen¹, Janina Maultzsch¹¹Department Physik, FAU Erlangen, Germany

We computed the theoretical bandstructures and absorption spectra of bilayer MoSe₂-WSe₂ and MoS₂-WSe₂ heterostructures with different stacking orders by solution of the excitonic Bethe-Salpeter equation with GW corrections [1] and inclusion of spin-orbit-coupling. We find two spin-orbit split Rydberg series of low oscillation strength and a surprisingly large binding energy below the absorption onset of the monolayer materials, which arise from a type-II alignment of the monolayer bands. Together with the indirect electronic band gap of the heterostructures, our results confirm the recent experimental observation of a doublet nature of the interlayer photoluminescence. We further show that the local stacking order leads to small variations in the hybridization between the MoSe₂ and WSe₂ bands and has a decisive effect on the polarization dependence of the interlayer excitonic absorption [2]. Our results motivate detailed studies of electron-phonon coupling effects and exciton dynamics in TMDC heterostructures by time-resolved optical experiments and ab initio methods.

[1] Gillen et al., IEEE JSTQE 23, 1 (2017); arXiv:1801.06310

[2] Gillen et al., Phys. Rev. B 97, 165306 (2018)

MON 25**Berry Curvature and Nonlocal Transport Characteristics of Antidot Graphene**Jie Pan¹, Ting Zhang¹, Haijing Zhang¹, Bing Zhang¹, Zhen Dong¹, Ping Sheng¹¹HKUST, Hong Kong

Antidot graphene denotes a monolayer of graphene structured by a periodic array of holes. From the tight-binding calculations, its energy dispersion is known to display a gap at the Dirac point. However, antidot graphene does not have the necessary symmetry requirement, such as that embedded in the 2D massive Dirac equation, for opening a bandgap. From inversion and time-reversal-symmetry considerations, antidot graphene should therefore have zero Berry curvature. In this work, we derive the effective Hamiltonian of antidot graphene from its tight-binding wave functions. The resulting Hamiltonian is a 4×4 matrix with a nonzero intervalley scattering term, which is responsible for the gap at the Dirac point. Furthermore, nonzero Berry curvature is obtained from the effective Hamiltonian, owing to the double degeneracy of the eigenfunctions. Since the Berry curvature is expected to induce a transverse conductance, we have experimentally verified this feature through nonlocal transport measurements, by fabricating three different antidot graphene samples. All the samples display topological nonlocal conductance, with excellent agreement with the theory predictions.

MON 26**Carbon nanotube-based saturable absorbers for ultrafast lasers in a spectral range 1.0-2.1 μm**

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The advantages of single-wall carbon nanotubes as material for ultra-fast stable saturable absorbers for a wide class of solid state lasers (including the fiber ones) have been demonstrated earlier [1-4]. However, not many publications concern the spectral range exceeding 2 μm . Here we demonstrate the universal approach to formation of saturable absorbers in shape of carboxymethylcellulose matrix with dispersed inside individual single-wall carbon nanotubes. Depending on tube diameter they provide realization of mode-locking regime for any laser with working wavelengths ranging from 1 μm (Yb) [2] to 2.1 μm (Ho)[5]. The final pulse duration varied between 100 fs and 1.5 ps. The thermal degradation threshold of such absorbers was about 10⁹ W/cm².

The work was supported by RFBR projects 18-42-130001 and 18-29-19113.

References

1. N.N. Il'ichev, E.D. Obraztsova, et al., Quant. Electron. 34(2004)572.
2. M. Zhang, E.J.R. Kelleher, et al., Optics Lett 36(2011) 3984.
3. M.A. Solodyankin, E.D. Obraztsova, et al., Optics Lett. 33(2008)1336
4. A.A. Krylov, D.S. Chernykh, et al., Optics Letters 42 (2017) 2439.
5. S.A. Filatova, V.A. Kamynin, et al., JOSA B 35(12)(2018)3122.

MON 27**Electronic Dipole Spin Resonance of 2D Semiconductor Spin Qubits**

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¹University of Konstanz,

Monolayer transition metal dichalcogenides (TMDs) offer a novel two-dimensional platform for semiconductor devices. One such application, whereby the added low dimensional crystal physics (i.e. optical spin selection rules) may prove TMDs a competitive candidate, is quantum dots as qubits. The band structure of TMD monolayers offers a number of different degrees of freedom and combinations thereof as potential qubit basis, primarily electron spin, valley isospin and the combination of the two due to the strong spin orbit coupling known as a Kramers qubit. Pure spin qubits in monolayer MoX_2 (where $X = \text{S}$ or Se) have been shown to be achievable by energetically isolating a single valley and tuning to a spin degenerate regime within that valley by a combination of a sufficiently small quantum dot radius and large perpendicular magnetic field. Within such a TMD spin qubit, we theoretically

induce and analyse single qubit rotations with an electric dipole spin resonance. We employ a rotating wave approximation within a time dependant Schrieffer-Wolf approximation to derive analytic expressions for the Rabi frequency of single qubit oscillations, and compare this with numerics.

MON 28

Nematic mesomorphous systems based on suspensions of carbon nanotubes and goethite

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²Saint-Petersburg State University, St.Petersburg

Fluid systems containing nanocarbon and mineral particles are in the focus of research interest. Relatively recent potential application of such systems would concern getting stable biaxial nematic phase, anticipated to have promising abilities in display technologies owing to the shortened response time of particles' medium axis with respect to the external field. Mixtures of single walled carbon nanotubes (SWCNT) and goethite in aqueous media have been under view. We discuss a long-standing issue of getting a biaxial nematic phase and its stabilization by an extremely elongated moieties (SWCNT) with regard to decay into a blend of uniaxial nematics. We report on the statistical-thermodynamic description of the phase diagram in ternary mixtures of particles with D4h symmetry on the platform of the restricted-orientation Zwanzig model on the 3rd virial level. We also give an account of processing regular nematic suspensions of SWCNT and goethite as pre-requisites of getting ternary suspensions with biaxial ordering.

A.V.V. acknowledges financial support by the RFBR (# 16-33-60208).

MON 29

Interface electroluminescence from in-plane heterostructures based transition metal dichalcogenide monolayers

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Here, we report a growth processes of high-quality in-plane heterostructures based on transition metal dichalcogenide (TMDC) monolayers and the anomalous electroluminescence (EL) from their one-dimensional (1D) interface. WS_2/MoS_2 and $WSe_2/MoSe_2$ in-plane heterostructures were grown on sapphire substrates by salt-assisted chemical vapor deposition (CVD). To observe electroluminescence from the heterointerface, we have fabricated the electric double layer light emitting diodes (EDLEDs) with ion gel. The devices show linear light emission from the interface by applying voltage. Interestingly, the EL spectra show different peaks from photoluminescence spectra measured around the interface. In the presentation, we will show

the details of sample preparation and discuss possible origins of EL peaks in the present EDLEDs.

MON 30

Exclusion of the first order electron-phonon interaction in special structures

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There is a special class of crystalline compounds with particular electronic states not bound to the nuclear dynamics in the first order perturbation theory. Such systems and electronic states are singled out by symmetry based conditions: (a) Duality between the geometries of the system and the star in Brillouin zone corresponding to the exceptional electronic states; (b) The stabilizers of the orbits of the system are maximal; (c) Invariance under spatial inversion. A consequence is that in these systems the Jahn-Teller theorem is broken, which is the first evidence of the adiabatic stability in nonlinear systems. It turns out that such crystals are already distinguished by a number of properties. Other physical implications are discussed.

MON 31

Optical determination of the Fermi level in the intercalated graphene

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The FeCl₃ intercalated graphene has a long-term stability at ambient conditions and the potential do induce extremely strong doping, which is highly attractive for electronic and plasmonic applications. The FeCl₃ molecules penetrate the space between the graphene layers and form ordered crystalline-like monolayers. The FeCl₃ deprives the graphene electrons, thus increasing the concentration of holes. The determination of charge carriers remains a challenging task due to the high complexity of the hybrid structure. In this work, we investigated the modified electronic structure of graphene by resonant Raman spectroscopy. The Raman intensity of the G mode was investigated as a function of excitation energy. The intensity of the G mode resonantly increases when the excitation energy approaches twice the Fermi energy. The increase in intensity occurs due to the blocking of the negatively interfering Raman process. We obtain Fermi energies of 0.98 and 1.04 eV in an intercalated graphene bilayer by fitting the resonance Raman profiles. The different doping levels correspond to different intercalant phases revealed by scanning transmission electron microscopy (STEM).

MON 32**Proximity and dephasing effects of single layer molecular superconductor on Ag(111) surface**Abdou Hassanien¹¹Condensed Matter Physics, Jozef Stefan Institute, Ljubljana

Using scanning tunneling microscopy and spectroscopy, we study how a monolayer of single component molecular superconductor interacts with two dimensional electron gas at the atomic scale. The spatial variations of the local density of states show evidences of proximity and dephasing effects across the island/metal boundary reaching as far as 15 nm into the metal side. Interestingly, the confined states of Ag(111) are gaped by superconducting state and can only cross the Fermi energy above the transition temperature of 5K. The mild broadening of the coherence peaks on the metal side together with long penetration length at low temperature indicate that electron-electron interactions are weakly restricting the dephasing length of cooper pairs. This behavior may open opportunity for proximal manipulation of ground state superconducting properties.

References

1. A. Hassanien, *Advanced Electronic Materials*, DOI 10.1002/aelm.201800247.
2. A. Hassanien et al., *Phys. Status Solidi B* 252, No. 11, 2574–2579 (2015).
3. K. Clark et al., *Nature Nanotechnology*, 5, 261–265 (2010)

MON 33**Three-layer moiré superlattice and strain engineering in hBN-encapsulated graphene**Lujun Wang¹, Andreas Baumgartner¹, Simon Zihlmann¹, Péter Makk^{1,2}, Ming-Hao Liu³, Jan Overbeck¹, Kenji Watanabe⁴, Takashi Taniguchi⁴, Christian Schönenberger¹¹Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland²Department of Physics, Budapest University of Technology and Economics and Nanoelectronics Momentum Research Group of the Hungarian Academy of Sciences, Budafoki ut 8, 1111 Budapest, Hungary³Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan⁴National Institute for Material Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

It has been predicted that non-uniform strain can generate a pseudo-magnetic field in graphene which acts on the two different valleys with opposite signs [1]. We introduce a new technique and sample design to engineer strain in graphene, which is encapsulated with hBN in order to obtain ultraclean graphene, thereby avoiding valley mixing due to disorder. Such devices show state-of-the-art transport characteristics, which is exemplified by the formation of a three-layer moiré superlattice [2], where both the top and the bottom hBN are aligned to the graphene. In a sec-

ond step we use Raman spectroscopy to demonstrate that the overall strain and strain gradients can be deterministically generated using a fairly standard break-junction setup. We then report several strain effects in transport experiments at cryogenic temperatures that can be attributed to both strain-induced scalar potential and pseudo-magnetic field.

[1] Guinea et al., Phys. Rev. B 81, 035408 (2010).

[2] Wang et al., arXiv:1812.10031 (2018).

MON 34

Graphene stabilized (6x2) oxygen reconstruction on Cu (110), investigated by scanning tunneling microscopy

Dominik Szombathy¹, Chanyong Hwang¹, Levente Tapasztó¹, Péter Nemes-Incze¹
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The presence of a graphene layer significantly alters the oxidation of copper and other metals. Details of this process are important for applications of graphene as a corrosion barrier, as well as dry peeling of graphene from the Cu substrate via van der Waals forces. However, the atomic scale details of the oxidation and intercalation of oxygen are still poorly understood.

Here we investigate the result of oxygen intercalation, between a graphene layer grown via chemical vapor deposition and the (110) surface of a Cu single crystal. Using scanning tunneling microscopy at a base temperature of 9K, we show that the oxygen intercalated (110) surface prefers a (6x2) reconstruction. With continued exposure to ambient air, the (6x2) reconstructed areas grow in size, but the nature of the reconstruction remains unchanged. This result is all the more surprising since this type of reconstruction is only stable in a narrow temperature and pressure range. By measuring dI/dV maps of the sample surface we identify the hallmark electronic states of both the clean Cu(100)-graphene areas, as well as the reconstructed system.

MON 35

Steady State Monodomain of Liquid Crystal Elastomer by Aligned Carbon Nanotubes in Sheets

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Liquid crystal elastomers (LCEs) are liquid crystals with elastomeric behaviour. The liquid crystalline nature provides anisotropy in the properties which results in anisotropic actuation (shape change). By heating, a phase transition from the unidirectionally aligned nematic phase to the isotropic state induces the actuation as result

of molecular rearrangement for maximising polymer coil entropy, with a shrinkage along the direction of the alignment. This property is very interesting for applications such as soft robotics and artificial muscles. However, the induction of orientationally ordered monodomains is a key requirement. In this work we present a technique to macroscopically orient LCEs using sheets of uniformly aligned carbon nanotubes (CNTs) pulled from vertically grown forests. The aligned CNTs transfer their order onto the LCE, inducing planar-aligned state that recovers after thermally induced actuation. This allows the CNT-LCE composite to change its shape, fully reversibly, from a flat to a bent sheet or even into a macroscopic roll. We also found that the solvent used in the composite preparation has an impact on the LCEs even in presence of templating CNTs.

MON 36

Improved stability of confined small diameter 1D nanocarbons against high temperature oxidation

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1D nanocarbons such as linear carbon chains (LCCs), carbon nanotubes (CNTs), and graphene nanoribbons (GNRs) have for thin diameters below 0.8 nm a reduced stability against high temperature oxidation. Recently, we have synthesized LCCs [1], ultra-thin CNTs [2], and GNRs [3] encapsulated inside carbon nanotubes. Here, we compared the oxidization stability of those LCCs, CNTs, and GNRs confined inside CNTs by using the resonance Raman spectroscopy as probe. We found that they have an improved stability and can survive up to 500°C due to the protection of the host tubes. Also, the larger (6,5) CNTs is more stable than the smaller (6,4) CNTs and LCCs and GNRs are both more stable than the (6,4) CNTs. Interestingly, the longer LCCs are more stable than the shorter LCCs. This illustrates that the stability of nanocarbons do not depend on the size of the confined 1D nanocarbons alone, but also depends on the interaction to and confinement in the host tubes in a more complicated manner.

[1] L. Shi, et al. *Nature Mater.* 15, 634 (2016).

[2] L. Shi, et al. *Nanoscale.* 10, 21254 (2018).

[3] H. Kuzmany, et al. *Phys. Stat. Sol. (RRL)* 11(8), 1700158 (2017).

MON 37

Nanoscale Infrared Identification and Mapping of Chemical Functional Groups on Graphene

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Typical chemical characterisation of two-dimensional materials often relies on bulk techniques: FTIR and XPS being common examples. These techniques, combined with measurements by AFM, allow for elucidation of chemical structure, albeit indirectly. Raman spectroscopy often has a lateral resolution of around 500 nm and can only give detailed information pertaining to polarisable bonding. Here, we will report results on direct chemical mapping of functionalised monolayer reduced graphene oxide flakes at less than 30 nm resolutions. This is now possible using AFM coupled infrared spectroscopy, bypassing the diffraction limitations on the spatial resolution of FTIR. In analysing a system comprised of pyrene-derived molecules onto reduced graphene oxide flakes. By exciting the flake with a tuneable infrared source, and using an AFM probe to detect thermal expansion, a nanoscale IR spectrum of each surface can be found using AFM-IR. These spectra can be directly correlated to the bulk FTIR spectrum of the pyrene molecules. Further, by mapping the flake at responsive wavelengths, we can report chemical imaging far below the diffraction limit of IR photons, at less than 30 nm resolution.

MON 38

Electronic Instabilities in Semi-Metallic Linear Chains

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In 1929 Peierls theorized that a semi-metallic linear chain of equally spaced single electron atoms is unstable due to electron-phonon coupling at $T=0$: periodic lattice distortions along the longitudinal mode of vibration lead to the opening of an electronic band gap, leading to a charge-density wave (CDW) phase and stabilizing a semiconducting ground state.

Here we study two equidistant semi-metallic linear chains: the (hypothetical) hydrogen chain and the carbon chain (carbyne) by means of accurate ab initio calculations based on quantum Monte Carlo and density functional theory (DFT). For both cases we find that the CDW state is more stable than the metallic phase without any lattice distortion, i.e., the metallic state is electronically unstable. Using DFT with hybrid functionals, we show that the electronic instability is directly related to the non-locality of the exchange term. These results suggest that in 1D semi-metals there exists a purely electronic instability that opens a gap, leading to a CDW phase prior to Peierls distortion. We discuss the relations of our findings to the excitonic insulator picture and to a similar CDW mechanism in 2D TiSe_2 .

MON 39**Engineering disorder in charge density waves using electron-irradiation- induced lattice defects in 2D layers.**

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Understanding order-disorder transitions and the role played by defects in strongly correlated materials will contribute towards applications as well as understanding fundamental physics. Charge density wave (CDW) materials provide a suitable model system where effects of disorder on transport and ordering behavior can be investigated¹. We have investigated the influence of electron beam-generated lattice defects on the structure of periodic lattice distortion (PLD) which accompanies CDW modulation in $1T-TaS_2$ and $1T-TaSe_2$. Lattice defects were generated through high-energy electron beam irradiation in a transmission electron microscope (TEM). Using atomic resolved high-resolution TEM (HRTEM) imaging, we directly visualize the PLD structure. We observe formation of dislocation-like defects as well loss of long range order in the PLD structure with increased exposure to the electron beam². These results are further discussed and compared to density functional theory calculations.

¹P. Monceau, Adv. Phys. 61, 325 (2012).

²M. K. Kinyanjui, T. Björkman, T. Lehnert, J. Köster, A. Krasheninnikov, and U. Kaiser, Phys. Rev. B 99, 024101(2019)

MON 40**Molecular based unconventional Andreev-interferometers**

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Devices, in which two superconductive and one normal leads attached to the central molecule, are known as Andreev-interferometers. In these systems, the current flowing through the normal lead (called Andreev-current) is shown interference phenomenon that can be understood as a result of an interference effect between the possible transport paths of the charged particles.

In our work the Andreev-current is investigated theoretically and numerically in a device consisting of a pyrene, as a central molecule, and one-dimensional contacts. We give the description of the effect using non-equilibrium Green-function techniques. We also give the explanation of an unconventional interference phenomenon, where the Andreev-current has no minima but a maxima.

HÜBNER Photonics
Coherence Matters.



- 08:30 – 09:00 **A. Kis, Lausanne**
Exciton Manipulation in 2D TMDC Heterostructures
- 09:00 – 09:30 **J. Fabian, Regensburg**
Proximity spin phenomena in 2D materials
- 09:30 – 10:00 **S. Ryu, Pohang**
Redox-Governed Charge Doping in Two-Dimensional Materials Revealed by Optical Spectromicroscopy
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **T. Korn, Rostock**
Interlayer excitons in TMDC heterostructures
- 11:00 – 11:30 **X. Marie, Toulouse**
Exciton Linewidth Approaching the Homogeneous Limit in MoS₂ based Van der Waals Heterostructures
- 11:30 – 12:00 **M. Koperski, Manchester**
Strained bubbles in van der Waals heterostructures as local emitters of photoluminescence with adjustable wavelength
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **A. Zettl, Berkeley**
1-D transition-metal-trichalcogenides in the single-chain limit
- 19:00 – 19:30 **C. Mattevi, London**
Direct solution-phase synthesis of 1T' WSe₂ nanosheets
- 19:30 – 20:00 **X. Feng, Dresden**
Polymer Synthesis Enabled by Interfaces: Towards a world of organic 2D materials
- 20:00 **Poster Session II**

Tuesday, March 12th

2D materials, excitons, synthesis

08:30**Exciton Manipulation in 2D TMDC Heterostructures**Andras Kis¹¹School of Engineering, EPFL, Lausanne

The discovery of graphene marked the start of research in 2D electronic materials which was expanded in new directions with MoS₂ and other layered semiconducting materials. They have a wide range of interesting fundamental properties and potential applications. New opportunities are enabled by the band structure of transition metal dichalcogenides (TMDCs) in which we could harness the valley degree of freedom for valleytronics and next-generation photonics. Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for this, allowing control over exciton diffusion length, energy and polarisation. I will show here how by using MoS₂/WSe₂ van der Waals heterostructures, we can realize excitonic transistors with switching action, confinement and control over diffusion length at room temperature in a reconfigurable potential landscape. Heterostructures with a long-range moiré potential such as in MoSe₂/WSe₂, on the other hand, offer the way to control polarization, emission and wavelength emitted by different optically active regions in the moiré.

09:00**Proximity spin phenomena in 2D materials**Jaroslav Fabian¹¹Department of Physics, University of Regensburg, Regensburg

Stacking graphene with other 2D materials opens up fascinating possibilities for spintronics. Transition metal dichalcogenides are of particular interest due to their strong spin-valley coupling. Placing graphene on, say, MoS₂, enables optospintronics, whereby optically generated spins in MoS₂ are transferred into graphene. Even more fascinating are proximity effects allowing spin manipulation. Spin-valley locking in the substrate is manifested via the valley Zeeman splitting in graphene which, in turn, yields giant spin relaxation anisotropy. Since the structure of intrinsic spin-orbit coupling is dramatically altered by the proximity effect, novel pseudohelical edge states can emerge in graphene nanoribbons and flakes, protected against backscattering by time reversal symmetry. Much greater playground for new physics is offered by bilayer graphene on 2D materials. Due to the locality of proximity effects, one can efficiently tune induced spin interactions via electric fields—gating. Thus, spin-orbit coupling as well as the exchange interaction can be turned on and off, opening prospects for novel spin transistors. Support from DFG, EU Graphene Flagship is acknowledged.

09:30**Redox-Governed Charge Doping in Two-Dimensional Materials Revealed by Optical Spectromicroscopy**Sunmin Ryu¹¹Department of Chemistry, POSTECH, Pohang 37673, Korea

Low dimensional carbon materials often undergo spontaneous hole doping in the ambient conditions, the detailed mechanism of which has yet to be revealed. In this work, we propose a mechanism based on a redox couple of O_2/H_2O and verified it for two model systems: photoluminescence (PL) modulation in single-layer WS_2 and thermally-activated phonon hardening in graphene with both supported on silica substrates. The PL modulation was directly correlated with the concentration of oxygen both in gaseous and aqueous states. Wide-field PL imaging, however, showed distinctively different spatial propagations of the modulation for the two states, revealing the microscopic picture of the charge doping in WS_2 . The mechanistic details and thermodynamic driving force for the charge doping will also be discussed in conjunction with the activated hole doping in graphene probed by Raman spectroscopy.

10:30**Interlayer excitons in TMDC heterostructures**Tobias Korn¹¹Institut fuer Physik, Uni Rostock, Rostock

Two-dimensional transition-metal dichalcogenides (TMDCs) have recently emerged as a promising class of materials. A fascinating aspect of these atomically thin crystals is the possibility of combining different TMDCs into heterostructures. For several TMDC combinations, a staggered band alignment occurs, so that optically excited electron-hole pairs are spatially separated into different layers. However, they can still form tightly bound, long-lived states, so-called interlayer excitons. The relative crystallographic alignment (twist angle) of the adjacent layers in our heterostructures offers a new degree of freedom, which allows us to control the alignment of band extrema in reciprocal space.

I will discuss how control of the twist angle enables us to identify the peculiar character of interlayer excitons in MoS₂-WSe₂ heterobilayers. For the MoSe₂-WSe₂ heterobilayer system, I will demonstrate engineering of the effective g factor for interlayer excitons based on crystallographic alignment.

11:00**Exciton Linewidth Approaching the Homogeneous Limit in MoS₂ based Van der Waals Heterostructures**Xavier Marie¹¹LPCNO, University of Toulouse - CNRS, Toulouse

The strong light matter interaction and the valley selective optical selection rules make monolayer (ML) MoS₂ an exciting 2D material for fundamental physics and optoelectronics applications. In this work we show that encapsulation of ML MoS₂ in hBN can efficiently reduce the inhomogeneous contribution to the exciton linewidth, as we measure in photoluminescence and reflectivity a FWHM down to 2 meV [2]. Similar results are obtained with encapsulated MoSe₂, MoTe₂, WSe₂ and WS₂ MLs [3]. This indicates that surface protection and substrate flatness are key ingredients for obtaining stable, high quality samples. Among the new possibilities offered by the well-defined optical transitions we evidence the optical selection rules for in-plane propagation of light. These studies yield a direct determination of the bright-dark exciton splitting [4]. We also uncover new information on exciton-exciton interactions [5] and exciton-photon weak coupling regime in these Van der Waals heterostructures.

[1] Cadiz et al, 2D Mat.3 , 045008 (2016)

[2] Cadiz et al, PRX 7,21026 (2017)

[3] Manca et al, Nat. Com. 8,14927 (2017)

[4] Wang et al, PRL 119,47401 (2017)

[5] Han et al, PRX 8, 31073 (2018)

11:30**Strained bubbles in van der Waals heterostructures as local emitters of photoluminescence with adjustable wavelength**A. V. Tyurnina^{1,4}, D. A. Bandurin¹, E. Khestanova¹, V. G. Kravets¹, M. Koperski^{1,2}, F. Guinea^{1,3}, A. N. Grigorenko^{1,2}, A. K. Geim^{1,2}, I. V. Grigorieva^{1,2}¹School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, UK²National Graphene Institute, University of Manchester, Manchester M13 9PL, UK³IMDEA Nanociencia, Faraday, 9, Cantoblanco, 28049 Madrid, Spain⁴Skolkovo Institute of Science and Technology, Nobel St 3, 143026 Moscow, Russia

The possibility to tailor photoluminescence (PL) of monolayer transition metal dichalcogenides (TMDCs) using external factors such as strain, doping and external environment is of significant interest for optoelectronic applications. Strain in particular can be exploited to continuously vary the bandgap. Here we describe room-temperature PL from hydrocarbon-filled bubbles which provide predictable, localized PL from well-separated submicron areas. Their emission energy is determined by the built-in strain controlled only by the substrate material, such that both the maximum strain and the strain profile are universal for all bubbles on a given substrate, i.e., independent of the bubble size. We show that for strained monolayer MoS₂, PL can be tuned between 1.72 to 1.81 eV by choosing PtSe₂, WS₂, MoS₂ or graphite as a substrate and its intensity is strongly enhanced by the funneling effect. Strong substrate-dependent quenching of the PL in areas of good contact between MoS₂ and the substrate ensures localization of the luminescence to bubbles only; by employing optical reflectivity measurements we identify the mechanisms responsible for the quenching.

18:30

1-D transition-metal-trichalcogenides in the single-chain limit

Alex Zettl^{1,2}

¹Department of Physics, University of California at Berkeley

²Materials Sciences Division, Lawrence Berkeley National Laboratory

The successful realization of single-layer or few-layer specimens of two-dimensional materials such as graphite, BN, and transition-metal-dichalcogenides has led to a wealth of exciting fundamental science and technical innovation. In their bulk form, quasi-ONE-dimensional materials such as the transition-metal-trichalcogenides support unusual electronic and structural ground states. In this talk I explore experimentally and theoretically the properties of some representative 1-D materials as they approach the few- to single-chain limit.

19:00**Direct solution-phase synthesis of 1T' WSe₂ nanosheets**cecilia mattevi¹¹Department of Materials, Imperial College London

Crystal phase control in layered transition metal dichalcogenides is paramount for exploiting their different electronic properties. However, the direct synthesis of metastable phases is challenging, restricting the spectrum of reachable materials. We demonstrate the direct synthesis of the metastable distorted octahedrally coordinated structure (1T' phase) of WSe₂ nanosheets [1]. 1T' WSe₂ branched few-layered nanosheets are produced in solution by designing a kinetically-controlled regime of colloidal synthesis. We show that the 1T' phase is fully convertible into the semiconducting 2H phase upon thermal annealing at 400 °C. The 1T' WSe₂ nanosheets have a metallic nature exhibited by an enhanced electrocatalytic activity for hydrogen evolution reaction as compared to the 2H WSe₂ nanosheets and comparable to other 1T' phases. We then discuss tuneability between different phases at the synthesis level.

[1] M. Sokolikova et al. Nature Communications, 10, 712 (2019)

19:30

Polymer Synthesis Enabled by Interfaces: Towards a world of organic 2D materials

Xinliang Feng¹

¹cafed & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany

In this lecture, we will present our recent efforts on the bottom-up synthetic approaches towards novel organic 2D materials with structural control at the atomic/molecular-level or at the meso-scale.

TUE 1**The metallic nanoparticles integrated into thin layers of hydrogenated amorphous silicon**

Jiri Stuchlik¹, Ha The Stuchlikova¹, Zdenek Remes¹, Jan Cermak¹, Jaroslav Kupcik¹, Karel Kral¹

¹Institute of Physics CAS, Praha 8

We present PIN structures based on hydrogenated amorphous silicon (a-Si:H) thin films with embedded Sn NPs characterized by electron microscopy (SEM and HR-TEM), atomic force microscopy (AFM), photothermal deflection spectroscopy (PDS), constant photocurrent method (CPM), photoluminescence (PL) and electroluminescence (EL). The temperature dependence of the electrical conductivity and the changes of its activation energy of are discussed in the frame of the theoretical model of the transfer of the charge carriers in these structures. This work was supported by the CSF project 19-02858J, the MEYS project LTC17029 INTER-COST Action MP1406 and by the Operational Programme Research, Development and Education financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. SOLID21 - CZ.02.1.01/0.0/0.0/16 019/0000760).

TUE 2**Vibrational properties and charge transfer in the misfit-layer compound LnS-CrS₂ and nanotubes thereof**

Felix Kampmann^{1,2}, Roland Gillen¹, Leela S. Panchakarla³, Reshef Tenne⁴, Janina Maultzsch²

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²TU Berlin Festkörperphysik, Berlin, Germany

³IIT Bombay Department of Chemistry, Powai, India

⁴Weizmann Institute of Science, Dept. Materials and Interfaces, Rehovot, Israel

Misfit-layer compounds of LnX-TX₂ consist of alternately stacked layers of a two-atom thick slice of a rocksalt structure and a single-layer of a transition metal dichalcogenide (TMD) that is either trigonal prismatic or octahedral. Here Ln is an element of the lanthanides and the TX₂ principally covers the whole range of the TMDs and similar structures like CoO₂. The misfit in the crystal lattice parameters of the two subsystems results in bending of the superstructure and can lead to the formation of multi-walled nanotubes and nanoscrolls.

In this study we investigate the formation of LnS-CrS₂ where the CrS₂-layer has not been reported as a single layer or a bulk material. We compare the Raman spectrum of CrS₂-based MLC nanotubes and bulk material with DFT calculations of their vibrational properties. Therefore we compute the Γ -point phonons of the full supercell of LaS-CrS₂ and compare it to the isolated subsystems LaS and CrS₂ as a single layer. The calculation of the Loewdin charges of both systems enables us to

connect the charge transfer between the two layers upon formation of the supercell with the shift of the phonon frequencies.

TUE 3

Individualization of Single Wall Carbon Nanotubes bundles out of surfactant.

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Single-wall carbon nanotubes (SWCNT) have drawn significant attention due to their exceptional properties which are determined by their diameter and chirality. SWCNT grow in bundles of diverse morphologies and one must separate them to particularly address their electronic properties. The main existing routes for SWCNT individualization are based in the use of surfactants or sidewall functionalization which affect their intrinsic electronic properties. In this work we address the development of a new individualization method for SWCNT that does not require the use of surfactants but a polar solvent instead (THF and DMF). This methodology is based in an in-situ charge transfer effect on carbon nanotubes via the intercalation with alkali metals (Na and K) followed by a chemical exfoliation process. We have obtained a high yield of individualized crystalline SWCNT as confirmed by the Raman radial-breathing mode, atomic force and scanning electron microscopy. In addition, our analysis revealed a functionalization degree dependence based on the solvent and sonication time employed. Which excels as a new way to obtain individual carbon nanotubes with or without surface functionalization.

TUE 4

Evolution of Metastable Defects in Monolayer and Few-Layer Films of MoS₂

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Italy

We report on structural and electronic properties of defects in chemical vapor-deposited monolayer and few-layer MoS₂ films. We use scanning tunneling microscopy, Kelvin probe force microscopy and transmission electron microscopy in order to obtain high resolution images and measurements of the local density of states, work function and nature of defects in MoS₂ films. We track the evolution of defects that are formed under annealing and electron beam irradiation in ultra-high vacuum conditions. We observe formation of metastable domains with different work function values after heating the material in ultra-high vacuum to moderate temperatures. The experiments show that sulfur vacancies formed after exposure to elevated temperatures diffuse, coalesce, and migrate bringing the system from a metastable to equilibrium ground state. The process could be thermally or e-beam activated with estimated energy barrier for sulfur vacancy migration of 0.6 eV in single unit cell MoS₂. The results provide estimates of the thermal budgets available for reliable fabrication of MoS₂-based electronics and indicate the importance of defect control and layer passivation.

TUE 5**Optical properties of various graphene quantum dots**

Lucile Orcin-Chaix^{1,2}, Shen Zhao¹, Loïc Rondin¹, Julien Lavie², Klaus Müllen³, Akimitsu Narita³, Christophe Voisin⁴, Stéphane Campidelli², Jean-Sébastien Lauret¹

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Graphene plays a key role as a central material for nanoelectronics. Nevertheless, graphene has a zero band gap that makes it unusable for semiconductor applications. Therefore, a lot of efforts are being made to develop materials with sizeable band gap compatible with the hexagonal lattice of graphene. In this context graphene quantum dots and nanoribbons have a lot of assets. Indeed, the so-called bottom-up synthesis allows a precise control of the size, shape and edges of these objects [1], which is a key issue in order to be able to reach the desired properties.

Recently, our groups have reported on the single photon emission of the C96 graphene quantum dot at room temperature [2]. In this poster, we will show our last results on the optical properties of different types of graphene quantum dots synthesized by bottom-up chemistry.

[1] R. Rieger and K. Müllen, *J. Phys. Org. Chem.* 23, 315-325 (2010).

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

TUE 6**Know more about your 2D Material with Tip-enhanced Raman spectroscopy combined to other Scanning Probe Microscopy Techniques**

Jana Kalbacova¹, Marc Chaigneau¹, Andrey Krayev¹

¹HORIBA Scientific

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS₂, MoSe₂, WSe₂, have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 – 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.

TUE 7**Influence of Sulphur vacancy defect density and arrangement on the electronic properties of MoS₂ sheets**

Geza I. Mark¹, Peter Vancsó¹, Pauline Castenetto², Philippe Lambin², Levente Tapasztó¹

¹Nanostructures Departement, Institute of Technical Physics and Materials Science, Centre of Energy Research, Budapest, Hungary

²Department of Physics, University of Namur, Belgium

We studied the influence of different densities of Sulphur vacancies [1] on the electronic structure and transport properties of monolayer MoS₂ by theoretical techniques, Density Functional Theory (DFT), Tight Binding (TB) and Wave Packet Dynamics (WPD). By the help of matching the TB results to DFT calculations we obtained TB parameters suitable for calculating for large sample sizes, allowing us to investigate the effect of the defects on the band structure. We found that the interaction of the S vacancies is negligible for supercell sizes larger than 4x4 unit cells, due to the local character of the defect states. In the WPD calculations we accounted for the pristine MoS₂ lattice by incorporating its E(k) dispersion relation obtained from DFT into the kinetic energy operator [2] and the S vacancies by local potentials in the potential energy operator. We found that the WP scattering on the defect is anisotropic, hence not only the defect density but also the angular order of defects influences the transport properties.

- 1: P Vancso et al; Sci. Rep., 6(June), 7. <https://doi.org/10.1038/srep29726>
2. GI Mark et al; Phys. Stat. Sol. B 254, 1700179(2017)

TUE 8

Momentum resolved valence band excitations in graphenes in the electron microscope

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¹Fakultät für Physik, University of Vienna, Vienna

²AIST Tuskuba, Japan

Recent advances in electron optics and spectroscopy have unlocked the door to map the entire excitation spectrum in freestanding 2D materials with unprecedented spatial, energy and momentum resolution. This allows to trace the phonon dispersion in graphene nanostructures [1]. Here we present recent results on the anisotropic valence band excitations and momentum dependent energy gap across the first and second Brillouin zone along ΓM and ΓK direction in few (5-10) layer graphene. These results are quantitatively compared to previous momentum resolved measurements on nanotubes [2], graphite [3], and graphene [4], performed at lower energy and momentum resolution.

[1] Senga et al, arxiv.org/abs/1812.08294

[2] Kramberger et al, 10.1103/PhysRevLett.100.196803

[3] Zeppenfeld, 10.1007/BF01379961

[4] Kinyanjui et al, 10.1209/0295-5075/97/57005

TUE 9

Vibrational properties of diamondoid dimers with exceptionally long carbon-carbon bonds

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We analyze the vibrational properties of diamondoid compounds via Raman spectroscopy. The compounds are lower diamondoids interconnected with carbon-carbon bonds exhibiting exceptionally long bond lengths up to 1.71 Å [1, 2]. Attractive dispersion interactions caused by pronounced intramolecular H···H contact surfaces determine their very long bond lengths and overall structures. The intramolecular

van-der-Waals interactions alter the vibrational properties of the compounds in comparison to pristine diamondoids. Supported by dispersion-corrected DFT (density functional theory) computations, we analyze and explain their experimental Raman spectra with respect to individual diamondoids. We find a new set of dispersion-induced vibrational modes comprising characteristic CH/CH₂ vibrations. Further, we find structure-induced dimer breathing modes that are indicative for the sizes of the dimers.

[1] P. Schreiner et al., *Nature*, 477, 308-311 (2011)

[2] A. A. Fokin et al., *JACS*, 134 (33), 13641-13650 (2012)

TUE 10

Fabrication of gate-tunable 2D heterostructures

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¹Physik LS Kotthaus Ag Högele, LMU, München

Transition metal dichalcogenides represent novel two-dimensional semiconductor materials with unique optoelectronic properties (1). Due to weak interlayer van der Waals bonding, bulk semiconductors can be exfoliated down to the monolayer limit and used to build 2D heterostructures consisting of multiple layers of different crystals stacked on top of each other (2). We demonstrate how the so-called “hot-pick-up” transfer technique (3) can be used to realize stacked devices based on the thermal control of van der Waals interactions at the interfaces of 2D crystals involved. Specifically, we implement this method to fabricate gate-tunable monolayer and bilayer encapsulated in hexagonal boron nitride. We show how active control of doping in such devices facilitates the interpretation of rich spectral signatures of monolayer and bilayer transition metal dichalcogenides at low temperatures.

[1] T. Cao et al., *Nature Communications*, 3, 887 (2012)

[2] Y. Liu et al., *Nature Reviews Materials* 1, 16042 (2016)

[3] F.Pizzocchero et al., *Nature Communications* 7, 11894 (2016)

[4] Geim, Andre K., und Irina V. Grigorieva. arXiv:1307.6718 (2013)

TUE 11

Growth, characterisation and transfer of 1D and 2D carbon nanomaterials for optoelectronics

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Carbon nanomaterials, i.e. carbon nanotube for the 1D geometry and graphene for the 2D one, hold great promise for optoelectronics and quantum technologies. Nevertheless their growth and their integration into optoelectronic circuits need a good control due to their sensitivity to contamination and defects. The nano-object as well

as its surface need to be and stay intact.

I will present the recent development for the CVD growth and transfer we did at LPENS.

For nanotubes, we have developed a very efficient integration process by transferring the nanotube onto a target substrate under vacuum conditions. This process allows the fabrication of spin-qubit devices with a decoherence time 2 orders of magnitude larger than previous C-based qubit. We also developed their structural characterization by Raman and Rayleigh scattering spectroscopy, with cross-correlation with TEM.

For graphene, we have developed the growth of 50 μ m-large flakes on Cu foil and the dry transfer directly from the Cu on BN. We are in fine able to fabricate a FET made of graphene encapsulated in BN and measure its electron mobility and compare our results with recent reports in the literature.

TUE 12

Level Crossings in Bilayer Graphene

Hiske Overweg¹, Angelika Knothe², Thomas Fabian³, Lukas Linhart³, Peter Rickhaus¹, Lucien Wernli¹, Kenji Watanabe⁴, Takashi Taniguchi⁴, David Sánchez⁵, Joachim Burgdörfer³, Florian Libisch³, Vladimir I. Fal'ko², Klaus Ensslin¹, Thomas Ihn¹

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A precise understanding and control of quantized energy levels in two-dimensional materials is key to exploit the quantum nature of layered nanodevices. We consider electrostatic confined quantum point contacts in bilayer graphene. We measure and simulate the behaviour of subbands in gapped bilayer graphene in a magnetic field [1]. At zero magnetic field conduction quantization steps of $4 e^2/h$ appear due to the valley and spin degeneracy in bilayer graphene. A perpendicular magnetic field lifts the valley degeneracy, leading to quantization steps of $2 e^2/h$. Since the magnetic field breaks time reversal symmetry, the quantization steps related to the two valleys evolve differently for increasing magnetic field. Subbands N and N+2 from the two valleys eventually join in the Landau regime in a topologically stable fashion and quantization steps of $4 e^2/h$ reappear.

[1] Physical Review Letters 121, 257702 (2018)

TUE 13**Increase of liquid crystal local order parameter due to carbon nanotubes**Giusy Scalia¹, Hakam Agha¹¹University of Luxembourg, Luxembourg

Liquid crystal (LC) phase exists between the isotropic and crystalline states of matter. The nematic phase is characterised by mainly orientational order and the order parameter S quantifies the degree of orientational order possessed by a specific LC and at a certain temperature. The order parameter changes with temperature since this affects the distribution function of the orientation of the molecular axes, broadening with the increase of temperature. The change in order parameter manifests with different birefringence colors as temperature varies. We discuss the effect of carbon nanotubes (CNTs) on the LC phase transition estimating the transition temperature of LC with code name 5CB or K15 mixed with CNTs. The presence of carbon nanotubes can increase locally the phase transition temperature, i. e. close to the nanotube surface, of about 0.1°C and in some cases 0.2°C . The LC molecules anchor at the nanotube surface which induces a local increase of order. Noticeably the effect is visible on macroscopic scale influencing LC molecules at distances, in some cases, much larger than the apparent aggregate dimension.

TUE 14**Spin transport in BiTeBr/graphene heterostructures**Zoltán Kovács-Krausz¹, Péter Makk¹, Bálint Szentpéteri¹, Anamul Md Hoque², Bálint Fülöp¹, Michael Yakushev³, Saroj Prasad Dash², Szabolcs Csonka¹¹Budapest University of Technology and Economics, Budapest, Hungary²Chalmers University of Technology, Gothenburg, Sweden³University of Strathclyde, Glasgow, UK

Graphene is a promising spin transport channel candidate due to long spin relaxation time and micrometer-scale spin signal transmission, but mechanisms for manipulating the spin signal without the use of an external magnetic field are needed. The class of polar semiconductors BiTeX (where X=Br,I) has attracted interest due to its giant built-in Rashba spin-orbit interaction.

We present fabrication methods of BiTeX/graphene heterostructures using different approaches, where BiTeX is expected to change the spin transport in the underlying graphene layer. To characterize the spin transport properties of the heterostructures, low temperature weak localization, along with room temperature nonlocal spin valve and Hanle spin precession measurements are performed. Using BiTeX as an injector electrode, we observe evidence of spin injection into graphene.

TUE 15**Engineering the structure and properties of single-layer MoTe₂: from point to extended defects**

Tibor Lehnert¹, Mahdi Ghorbani-Asl², Janis Köster¹, Zhongbo Lee¹,
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Aberration-corrected high-resolution transmission electron microscopy (TEM) experiments combined with first-principles calculations are performed to investigate defect-induced structural transformations and their properties. To increase contrast and still maintain sub-Angström resolution TEM data were acquired with the Cc/Cs-corrected SALVE (Sub-Angström Low-Voltage Electron microscopy) instrument at 40 kV [1,2].

We show electron-beam driven atom-by-atom evolution of single-Te vacancies and column divacancies into different types of Te tetravacancies and trefoil-like structures. Moreover, we report on the formation of single Te vacancy lines originating from agglomeration of single Te vacancies. The driving force for the reported defect evolutions is minimization of the free energy of the system.

Furthermore, we show that the electron-beam-driven formation of Te-deficient inversion domains with 4|4P and 4|4E mirror twin boundaries and strain induced local phase transformations from the 2H to the 1T' MoTe₂ phase.

[1] M. Linck et al., Phys. Rev. Lett. 2016, 117, 076101

[2] Z. Lee et al., Ultramicroscopy 2012, 112(1), 39-46

TUE 16**Magnetic Proximity Effects in Two-Dimensional Materials**

Igor Zutic¹

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Proximity effects can transform a given material through its adjacent regions to become superconducting, magnetic, or topologically nontrivial [1]. In bulk materials, the sample size often greatly exceeds the characteristic lengths of proximity effects allowing their neglect. However, in 2D materials such as graphene, transition-metal dichalcogenides (TMDs) and other atomically thin monolayers, the situation is drastically different. Even short-range magnetic proximity effects exceed their thickness and we show how they strongly modify transport and optical properties [2,3], or change the band topology [4]. In TMDs rotating the magnetization of the substrate can convert between optically inactive and active excitons [3] and we discuss how it

could enable novel functionalities of spin lasers we have discovered in conventional semiconductors [5].

1. I. Zutic et al., *Materials Today*, in press <https://doi.org/10.1016/j.mattod.2018.05.003>
2. P. Lazic, K. D. Belashchenko, I. Zutic, *Phys. Rev. B* 93, 241401(R) (2016)
3. B. Scharf et al., *Phys. Rev. Lett.* 119, 127403 (2017)
4. T. Zhou et al., *npj Quant. Mater.* 3, 39 (2018)
5. M. Lindemann et al., arXiv:1807.02820, to appear in *Nature*

TUE 17

Electrophysical properties of single-walled carbon nanotubes separated by type of conductivity

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Possessing amazing properties due to their unique structure, single-walled carbon nanotubes (SWCNT) can be found considerably attractive in many fields of research. As the yield of most synthesis techniques is the mixture of semiconducting and metallic nanotubes, the important point is to achieve the high quality of solely metallic or solely semiconducting nanotubes. In this research, we demonstrated that the separation of large diameters SWCNT can be very effectively achieved with an aqueous two-phase extraction technique. The purity of separated metallic and semiconducting nanotubes are up to 98%.

Separated by type of conductivity SWCNTs were used for investigation of a variety of their electrophysical properties starting with a CNTFET sensor on 2-chlorophenol, probing field emission from solely metallic and solely semiconducting SWCNT films, and ending with a highly correlated behaviour of charge carriers in SWCNT films doped with copper chloride.

TUE 18**Synthesis, characterization and field emission from $\text{Mo}_{1-x}\text{W}_x\text{S}_2$ nanotubes**Luka Pirker¹, Bojana Višić^{1,2}, Maja Remškar¹¹Institut Jozef Stefan, Ljubljana, Slovenia²Institute of Physics Belgrade, Belgrade, Serbia

Semiconducting MoS_2 and WS_2 nanotubes have been studied in the last decades for their interesting electrical, optical and structural properties. Recently it has been shown that MoS_2 nanotubes can enhance the performance of sodium-ion batteries and act as optical resonators while the WS_2 nanotubes have shown enhanced field emission properties. [1,2,3] Alloys from transition metal dichalcogenides, such as $\text{Mo}_{1-x}\text{W}_x\text{S}_2$, show interesting properties due to the tunable physical properties by changing the ratio of the transition metals components.

Here we present $\text{Mo}_{1-x}\text{W}_x\text{S}_2$ nanotubes synthesised by the chemical transport reaction for the first time. The nanotubes have been characterized with SEM, TEM, Raman spectroscopy, STM and Kelvin probe microscopy. Field emission properties and the work function were measured on single nanotubes in UHV.

[1] T. Zheng et al., Inorg. Chem. Front. 5, 1587-1593 (2018)

[2] D. R. Kazanov et al., APL 113, 101106 (2018)

[3] Viskadourous, G. et al., Small, 10, 2398-2403 (2014)

TUE 19**Indirect to Direct Gap Crossover in Two-Dimensional InSe Revealed by Angle Resolved Photoemission Spectroscopy**Matthew Hamer^{1,2}, Johanna Zultak^{1,2}, Alexei Barinov³, Neil Wilson⁴, Roman Gorbachev^{1,2}¹Physics and Engineering, University of Manchester, Manchester, UK²National Graphene Institute, University of Manchester, Manchester, UK³Elettra Sincrotrone, Trieste, Basovizza, Italy⁴Department of Physics, University of Warwick, Coventry, UK

Atomically thin films of III-VI post-transition metal chalcogenides (e.g. InSe) form an interesting class of two-dimensional semiconductor that feature a strong variation of their band gap as a function of the number of atomic layers. Specifically for InSe, there is an expected crossover from a direct gap in the bulk to a weakly indirect band gap in monolayers and bilayers [1].

Here, we apply angle resolved photoemission spectroscopy with submicrometer spatial resolution (μ ARPES) to visualise the layer-dependent valence band structure of mechanically exfoliated crystals of InSe. Due to the high-quality glovebox encapsulated samples, we show that for 1 layer and 2 layer InSe the valence band maxima is away from the Γ -point, forming an indirect gap. In contrast, for four or more layers the bandgap becomes direct, in good agreement with theoretical predictions and photoluminescence observations. These results are important as an

increased understanding of InSe's band structure could lead to advances in InSe based optoelectronic applications.

[1] Bandurin et al. Nature nanotechnology 12.3 (2017): 223.

TUE 20

Superconducting proximity effect in hBN-graphene moiré superlattice

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The alignment of the crystallographic axes of graphene and hexagonal boron-nitride (hBN) generates an additional periodic potential, which leads to a change in graphene's bandstructure. This change manifests in the appearance of so-called satellite Dirac points, van Hove singularities and renormalization of the Fermi velocity. While such systems have been widely studied with normal contacts and scanning techniques, there are only a few reports investigating proximity induced supercurrent in a Josephson junction (JJ) geometry. In the long junction limit, where the transport channel length exceeds the coherence length, the product of the critical current and the normal state resistance is proportional to the Thouless energy. In our work [1] we show that the combined measurement of the critical current and the normal state resistance reveals signatures of the modified density of states in a hBN-graphene superlattice. Further, we studied the dependence of the critical current on the normal state resistance in a ballistic superlattice by forming a p-n junction in the graphene transport channel.

TUE 21

Interacting Electrons in Bilayer Graphene and Bilayer Graphene/hBN Moiré Superlattices

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We will present our magnetotransport measurements of graphene bilayers [1] at large D , up to ~ 1.5 V/nm, where we observe crossings between Landau levels with different orbital quantum numbers. For particular crossings at large displacement fields, we observe resistivity hysteresis, indicating the presence of easy-axis quantum Hall ferromagnetism. Moreover, we study dual-gated graphene bilayer/hBN moiré superlattices. We observe additional resistance peaks as the charge density varies. The peaks' resistivities vary approximately quadratically with D . Data fits to a continuum model yield a bilayer/hBN interaction energy scale $\sim 30 \pm 10$ meV. Under a perpendicular magnetic field, we observe Hofstadter butterfly spectra as well as symmetry-broken- and fractional Chern insulator states characterized by their Chern number t and miniband index s [2, 3]. Their topology and lattice symmetry breaking is D -tunable, enabling the realization of new topological states in this system.

[1] A. H. Castro Neto, et al., Rev. Mod. Phys., 2009, 81, 109.

[2] E. M. Spanton, et al., Science, 2018, 360, 62.

[3] L. Wang, et al., Science, 2015, 350, 1231.

TUE 22

Pseudo magnetic field and non-superlattice minigaps in corrugated graphene

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We show the emergence of minigaps in the Dirac cone of corrugated graphene which are not related to the superlattice potential using a band unfolding approach based on first principles. To get more insight into the revealed phenomenon, we attempt to couple two different scenarios and we explain the pseudo-magnetic field induced pseudo-Landau level quantization by the opening of a non-superlattice related sequence of minigaps in the unfolded energy spectra in strained graphene systems which are consistent with accurate density of states (DOS). We also argue that in corrugated graphene above a certain threshold curvature Dirac fermions open minigaps which could be general in most of the strained and/or curved Dirac materials. A related scanning tunneling spectroscopy (STS) spectrum is also shown recorded on artificially corrugated graphene which is as designed not periodic; therefore the emerging measured LDOS dips are primarily not in superlattice crossing replica band origin nor related to superlattice Dirac points.

P. Süle, et al., Nano Lett. 15, 8295. (2015), A. Pálinkás et al., Carbon 107, 792. (2016).

TUE 23

Controlled synthesis of horizontally and vertically aligned MoS₂ films

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MoS₂ is a semiconductor with an indirect bandgap, however, the monolayer MoS₂ is a direct gap semiconductor. This is important for photovoltaic and photocatalytic applications due to its strong absorption in the solar spectral region. Other applications include photodetectors, photovoltaic cells, light-emitting diodes, catalysts and biosensors.

In most cases, MoS₂ films are grown horizontally with c-axis perpendicular to substrate plane. Some groups have presented also vertically aligned MoS₂ films where c-axis is oriented parallel to the substrate plane.[1,2] Since some applications such as water splitting or disinfection require vertically grown MoS₂, the controllable growth is an important issue.

Here we present fabrication of MoS₂ thin films using one zone sulfurization of Mo films on the c-plane sapphire. Changing the synthesis conditions, we are able to prepare vertically or horizontally aligned films starting from the same thickness of initial molybdenum film. Prepared films were characterized by GIWAX, AFM, Raman and optical measurements.

[1] Y. Jung et al., Nano Letters 2014, 14, 6842.

[2] S.-Y. Cho et al., ACS Nano 2015, 9, 9314.

TUE 24

Characterization of Atomically Precise Graphene Nanoribbons by Raman Spectroscopy

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Graphene nanoribbons (GNRs) exhibit an electronic bandgap due to the lateral confinement of charge carriers and edge effects. They can be fabricated by bottom-up on-surface synthesis from molecular precursors resulting in atomically precise structures [1]. This approach promises tunable optical and electronic properties [2]. We use Raman spectroscopy to characterize different types of GNRs and investigate their interaction with growth and devices substrates. In particular, we investigate new geometry-dependent signatures beyond the radial breathing like mode (RBLM).

[1] Cai, J. et al. (2010), Nature 466, 470–473

[2] Chen, Y.-C et al. (2013), ACS Nano 7, 7, 6123–6128

TUE 25**Exploring the Catalytic Properties of 2D-Pnictogens Sb and BP**

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⁵Instituto de Ciencia Molecular, Universitat de València, Catedrático José Beltrán 2,46980, Paterna, Spain.

The novel 2D-materials of group 15, also called 2D-pnictogens, exhibit in comparison to Graphene a more pronounced reactivity as organic catalysts. More concretely, the novel layered materials Black Phosphorus (BP) and Antimonene (Sb) offer excellent properties for catalytic reactions. The high degree of exfoliation in our materials and the protection against oxidation given by the ionic liquid (IL) allows the alkylation of soft nucleophiles with esters by using BP or Sb as catalyst.^[1] Nevertheless, the use of IL limits the number of reactions that can be studied. Therefore, our groups have investigated the exfoliation of BP in different solvents in order to explore further reactions that these materials can catalyze. Remarkably, BP dispersions in THF promote the free radical addition of CBrCl₃ to alkenes. These results confirm that BP can be used as an effective halogen transfer agent and give further insights into the unexplored catalytic properties of this 2D material, broadening the number of its applications.

[1] G. Abellán et al. Nat. Communications 2019, 10, 509

TUE 26**Electrical resistance of carbon nanotube sheets in presence of nematic liquid crystal 5CB**

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Liquid crystals (LCs) are fluids with some degree of order which, together with the molecular characteristics, affects their macroscopic properties. LCs align dispersed carbon nanotubes (CNTs) [1] and they can even impose some degree of orientational order onto networks of nanotubes. In this work we aim to investigate the

influence of LC on the electrical properties of networks of CNT. Cells with LCs and CNTs have been realized with two glass substrates one of which is coated with in-plane electrodes of indium tin oxide and multi-wall CNTs, drawn from spinnable forests, deposited on the other surface. The nematic LC(5CB) is filled by capillarity action into the cell covering the CNTs. The resistance of the network was monitored before, with the CNTs overlaid by air, and after the insertion of LC. The temperature was then changed for investigating the contribution of the variation in dielectric constant, occurring with temperature, until the isotropic phase. Finally, the behaviour of the resistance of CNT sheet was also investigated during the application of pressure on the LC cell.

References: [1] G. Scalia et al Adv. Mat., 16 11 June 2004, 865 869

TUE 27

A screening method for MoS₂ nanosheets using metal ions in solution

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MoS₂ nanosheets have been widely studied for electronic devices, which nanomaterials are mainly synthesized by sonication. But solution-exfoliated MoS₂ nanosheets are nonuniformly distributed in size from one nanometer to a few hundred nanometers, and these nanosheets as a complex composite were applied in reported devices. Therefore, a composite consisting of MoS₂ nanosheets with same size exhibit the same electronic and thermal properties for potential applications. Here, we suggest a method to screen MoS₂ nanosheets by metal ions. MoS₂ nanosheets with the same potential energy precipitate at the same rate when the same amount metals ions are attached to their surface, due to the fact that the MoS₂ nanosheets cannot exist in the colloidal dispersion system after metal ions introduced into their solution. Hence, MoS₂ nanosheets with the same potential energy could be selected according to the density of metal ions and the reaction time. Finally, the precipitated MoS₂ nanosheets could be separated from the metal ions and dissolved again by sonication. We will further study the electronic and thermal properties of nanomembranes by the selected MoS₂ nanosheets with a similar size.

TUE 28

On the anomalous spin-relaxation in graphite

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The anomalous temperature dependence of the spin-relaxation time, its anisotropy, and g -factor in graphite poses a 60-year-old problem albeit it is one of the best known materials. The spin-relaxation time in graphite is deduced from the electron spin resonance (ESR) line-width and it increases with decreasing temperature contrary to that expected from the conventional Elliot-Yafet model. High field ESR (at 5.6 T) measurements show that the ESR line is homogeneously broadened and the line-width has negligible magnetic field dependence. This rules out a number of explanations and shows that the anomalous temperature dependence has a true electronic origin. The ESR linewidth has an anomalous 2:1 anisotropy for magnetic field out- ($B||c$) and in-the plane ($B||(a, b)$) and the g -factor shift is strongly temperature dependent for $B||c$ whereas $B||(a, b)$ is constant. We show that the anomalous temperature dependence of both the spin-relaxation and the g -factor are explained by the near band degeneracy around the Dirac point in the graphite band structure.

TUE 29

Significant enhancement of electrical transport in SWCNT network-graphene hybrid system

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The electrical transport in carbon nanotube networks vary in a wide range of values as the structure of tubes and the morphology of networks differ. The fundamental importance lies in the properties of the individual nanotubes: electronic structure, tube length and defect concentration. The bottle neck for electrical transport is, nevertheless, a network morphology determining efficiency of charge tunneling between tubes. We compare conductivities of SWCNT networks, where the tube-to-tube tunneling is modified by substrates: a bare or graphene covered silicon surface. We observe an enhancement of conductivity 50% in the SWCNT-graphene system relative to a SWCNTs. Since graphene's conductivity was 20 times lower than that of SWCNTs, its parallel contribution to the total value would be negligible. Doping from graphene to SWCNTs was also excluded: Raman spectra showed no additional Raman shift due to doping. We interpret the significant conductivity enhancement

based on Van der Waals (VdW) interactions between tubes and graphene which enhances the efficiency of the charge tunneling. We demonstrate the enhanced VdW interactions between SWCNTs and graphene by SEM and TEM images.

TUE 30

Directionality and energetics of the nickel-induced graphitization of amorphous carbon thin films

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The catalytic graphitization with layer exchange (LE) of amorphous carbon in thin film stacks with Ni was investigated as a function of the initial stacking order. Bilayer and triple layer stacks were exposed to heating ramps up to 700 °C. Raman spectroscopy showed the formation of a layered graphitic structure after the annealing. During outwards LE, as C is transported towards the sample surface, a smooth layer with graphitic planes parallel to the interface with the substrate has formed through a 2D growth. A significant restructuring of the Ni layer appeared during inwards LE, as C is transported towards the substrate. Here, the fragmentation of the Ni layer, as well as the regions with turbulence-like and folding defects indicated a 3D growth. The degree of LE, quantified by ion beam analysis, is 95 % and 80 % for the out- and inwards direction, respectively. Based on the calculation of surface and interface energies of the initial and final states, thermodynamic estimations pointed to the wetting of Ni grain boundaries by C atoms as the initial driving force for the LE and allowed a consistent understanding of the LE directionality and of the final thin film microstructure.

TUE 31

IR and THz near-field spectroscopy for nanoscale free-carrier profiling

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IR and THz spectroscopy is an important tool to characterize vibrational resonances and low-energy dynamic processes in solid-state matter. However, the spatial resolution of conventional spectroscopy is limited by diffraction. Scattering-type scanning near-field optical microscopy (s-SNOM) overcomes the diffraction limit by employing a sharp metallic AFM tip as near-field probe. The laser-illuminated tip acts as an antenna, concentrating the light in a nanofocus at its apex. By detecting the tip-scattered light the local optical properties of the sample with nanoscale resolution

can be recorded. Here we present the implementation of a THz-Time Domain Spectroscopy system in an s-SNOM enabling to record nanoscale resolved, quantitative THz-TDS near-field spectra and consequently to measure the free-carrier concentration in semiconductor devices without any prior calibration. Further, we present application examples for the electrical characterization of graphene, and the measurement of absorption bands of molecular resonances. In the future we expect outstanding insights into low-energy dynamics and transitions by the recent system integration into a closed-cycle cryostat.

TUE 32

Temperature dependent Raman spectroscopy of pristine and Cu-doped TiSe₂

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Titanium diselenide, TiSe₂, is a compound from the family of transition metal dichalcogenides. It is a two-dimensional material that exhibits a transition to a charge-density wave (CDW) state below 200 K. Upon doping with copper, Cu_xTiSe₂ becomes a superconductor at dopings $x \geq 0.04$, with a maximum transition temperature of 4.2 K for $x = 0.08$. Emerging superconductivity is accompanied with the suppression of the CDW state.

We present Raman measurements of pristine and Cu-doped TiSe₂ single crystals performed down to 7 K and for series of dopings of up to $x=0.08$. Besides the normal state Raman modes of TiSe₂ at 136 and 200 cm⁻¹, CDW-related A_{1g} and E_{1g} lines were observed at 118 and 80 cm⁻¹, respectively, at temperatures below 150 K. The CDW modes of TiSe₂ soften and broaden with the increasing temperature. At low doping levels, the CDW modes are present in the spectra while they are completely absent at $x = 0.08$. The CDW A_{1g} line softens and broadens with increased copper doping. We will discuss other effects such as strong background dependent on x , asymmetrical shape of the Raman lines at higher doping levels and lines that have not been reported so far.

TUE 33

One dimensional van der Waals heterostructures wrapped around single-walled carbon nanotubes

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We have synthesized a new coaxial nanotube structure, in which mono- or few-layer hexagonal boron nitride nanotube (BNNT) seamlessly wrap around a single-walled carbon nanotube (SWCNT), and result in an atomically smooth coaxial tube consisting two different materials. TEM-EELS clearly demonstrated the BNNT-SWCNT coaxial structure. We have tried various morphologies of SWCNTs as starting material, e.g. vertically aligned array, horizontally aligned array, suspended SWCNTs, and dry-deposited random network films. We can clearly observe the coaxial structure from originally isolated SWCNTs. We found no correlation between chiral angle of inner SWCNT and outer BNNT for 'double-walled' SWCNT-BNNT. We concluded that these are one-dimensional van der Waals heterostructure. We have further developed the 1D coating CVD for transition metal dichalcogenide nanotubes, such as MoS₂ nanotube. We can grow MoS₂ nanotubes around relatively large diameter SWCNT or SWCNT@BNNT [1]. We will discuss properties of the 1D heterostructures through optical absorption, Raman scattering, photoluminescence, FT-IR, and cathode luminance.

Reference: [1] Rong Xiang et al., arXiv:1807.06154 (2018).

TUE 34

Functionalized graphene transistor detects traces of carbon-quantum dots at ppm level

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The omnipresent carbon nanomaterials pose a great potential for the emerging technologies as well as threat for human health at the end of their lifecycle, especially when introduced into waste or ground waters. A graphene field-effect transistor (GFET) is employed for detecting sub-monolayer of carbon quantum dots (CQDs) in water. We validate both the exfoliated as well as the chemical vapor deposited (CVD) graphene as an effective GFET channel. The adsorption of CQDs is followed by the conductance changes of GFET. A readily measured shift in the Dirac voltage is observed after the graphene channel functionalized by (3-Aminopropyl)triethoxysilane is exposed to CQDs. The affinity of CQDs carboxyl terminal groups towards the amino-functionalized graphene channel enabled a highly sensitive detection based on alteration of GFET conductivity. The adsorption of CQDs induce a positive shift of Dirac point having a limit of detection at the concentration of 80 ppm and 20 ppm for exfoliated and CVD graphene, respectively. Supporting study of CQDs adsorption is performed by real time in-situ confocal Raman microscopy and ex-situ X-ray photoelectron spectroscopy.

TUE 35**Modification of the electronic properties of single-walled carbon nanotubes by encapsulation of electron acceptor and donor substances**

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The filling of internal channels of single-walled carbon nanotubes (SWCNTs) is a promising method of controllable modification of their electronic properties, because a variety of substances with appropriate physical and chemical properties can be encapsulated inside SWCNTs [1]. In this work, we perform the filling of SWCNTs with a mean diameter of 1.4 nm with lead halogenides (PbCl₂, PbBr₂ and PbI₂) and rubidium iodide (RbI) by the melt method. We investigate the morphology and atomic structure of the filled SWCNTs by scanning transmission electron microscopy and show that one-dimensional nanocrystals with well-ordered structure are formed within SWCNTs. Raman spectroscopy and X-ray photoelectron spectroscopy investigations of the filled SWCNTs show that lead halogenides cause hole doping of SWCNTs accompanied by a downshift of their Fermi level. In contrast, the encapsulated rubidium iodide leads to electron doping of host SWCNTs with an upshift of their Fermi level. The observed differences are explained by different work functions of the salts.

[1] M.V. Kharlamova, Prog. Mater. Sci. 77, 125-211 (2016)

TUE 36**Transmission Electron Microscope Specimen Polymer Preparation of Mn/FePS₃ and Electron Beam Induced Defect Dynamics in Two-Dimensional MoTe₂**

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The Sub-Ångström Low-Voltage Electron Microscope (SALVE) [1,2], which is a Cc/Cs-corrected TEM, enables the analysis of electron beam induced defect dynamics in two-dimensional (2D) materials on an atomic level. Therefore, sample preparation is a crucial part and one of the defining factors for high quality results. The common sample preparation method (e.g. scotch-tape method, wet-etching with potassium hydroxide (KOH) solution [3]) was used for producing molybdenum ditelluride (MoTe₂) monolayers, but it faces problems of fast oxidation of the material.

With MnPS_3 and FePS_3 , we were able to demonstrate a gentle way to enhance the quality of the 2D-TEM samples with respect to oxidation. Polymer coating (PMMA and PVA) enables to avoid KOH, the main reason for oxidation.

Furthermore, in first SALVE experiments we observe migration of tellurium (Te) vacancies in freestanding 2D MoTe_2 under electron irradiation. First-principles calculations were conducted to rationalize the TEM results.

[1] Z. Lee et al., Ultramicroscopy 2012, 112(1)

[2] M. Linck et al., Phys. Rev. Lett. 2016, 117

[3] J. C. Meyer, et al., Appl. Phys. Lett. 2008, 92

TUE 37

Raman spectroscopy monitoring of the integration process of individual single-walled carbon nanotubes into sensing devices

Miroslav Haluska¹, Lalit Kumar¹, Laura V. Jenni¹, Seoho Jung¹, Christofer Hierold¹

¹Micro and Nanosystems D-MAVT, ETH Zurich, Tannenstrasse 3, 8092 Zurich

Raman spectroscopy was applied to identify processing steps with dominant impact on single-walled carbon nanotubes (SWCNTs) during their integration into sensing devices. It was used for CNT's localization and characterization with respect to their size, structural quality and metallicity too. SWCNTs were synthesized on SiO_2/Si substrates or oxidized SOI MEMS structures with beams from ferritin-based Fe catalyst nanoparticles by CH_4/H_2 -CVD at 825-860°C [1]. Devices with CNTFET architecture based on individual tubes were fabricated either by standard photo- or electron-beam lithography, or by ultra-clean mechanical transfer from dedicated growth substrates onto the final device structures. The use of a mechanical dry-transfer allows for a straight-forward integration of suspended CNTs [2]. In the case of substrate-bound nanotubes, the application of Raman monitoring lead to an optimized process flow producing devices with eight times reduced variation of their electrical resistance [3].

References

[1] L. Durrer, et al., Nanotech. 20, 355601 (2009).

[2] M. Muoth, et al., IEEE MEMS, 1352 (2012).

[3] W. Liu, et al., Nanotechnology 27, 015201 (2016).

TUE 38

Topological phase diagram of BiTeX graphene hybrid systems

Zoltán Tajkov¹, László Oroszlány², János Koltai¹

¹Department of Biological Physics, Eötvös Loránd University, Budapest

²Department of Physics of Complex Systems, Eötvös Loránd University, Budapest

Tuning spin-orbit interaction in graphene samples promises several revolutionary

applications. One of the most striking effects is the appearance of a quantum spin hall phase as proposed by Kane and Mele. Since the intrinsic spin-orbit coupling (SOC) is weak in graphene one needs to turn to alternative methods in order to reach the topological phase. Combining graphene with other novel layered materials is a possible way for engineering the band structure of charge carriers. Strong spin-orbit coupling in BiTeX compounds and the recent fabrication of a single layer of BiTel points towards a feasible experimental realization of a Kane-Mele phase in graphene based heterostructures. In our work we explore the electronic structure and topological phase diagram of hybrid systems built from graphene and BiTeX (X=I,Br,Cl) layers. We show that structural stress inherently present in fabricated samples could easily induce a topological phase transition thus turning the sample in a novel experimental realization of a time reversal invariant topological insulator.

TUE 39

Electron-Beam Manipulation of Silicon Impurities in Single-Walled Carbon Nanotubes

Kimmo Mustonen¹, Mukesh Tripathi¹, Alexander Markevich¹, Heena Inani¹, Aqeel Hussain², Er-Xiong Ding², Clemens Mangler¹, Esko I. Kauppinen², Jani Kotakoski¹, Toma Susi¹

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The recent discovery that heteroatoms in graphene can be manipulated with focused electron irradiation has opened novel avenues for top-down atomic engineering. These achievements have been enabled by largely by advances in electron optics and microscope stability, but also in the preparation of suitable crystalline materials with impurity elements incorporated via ion and electron-beam irradiation or other means. Here, starting with silicon impurity introduction into the lattice of single-walled carbon nanotubes (SWCNTs), we show their positions can be manipulated using a focused 55–60 keV electron probe aimed at a neighboring carbon site. Moving the silicon atom mainly along the longitudinal axis of ~ 2.7 nm tubes, more than 90 controlled lattice jumps were recorded and the relevant scattering cross sections estimated. Molecular dynamics simulations show that even in ~ 2 nm SWCNTs, depending on the local geometry around the electron-beam-displaced carbon atom with respect to the tube axis, the threshold energies for out-of-plane dynamics are different than in graphene.

TUE 40

Binary molecule encapsulation for precise carrier density control of SWCNTs

Guowei Wang¹, Takeshi Tanaka¹, Atsushi Hirano¹, Hiromichi Kataura¹

¹Nanomaterials Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8565, Japan

We are developing electric power generation devices using semiconducting single-wall carbon nanotube (SWCNT) films. In this method, current can be generated by moving an electrolyte droplet on the film. To optimize the system, carrier density of the SWCNT has to be controlled precisely. In this study, we tried to control the carrier density of SWCNT precisely using chemical doping by encapsulating dopant molecules. For this purpose, usually, we need to control the number of dopant molecules inside SWCNTs. Our new method is to control the number of dopant molecules precisely by changing the concentration ratio of dopant and dummy molecules. We selected 2,4-bis[4-(N,N-diphenylamino)-2,6-dihydroxyphenyl] squaraine (DPSQ) and coronene as hole dopant and dummy molecules, respectively. SWCNTs (EC1.5, Meijo Nano Carbon, unsorted) were refluxed in 1,4-dioxane for 3 h with pre-dissolved dopant and dummy molecules. By changing concentration ratio of DPSQ to coronene, we have prepared several SWCNTs encapsulating DPSQ molecules with different density. Since the dummy molecules do not affect the electronic properties of SWCNTs, this method can be useful to control carrier density precisely.

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- 08:30 – 09:30 **TUTORIAL: E. Andrei, New Jersey**
Strategies for band structure engineering in 2D materials
- 09:30 – 10:00 **P. Rickhaus, Zurich**
Transport in Twisted Bilayer Graphene at Extreme Angles
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **J. R. Ahn, Suwon**
Dirac electrons in a dodecagonal graphene quasicrystal
- 11:00 – 11:30 **P. Hommelhoff, Erlangen**
Ultrafast coherent electron physics in graphene and in a graphene-SiC Schottky junction
- 11:30 – 12:00 **A. Jorio, Belo Horizonte**
Photonic Cooper Pairs and TERS in 2D systems
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **S. Eigler, Berlin**
Oxo-functionalization of graphene and functionalization
- 19:00 – 19:30 **L. Hornekær, Aarhus**
Controlling the Electronic and Chemical Properties of Graphene via Functionalization and Intercalation
- 19:30 – 20:00 **D. R. Klein, Cambridge**
Magnetism in the Ultrathin Chromium Trihalides
- 20:00 – 20:30 **T. Heine, Dresden**
Two-Dimensional Topological Polymers

Wednesday, March 13th

Graphene, new materials

08:30**Strategies for band structure engineering in 2D materials**Eva Y. Andrei¹¹Rutgers University, New Jersey

A new era of materials started with the breakthrough isolation of the first free standing 2D material, graphene, followed by dozens of new 2D materials since. The distinctive characteristic of these layers is that, with all the atoms residing at the surface, it is possible to access and manipulate their properties with non-chemical "knobs" such as strain, twist, electric and magnetic fields. I will discuss experiments that utilize such knobs to transform the electronic structure of graphene: inducing magnetism and Kondo screening by removing single Carbon atoms; generating flat bands and pseudo-magnetic fields by twist, strain and buckling.

References

- [1] Y. Jiang et al., "Inducing Kondo screening at point defects in graphene with gating and local curvature", Nature Communications 9, (2018) 2349
- [2] D. May, et al., Modeling of the gate-controlled Kondo effect at carbon point defects in graphene, Phys. Rev. B 97, 155419 (2018)
- [3] Y. Jiang, Visualizing Strain-Induced Pseudo Magnetic Fields in Graphene through an hBN Magnifying Glass , Nano Lett., 17 , 2839 (2017)

09:30**Transport in Twisted Bilayer Graphene at Extreme Angles**

Peter Rickhaus¹, J. R. Wallbank², Sergey Slizovskiy², Riccardo Pisoni¹, Hiske Overweg¹, Yongjin Lee¹, Marius Eich¹, Ming-Hao Liu³, Thomas Ihn¹, Klaus Ensslin¹

¹Department of Physics, ETH Zürich, Zürich

²National Graphene Institute, University of Manchester, Manchester, M13 9PL,

³Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Two misaligned layers of graphene exhibit intriguing transport properties that depend drastically on the twist angle. Here we investigate the properties at extreme angles. On the one hand we study the regime of tiny twist angles, where large regions of strongly coupled bilayer graphene dominate the transport. By gating, these regions can become gapped. This leads to a triangular network of topological channels which we investigate [1] by an electronic Fabry-Pérot interferometer [2,3]. We observe coherent oscillations which originate from loops in the topological network. The length of the corresponding loops is in the micron range and the oscillations are robust in magnetic fields up to 8 Tesla. On the other hand, we investigate transport in large-angle twisted graphene. Here we demonstrate that the wavefunctions in the upper and lower layer are strongly decoupled but remain coherent and we measure an ultra-high capacitance between the two layers [4].

[1] P. Rickhaus, et. al, Nano Lett. 18, 11, 6725 (2018)

[2] P. Rickhaus et. al. Nat. Commun. 4, 1 (2013)

[3] P. Rickhaus et. al., Nat. Commun. 6, 6470 (2015)

[4] P. Rickhaus et. al., in preparation

10:30**Dirac electrons in a dodecagonal graphene quasicrystal**Joung Real Ahn¹¹Department of Physics, Sungkyunkwan University, Suwon

Quantum states of quasiparticles in solids are dictated by symmetry. Thus, a discovery of unconventional symmetry can provide a new opportunity to reach a novel quantum state. Recently, Dirac and Weyl electrons have been observed in crystals with discrete translational symmetry. Here we experimentally demonstrate Dirac electrons in a two-dimensional quasicrystal without translational symmetry. A dodecagonal quasicrystal was realized by epitaxial growth of twisted bilayer graphene rotated exactly 30 degree. The graphene quasicrystal was grown up to a millimeter scale on SiC(0001) surface while maintaining the single rotation angle over an entire sample and was successfully isolated from a substrate, demonstrating its structural and chemical stability under ambient conditions. Multiple Dirac cone replicated with the 12-fold rotational symmetry were observed in angle resolved photoemission spectra, showing its unique electronic structures with anomalous strong interlayer coupling with quasi-periodicity. Our study provides a new way to explore physical properties of relativistic fermions with controllable quasicrystalline orders.

11:00

Ultrafast coherent electron physics in graphene and in a graphene-SiC Schottky junction

Peter Hommelhoff¹

¹Physics Department, University of Erlangen, Erlangen

We focus two-cycle short laser pulses at graphene and observe the resulting carrier envelope phase-dependent current. (The carrier envelope phase, CEP, describes the phase difference between the optical carrier field and the envelope of a laser pulse.) We observe a CEP-dependent current in graphene, whose direction changes when we increase the laser field strength above 2 V/nm. We can explain this by a transition from the photon-driven weak-field regime to the strong-field regime, in which intraband motion and interband transitions are coupled. Moreover, we observe fully coherent electron physics inside of graphene in the form of Landau-Zener-Stückelberg interference.

In the second part of the talk we will discuss the ultrafast charge transfer across a graphene-silicon carbide Schottky junction. We observe a record-fast charge transfer time of 300 attoseconds, which is tuneable by virtue of the bias voltage over three orders of magnitude.

11:30

Photonic Cooper Pairs and TERS in 2D systems

Ado Jorio¹

¹Physics, UFMG, Belo Horizonte

In this talk I will address two new achievements in the field of Raman spectroscopy: (i) the photonic counterparts of superconducting Cooper pairs; (ii) tip-enhanced Raman spectroscopy (TERS) in two-dimensional systems. The photonic Cooper pairs are due to a virtual-phonon mediated photon-photon interaction, which happens in any material, and it seems to be superior in engineered graphene. The TERS in two-dimensional systems (graphene, transition metal mono/di-chalcogenides) are enabled by the ultra-high enhancements achieved with plasmon-tuned tip piramides. With this ultra-high enhancement, the local Raman is much more intense than the response from the large surface area illuminated by the confocal system, allowing us to probe local effects in the pristine two-dimensional structure.

18:30**Oxo-functionalization of graphene and functionalization at defect sites**Siegfried Eigler¹¹Freie Universität Berlin, Berlin

The development of versatile functionalization concepts for graphene are currently in the focus of research. With oxo-functionalization of graphite the full surface of graphene becomes accessible for C-C bond formation to introduce out-of-plane functionality. Several synthetic strategies are presented leading to oxo-functionalized graphene.[1] Moreover, we present the arylation of graphene by arylazocarboxylic tert-butylesters, which generates aryl radicals after activation by acids. Surprisingly, the degree of functionalization is related to the concentration of lattice vacancy defects of graphene.[2] Consequently, graphene, which is free from lattice defects is not reactive. The presented method paves the way to functional graphene derivatives with the density of defects determining the degree of functionalization.

[1] S. Seiler, C. E. Halbig, F. Grote, P. Rietsch, F. Börrnert, U. Kaiser, B. Meyer, S. Eigler *Nature Commun.* 2018, 9, 836.

[2] C. E. Halbig, R. Lasch, J. Krüll, A. Pirzer, Z. Wang, J. N. Kirchhof, K. I. Bolotin, M. R. Heinrich, S. Eigler, *Angew. Chem. Int. Ed.* DOI: 10.1002/anie.201811192

19:00

Controlling the Electronic and Chemical Properties of Graphene via Functionalization and Intercalation

Liv Hornekær¹

¹Dept. Physics and Astronomy; iNANO , Aarhus University, Aarhus

Extensive control of the electronic and chemical properties of graphene on Ir(111) is available through chemical functionalization and intercalation. Combined Scanning Tunneling Microscopy, (Standing Wave) X-ray Photoemmission Spectroscopy and Density Functional Theory calculations show how on one hand, functionalization structures can be controlled via intercalation, while conversely, intercalation can be hindered via chemical functionalization. Furthermore, unique oxygen functionalization structures and molecular hydrogen dissociative adsorption pathways are available in this system. Overall this allows for extensive control of electronic properties for band gap engineering, as well as control of the graphene-substrate interaction, providing proof-of-principle pathways to e.g. enhance the coating properties of graphene on metal surfaces.

19:30**Magnetism in the Ultrathin Chromium Trihalides**Dahlia R. Klein¹¹Physics, Massachusetts Institute of Technology, Cambridge

Recently, the family of layered 2D crystalline materials has expanded to include the chromium trihalides (CrX_3), a class of insulating magnets. We first employ the magneto-optical Kerr effect to probe the magnetic ordering of CrI_3 down to the monolayer limit. Beyond optical techniques, we present a new approach to probe the layer-dependent magnetic ordering of these materials using electrical transport. We fabricate spin-filter magnetic tunnel junctions from two graphite contacts separated by a few-layer crystal of CrX_3 that serves as the insulating tunnel barrier. By measuring the differential conductance across the junction, we can electrically detect the magnetic ordering as a function of applied magnetic field and bias voltage. These results reveal interesting magnetic properties in ultrathin CrX_3 differing from the bulk crystals. This new concept of magnetic tunnel junctions constructed by stacking 2D materials paves the way for discovering novel magnetic phenomena in the many unexplored layered magnetic insulators, as well as integration of these junctions in the spintronics community due generation of highly spin-polarized currents and large magnetoresistances.

20:00**Two-Dimensional Topological Polymers**Thomas Heine^{1,2}, Yu Jing¹, Maximilian Springer², Agnieszka Kuc²¹Theoretical Chemistry, TU Dresden, Dresden²Helmholtz Center Dresden-Rossendorf, Dresden

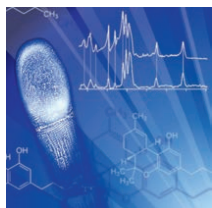
In 1643, Johannes Kepler identified 11 possibilities to regularly tile 2D space. These crystalline networks with translational symmetry are the so-called Kepler nets. Nature only knows few of these networks. However, artificial 2D networks of any topology can be created and studied in the laboratory by placing atoms at flat surfaces under cryogenic conditions. While this allows to explore the physical phenomena of such networks (and there are many!) in principle, experiments are difficult, expensive, and any exploitation of these phenomena is essentially impossible.

On the other hand, chemistry knows molecules that can act as 2D building blocks. They can be readily connected to form such regular tilings which are stable at ambient conditions. I will present the progress that has been made in chemistry in order to form crystalline semiconducting 2D polymers, discuss the challenge of achieving high charge carrier mobilities, and present first results on exotic networks, such as kagome lattices and others, which expose intriguing relations between lattice topology and electronic topology.



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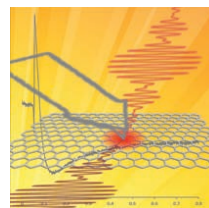
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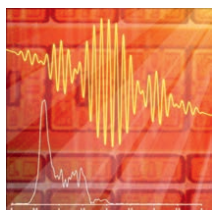
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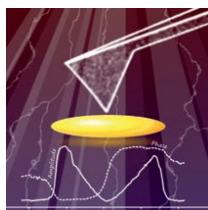
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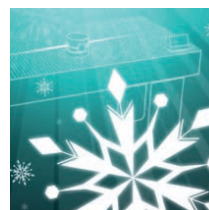
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- 08:30 – 09:00 **D. Prezzi, Modena**
Light Emission from Graphene Nanoribbons: Insights from Ab Initio Simulations
- 09:00 – 09:30 **G. Borin Barin, Dübendorf**
Bottom-up fabrication of graphene nanoribbons: From molecules to devices
- 09:30 – 10:00 **A. Mugarza, Barcelona**
Tailoring structural and electronic properties of graphene nanostructures with atomic precision
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **U. Kaiser, Ulm**
Dynamics of Advanced Low-Dimensional Materials by Low-Voltage Atomic-Scale TEM experiments
- 11:00 – 11:30 **E. Besley, Nottingham**
Effects of encapsulation on molecular damage under electron irradiation
- 11:30 – 12:00 **M. Grifoni, Regensburg**
Majorana fermions in carbon nanotubes
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **G. Abellán, Erlangen**
Chemistry of 2D-Pnictogen Nanomaterials
- 19:00 – 19:30 **C. Casiraghi, Manchester**
Water-based and biocompatible inks made of 2D-materials for fully printed electronics
- 19:30 – 20:00 **M. Drndic, Philadelphia**
Where did the missing atoms go? From local bandgap tinkering and antidots to nanoporous medley
- 20:00 **Poster Session III**

Thursday, March 14th

Carbon nanostructures, chemistry

08:30**Light Emission from Graphene Nanoribbons: Insights from Ab Initio Simulations**Deborah Prezzi¹¹Nanoscience Institute, National Research Council (CNR), Modena

Graphene nanoribbons (GNRs) have attracted increasing attention as a viable route for graphene-based nano- and opto-electronic applications, especially in view of the successful production of ultranarrow and structurally well-defined GNRs that allows to have tunable bandgaps. While absorption properties have been addressed in depth, emission properties are still largely unexplored.

We here report on the optical response of infinite and finite-length GNRs as resulting from state-of-the-art ab initio calculations beyond mean field[1,2]. Our results indicates that bulk-like excitations coexist with below-bandgap states localized at the GNR extremities, which are almost independent on the length. By investigating both the presence of defects and the effect of the substrate, our simulations allow us to identify unpredicted optical transitions in GNRs and to elucidate the origin of below-bandgap STM-induced light emission recently observed in suspended GNRs[1], providing a promising route for the realization of bright, robust, and controllable graphene-based light-emitting devices.

[1] M. Chong et al., Nano Lett. 18, 175 (2018).

[2] C. Cardoso, A. Ferretti, D. Prezzi, EPJB (2018)

09:00**Bottom-up fabrication of graphene nanoribbons: From molecules to devices**Gabriela Borin Barin¹, Pascal Ruffieux¹, Roman Fasel¹¹nanotech@surfaces Laboratory, Empa, Dübendorf, Switzerland

Atomically precise graphene nanoribbons (GNRs) have shown great potential to further stretch the upcoming scaling limit of integrated circuits technology. GNRs exhibit a sizeable bandgap[1], which is inversely proportional to their width, and are thus excellent candidates for room temperature switching applications such as field-effect transistors (FET). Despite their exceptional properties, significant challenges remain for GNR fabrication, processing and characterization. Bottom-up synthesis of graphene nanoribbons is most commonly performed under ultra-high vacuum conditions, which is one of the bottlenecks in the further technological advancement of this material. Additionally, little is known about the stability of ultra-narrow GNRs under ambient conditions or during device processing. In this talk I will address these critical challenges, focusing on GNR fabrication scalability, substrate transfer[2], ex-situ characterization, and show that gate and channel length optimization on GNR-FET allows for the fabrication of GNRs devices with high on/off ratios[3].

[1] J.Cai et al. Nature,466,2010

[2] A.Fairbrother et al. Nanoscale,8.2017

[3] J.P.Llinás et al. Nature Comm,8.2017

09:30**Tailoring structural and electronic properties of graphene nanostructures with atomic precision**Aitor Mugarza¹¹ICN2, Barcelona

Nanostructuring graphene confers multiple functionalities to this material, making it attractive to very diverse applications in electronics, molecular sensing and filtering. For instance, semiconducting gaps can be induced by reducing its dimensions to the nanometer scale, whereas introducing pores of similar sizes turns impermeable graphene into the most efficient molecular sieve membrane. In both cases, the interesting scale for applications is below 3-5 nm, a regime where bottom-up synthesis can be particularly efficient.

Here I report different on-surface methods to grow graphene quantum dots with controlled shape and edge structure [1], periodic arrays of nanoribbons with lengths exceeding 100 nm [2], and nanoporous graphene sheets that combine 1nm size ribbons and pores [3]. Their novel electronic states are correlated with the particular atomic structures by using STM. Their potential application in devices is illustrated by gate modulated transport measurements in nanoporous graphene sheets.

[1] S. O. Parreiras et al., *2D Mater.*, 4 25104 (2017).

[2] C. Moreno et al., *Chem. Commun.* 54, 9402 (2018).

[3] C. Moreno et al, *Science* (80-.). 360, 199 (2018).

10:30

Dynamics of Advanced Low-Dimensional Materials by Low-Voltage Atomic-Scale TEM experiments

Ute Kaiser¹

¹Central facility of Materials Science Electron Microscopy, University of Ulm, Ulm 89081, Germany

To obtain structural and electronic properties of advanced low-dimensional material at the atomic scale is a growing demand in materials science. A new type of transmission electron microscopes operating at electron energies between 80keV and 20keV was developed. It allows to undercut most of the materials knock-on damage thresholds and enables sub-Angstroem resolution in an 4000x4000 pixels, single-shoot image down to 40keV by correcting not only geometrical aberrations but also its chromatic aberration. We modify properties of low-dimensional materials by the use of the electron beam not only for imaging its original structure but also for engineering 2D transition metal dichalcogenide with new properties. We generate metal-atom-dimers encapsulated within single-walled carbon nanotubes and observe the dynamics of metallic bonds by exact measurements of the inter-atomic distance. We intercalate bilayer graphene by lithium and study the lithiation and delithiation between bilayer graphene, as well as the structure of the new high density crystalline Li- phase.

[1] We thank DFG and the MWK-B/W for SALVE, B/W Stiftung for CleanTech and EU for Graphene falgship.

11:00**Effects of encapsulation on molecular damage under electron irradiation**Elena Besley¹, Stephen T. Skowron¹¹School of Chemistry, University of Nottingham, Nottingham

We discuss encapsulation techniques providing some protection of a sample from radiation damage. The talk is focussed on chemical samples containing organic molecules encapsulated in carbon nanomaterials. As a framework for understanding effects of encapsulation, we use Fryer's experiments investigating the degree to which encapsulating carbon films reduce beam damage to three dimensional organic crystals, quantified by a 'protection factor' (PF). As bulk diffusion is believed to be the rate determining step of damage, encapsulation of organic crystals within carbon layers eliminates some diffusion routes, enhances recombination rates of radiation-displaced species and thus prolongs sample lifetime (a known 'cage effect'). As PF increases with decreasing thickness of crystal, this suggests promising protection for 2D materials. We consider damage rates in low dimensional encapsulated systems by separating the effects of dimensional reduction and the actual effects of encapsulation on the observed damage rates. In addition to the general protecting effects of encapsulation due to the increase in recombination rates we discuss confinement and temperature effects.

11:30**Majorana fermions in carbon nanotubes**Milena Grifoni¹, Magdalena Marganska¹, Lars Milz¹, Wataru Izumida²¹Faculty of Physics, University of Regensburg, Regensburg²Department of Physics, Tohoku University, Sendai

Engineering effective p-wave superconductors hosting Majoranaquasiparticles (MQPs) is of particular interest for fundamental research as well as for applications in fault-tolerant topological quantum computation. In quasi one-dimensional systems, the parameter space for topological superconductivity is significantly reduced by the coupling between transverse modes. Together with the requirement of achieving the topological phase under experimentally feasible conditions, this strongly restricts in practice the choice of systems which can host MQPs. Here we demonstrate that semiconducting carbon nanotubes (CNTs) in proximity with ultrathin s-wave superconductors, e.g. exfoliated NbSe₂, and in perpendicular magnetic field satisfy these needs. By atomic tight-binding calculations we show the emergence of localized zero-energy states at the CNT end of which we determine the full 3D spatial profile. We show that the chiral nature of the CNT lattice is imprinted in the MBS wave function which has a helical structure, anisotropic in the transverse direction. The local spin canting angle displays a similar spiral pattern. The experimental state of the art is discussed.

18:30**Chemistry of 2D-Pnictogen Nanomaterials**Gonzalo Abellán^{1,2}¹Institute of Advanced Materials and Processes, University Erlangen-Nuremberg, Erlangen²Institute of Molecular Science (ICMol), University of Valencia, Paterna

Two-dimensional (2D) materials have attracted great attention in the last years due to their outstanding physical properties and their potential applications in optoelectronics, sensors, energy storage, and catalysis. In contrast to the most studied material graphene, the layered allotropes of group 15 elements (P, As, Sb, and Bi, also called pnictogens) have been fairly less developed. 2D pnictogens exhibit a marked puckered structure with dative electron lone pairs located on the surface atoms, which results in semiconducting character and good electronic mobility, and also in an increased chemical reactivity. Indeed, 2D-BP (phosphorene) and 2D-Sb (antimonene) exhibit a great ability to easily adsorb and stabilize unsaturated organic molecules through van der Waals interactions. Herein we will show novel insights into the oxidation, chemical functionalization (both covalent and non-covalent), intercalation and passivation of 2D pnictogens. Moreover, we will prove that 2D-BP and 2D-Sb can act as catalysts in synthetic organic transformations involving unsaturated molecules, in a completely different way as graphene does.

19:00

Water-based and biocompatible inks made of 2D-materials for fully printed electronics

Cinzia Casiraghi¹

¹School of chemistry, University of Manchester, UK

Solution processing of 2D-materials allows simple and low-cost techniques such as inkjet printing to be used for fabrication of heterostructures of arbitrary complexity. However, the success of this technology is determined by the nature and quality of the inks used.

In this work we show a general formulation engineering approach to achieve highly concentrated, and inkjet printable water-based 2D crystal formulations, which also provide optimal film formation for multi-stack fabrication [1]. Examples of all-inkjet printed devices, such as large area arrays of photosensors on plastic [1], programmable logic memory devices [1], strain sensors on paper [2] and capacitors [3] will be discussed.

[1] McManus et al, Nature Nanotechnology, 2017, doi:10.1038/nnano.2016.281

[2] Casiraghi et al, Carbon, 2018, 129, 462

[3] Worsley et al, ACS Nano, accepted.

19:30**Where did the missing atoms go? From local bandgap tinkering and antidots to nanoporous medley**Marija Drndic¹¹Physics and Astronomy, University of Pennsylvania, Philadelphia

Atomic-defect engineering in 2D materials provides new opportunities from condensed matter physics to molecular filtration. Introducing atomic and nm-scale vacancies in 2D materials changes their electrical and optical properties (for example the bandgap, as in antidot lattices). When 2D materials are suspended, vacancies make the membranes permeable to ions and molecules in liquid or gas phases, allowing transport studies at atomic scales. While Ohm's law works well to describe ion current flow through nm-size holes, for sub-nm holes comprised of a handful of missing atoms, one measures non-linear current-voltage curves. Sub-nm holes allow the passage of smaller water molecules but block the larger hydrated salt ions which can be exploited for efficient water desalination. Raman and photoluminescence spectroscopy combined with aberration-corrected TEM, together with molecular-dynamics and DFT calculations, provide a comprehensive approach to characterize the holes and transport through them. Raman peak shifts can be used to quickly determine the density of vacancies, once those have been initially calibrated with electron microscopy data.

THU 1**Ultrafast terahertz spectroscopy of gated and chemically doped carbon nanotubes**

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Transient optical-pump terahertz - probe (OPTP) spectroscopy provides an ideal tool to investigate photoinduced charge generation. By varying the delay between the optical pump and the THz probe, the time evolution of the photoinduced conductivity on a picosecond time scale can be measured. The optoelectronic properties of carbon nanotubes can be tailored by doping, functionalization or by changing their geometry. For a better understanding of these properties we performed a full characterization (UV/VIS/IR absorption, Raman, FTIR, TDS-THz, OPTP spectroscopy and transmission electron microscopy) and a direct comparison of chemically doped and electrically gated samples. Doping allowed the suppression of the excitonic absorption transitions concurrently with an increase in the THz conductivity. Under optical excitation samples showed a photoinduced bleaching of the THz spectral conductivity, and distinctly different temporal recombination dynamics. This rarely observed negative photoconductivity can be understood by the exciton-induced screening of charge motion.

THU 2**Incidence of multilayers in chemically exfoliated graphene**

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An efficient route to synthesize macroscopic amounts of graphene is highly desired

for various applications and a bulk characterization of such samples, in terms of the number of layers, is thus equally important. We present a Raman spectroscopy-based method to determine the distribution of the number of graphene layers in chemically exfoliated graphene. We utilize a controlled, high vacuum vapor-phase potassium intercalation technique and identify a lightly doped stage, where the Raman modes of undoped and doped few-layer graphene flakes coexist. The spectra can be unambiguously distinguished from alkali doped graphite, and a modeling with the distribution of the layers yields an upper limit of flake thickness of five layers with a significant single-layer graphene content. Complementary, statistical AFM measurements on individual few-layer graphene flakes find a consistent distribution of the layer numbers, confirming our Raman based findings.

Paper available on arXiv:1807.09329

THU 3

First-principles theory of effective charges and piezoelectric response of graphene

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A single layer of ideal graphene is an homopolar material, with vanishing infrared effective charges and piezoelectricity. In contrast graphite and multilayered graphene can present a significant infrared activity. Here I will discuss different symmetry breaking mechanisms that can activate a finite infrared and/or a piezoelectric response. In such situations we use density functional theory to provide accurate estimations of effective charges and piezoelectric tensor. Our first-principles calculations predict extremely large values for such quantities that can influence the electron-phonon scattering processes and thus charge transport and the relaxation-dynamics of photoexcited carriers. We acknowledge the support of the EU graphene flagship program.

THU 4

2D-0D Hybrid heterostructures for single electron devices

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We report a simple and scalable fabrication route of new 2D material/0D clusters heterostructures, exploiting the self-organized growth over graphene of epitaxial flat aluminium based nanoclusters assemblies. We provide experimental evidence that 2D materials are unique promising alternative to skirt the challenging issue of contacting the nanoparticles one by one with external leads in the sake of developing single electron transport devices [1]. The spintronics properties of 2D–0D heterostructures are also unveiled [2]. An anisotropic magnetoCoulomb effect, mediated by spinorbit coupling within a single ferromagnetic electrode, provides tunable spinvalve like magnetoresistance signatures and controllable magnetic modulation of the device's singleelectron charge states, without need of spin coherent tunnelling transport. These heterostructures pave the way towards scalable nanospintronics device architectures at the crossroads of 2D material physics and spin electronics. Moreover, back gate control of the nanoclusters will open new prospects for multifunctional devices.

Références

[1]F. Godel et al. ,Adv Mat, 29,1604837(2017)

[2]L.D.N. Mouafo et al. ,Adv Mat,30, 1802478(2018)

THU 5

Spin and Valley polarization in gate defined quantum point contacts in bilayer graphene

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One of the most unique characteristics of bilayer graphene (BLG) is the possibility to tune the low-energy electron dispersion relation by applying an external electric field. This allows for opening up a band gap, modifying the band curvatures and even changing the topology of the Fermi surface. Recent improvements in the device fabrication, such as the encapsulation of BLG and the use of graphite gates, result in high-mobility devices with very little disorder, which allow to study mesoscopic transport in electrostatically confined BLG nanostructures, such as quantum point contacts (QPC) and quantum dots.

We present a study of a QPC with a subband spacing of $400\mu\text{eV}$ (width 250nm). By applying in-plane and perpendicular magnetic fields, we are able to lift the spin and valley degeneracies and study spin- and valley polarized modes. Using large

in-plane magnetic fields, we are able to polarize the QPC with up to 6 fully spin polarized transport channels.

Furthermore, at zero magnetic field, we observe an additional plateau at $2e^2/h$. The energy gap of this plateau scales linearly with the applied displacement field and most likely originates from a spin-valley coupling.

THU 6

Measuring the Entropy of a Mesoscopic system via Thermoelectric Transport

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Entropy is a fundamental thermodynamic quantity indicative of the accessible degrees of freedom in a system. While it has been suggested that the entropy of a mesoscopic system can yield nontrivial information on emergence of exotic states, its measurement in such small electron-number system is a daunting task. Here we propose a method to extract the entropy of a mesoscopic system from transport measurements. We prove analytically and demonstrate numerically the applicability of the method to a mesoscopic system of arbitrary spectrum and degeneracies. We then apply our procedure to measurements of thermoelectric response of a single quantum dot, and demonstrate how it can be used to deduce the entropy change across Coulomb-blockade valleys, resolving, along the way, a long standing puzzle.

THU 7

Enhancement of photocatalytic activity in zinc oxide/reduced graphene oxide nanocomposites due to annealing

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Metal oxide-based photocatalysts have emerged as versatile materials since the discovery of water splitting on TiO₂ electrodes in 1972. Such materials are characterized by low cost, biocompatibility, and ease of manufacturing. More recently, nano-sized heterostructures have been investigated to promote charge separation in photocatalysts, increasing recombination time and improving photocatalytic efficiency. In this work, composite nanoparticles for photocatalysis consisting of reduced graphene oxide (rGO) embedded in zinc oxide were synthesized by a facile co-precipitation method. The effect of annealing at different temperatures on the quality and dispersion of rGO in the ZnO matrix and on the crystalline structure of the ZnO are evaluated in situ using micro-Raman spectroscopy, and the resultant change in functional performance of the nanocomposite material is studied by measuring the photocatalytic degradation of rhodamine B in simulated sunlight using UV-vis spectroscopy. The annealing process is shown to significantly increase the degradation rate of the model dye, which is concomitant with a notably improved dispersion of the rGO in the ZnO matrix.

THU 8**Fermi Resonance in the Raman Spectrum of Graphene?**

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In Graphene grown on a chromium (Cr) coated copper foil, we report the observation of an intense anomalous peak in the Raman spectrum that cannot be attributed to structural defects. The unusual Raman spectrum displays an intense anomalous peak at 1608 cm⁻¹ associated to the presence of Cr metallic nanoparticles in contact with graphene (named U peak). Bombardment with an electron beam demonstrates that this U peak is clearly distinct from the well-studied D' peak appearing when defects are created in graphene. We argue that the bonding of Cr atoms with carbon atoms softens the frequency of the ZO phonon mode in such a way that the frequency of its overtone 2ZO reaches the frequency of the G mode. Thus, the observed U peak is attributed to the 2ZO mode which becomes Raman active within a mechanism known as Fermi resonance. First-principles calculations on vibrational and anharmonic properties on the graphene/Cr interface support this scenario [1].

References

[1] D. Kalita et al, submitted to PRL.

THU 9**Graphene oxide flake behavior under electric field in liquid crystal phase**

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Graphene flakes in water show macroscopic properties due to their self-organization making graphene attractive for applications not only in solid phase, but also in liquid phase. An easy and high yield method for producing graphene flake suspensions is the wet chemical exfoliation of graphite, having graphene oxide (GO) as an intermediate step. In aqueous suspension, GO flakes, due to their high aspect ratio and good dispersibility, form liquid crystal (LC) phases at very low flake concentrations. They show, as typical LCs, birefringence with uniform orientations within hundreds micrometer domain size. Interestingly, like standard LCs used in displays, their optical transmission can be tuned by the application of electric fields. The birefringence is generated by a common orientation of the flakes as we have proven by direct visualization of the flakes with confocal laser microscopy. By advanced polarizing optical method, we could follow the flake reorientation under the application of electric fields and also confirmed that the reoriented flakes are parallel to the field direction. Thus the graphene oxide LC is an optically negative material.

THU 10**Embedding of impurity atoms into graphene using low-energy ion implantation**

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Ion implantation is a well-established technique for modification of materials properties. It offers a lot of opportunities due to a variety of ion species, wide range of implantation energies and control over the dopant concentration. However, in the case of two-dimensional materials, such as graphene, ion implantation is quite challenging – an ion has to be trapped within a single atomic layer and only a narrow ion energy window is suitable for embedding of impurity atoms into a 2D lattice. The precise choice of ions energy is therefore essential for successful implantation. We have used molecular dynamics simulations (on quantum-mechanical and classical levels) to study direct implantation of various atomic species, ranging from light elements such as boron and nitrogen to heavy elements such as platinum, into single and double layer graphene. The most suitable implantation energies have been determined. Our results show that low-energy ion irradiation could be used for modifications of structural and electronic properties of graphene through precise doping of the material with a large variety of atomic species.

THU 11**Contactless Surface Resistance of 2D Materials Using a Rutile Resonator**

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The measurement of the electrical surface resistance of 2D materials without any contacts, will provide as a method for obtaining their intrinsic characterisation. Moreover, we know that the substrate has a strong influence, that can modify intrinsically the properties of the 2D materials, as found in graphene. A rutile dielectric resonator (RDR) is essentially a closed resonant cavity housing the small dielectric cylinder, two identical samples are placed axially, at the top and bottom of the rutile cylinder. The RDR can be used to measure the electrical surface resistance in conducting coatings deposited on isolating substrates, at the resonance frequency, in our case 9,1GHz [1]. The sample shape is a square 12x12 mm². Raman spectroscopy is used to check the quality of the samples. We used the RDR method on different samples of carbon nanotubes (bucky paper) and for graphene on different substrates: SiO₂/Si, on Quartz, on PET.

[1] P. Krkotić, A. Aguasca and J. M. O'Callaghan, "Small Footprint Evaluation of Metal Coatings for Additive Manufacturing," 2018, 48th European Microwave Conference (EuMC), Madrid, 2018. doi: 10.23919/EuMC.2018.8541442.

THU 12

On the growth of Linear Carbon Chains by laser annealing

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Several methods to create linear carbon chains (LCC) have been proposed over the last decades. Studies from 30 years ago could not define clearly the process of their formation: it was not clear and dangerous, because the reagents used are highly unstable and can explode. However, the study on this interesting material as the forerunner for carbyne -the truly 1D carbon allotrope- has continued to be developed given its interesting chemistry, electronic and thermophysical properties, and its promising potential applications [1,2]. In recent years, the use of Carbon Nanotubes (CN) to protect the LCC opened the possibility to create large stable chains [3]. In our study, we show the formation of LCC from single wall carbon nanotubes (SWCNT) using solvents as a carbon source and laser annealing to start the nano-chemical reaction that leads to the chain formation. The nano-reaction was monitored in situ step by step with Raman spectroscopy, where we can see the formation of a new peak that corresponds to the formation of long LCC of around ~ 100 atoms.

1 ACS nano 7, 10075, 2013.

2 Carbon 107, 217, 2016.

3 Nature Materials 15, 634, 2016.

THU 13

Isolation of Single-wired Transition-Metal Monochalcogenides by Carbon Nanotubes

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The successful isolation of single-layers from 2D van der Waals (vdW)-layered materials has opened new frontiers in condensed matter physics and materials science. Their discovery and unique properties laid the foundation for exploring 1D counterparts. However, the isolation of 1D 'vdW-wired' materials has thus far remained a challenge due to inefficient techniques. Theoretically, isolated wires of some vdW-wired materials could possess exotic properties distinct from their counterparts, although this has never been fully verified by experiments. Here we report the facile synthesis of isolated transition-metal monochalcogenide MoTe nanowires by using carbon nanotubes as molds. Individual nanowires are perfectly separated by a carbon nanotube with a minimal interaction, allowing easy handling and detailed characterization of the single-wires. Atomic-resolution TEM revealed unusual torsional motions absent in their bulk crystals. This finding indicates that isolated MoTe nanowires are unique building blocks for future electromechanical devices.

THU 14

Reversible hydrostatic strain in graphene/gold nanoparticles hybrid material induced by laser irradiation

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Gold nanoparticles (NPs) were prepared on SiO₂ substrate by local annealing of gold thin films using focused laser beam. CVD-grown graphene was transferred onto the prepared NPs. Subsequent Raman-spectroscopy measurements were performed on the samples using different laser powers. We used higher laser intensity (6 mW) to locally anneal the hybrid material. Low laser powers (0.6 mW) were used to characterize the doping and the strain formed in the same areas both before and after local heating. While we found that higher intensity laser irradiation increased gradually the doping and the defect concentration in SiO₂-supported graphene, the same irradiation procedure did not induce such irreversible effects in the graphene supported by Au NPs. Moreover, the laser irradiation induced dynamic hydrostatic strain in the graphene on Au NPs, which turned out to be completely reversible. These results point out the role of the substrate in the resistance of graphene against laser irradiation, and can have implications in the development of graphene/plasmonic nanoparticle based high temperature sensors. NANOSCALE 10, 13417 (2018)

THU 15

Evidence for room temperature quantum spin Hall insulator state in the air stable layered mineral jacutingaite

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Quantum spin Hall (QSH) insulators are two-dimensional topological materials that have recently attracted tremendous interest, due to the promise of applications from low-power electronics to quantum computing. A major challenge in this field is the identification of large gap QSH materials, which would enable room temperature dissipationless transport in their edge states. Here we show that the layered mineral jacutingaite (Pt_2HgSe_3) realizes the QSH state, within the framework of the Kane-Mele model. Using scanning tunneling microscopy, we measure a band gap of 110 meV and identify the hallmark edge states at single layer steps on top of the bulk crystal. As predicted previously by Marrazzo et al. (PRL 120, 117701 (2018)), we identify the topological nature of the gap by calculating the Z_2 invariant, using density functional theory. By scotch tape exfoliation, we prepare thin flakes of the material and show that it can be incorporated into heterostructures of 2D materials, using the well established dry stacking techniques.

THU 16

Tracking the Origin of Single Photon Emitters in WSe_2

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Single-photon emitters (SPEs) are critical for a range of leading quantum technologies. Several recent measurements of SPEs in monolayer WSe_2 have established this two-dimensional material as a promising candidate for a reliable single photon source. Despite empirical evidence that SPEs in WSe_2 are associated with some combination of strain and point defects, a comprehensive microscopic model explaining the underlying physics has proven elusive.

We present a multi scale tight-binding model for single photon emitters in WSe_2 including non-uniform strain, defects and two-particle interactions using the Bethe-Salpeter equation. We find that strain locally shifts excitonic energy levels into the band gap, where they overlap with inter-gap defect states. The resulting hybridization allows for efficient filling and subsequent radiative decay of localized defect states, explaining the observed brightness and lifetimes. Our model quantitatively reproduces and explains several empirical findings, including the evolution of the energy and polarization of the emitted photons with magnetic and electric fields.

THU 17

Magnetoluminescence of charge-controlled monolayer and bilayer semiconductors

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Layered transition metal dichalcogenide semiconductors exhibit valley Zeeman phenomena in response to an external magnetic field [1,2,3]. The characteristic exciton g-factors, however, are not unique for all materials but depend on different sample parameters such as the level of charge doping [4]. To quantify the valley Zeeman splitting of various photoluminescence peaks of tungsten-based dichalcogenides, we realized charge-tunable devices of WSe₂ monolayers and bilayers embedded in hexagonal boron nitride and performed magnetoluminescence experiments in perpendicular magnetic fields of up to 9 Tesla. The variety of g-factors suggests that different exciton species contribute to the rich emission spectra of tungsten-based dichalcogenides at low temperatures.

[1] A. Srivastava et. al., *Nature Physics* 11, 141–147 (2015)

[2] G. Aivazian et. al., *Nature Physics* 11, 148–152 (2015)

[3] Y. Li et. al., *Phys. Rev. Lett.* 113, 266804 (2014)

[4] M. Koperski et. al., arXiv:1803.00376 [cond-mat.mes-hall] (2018)

THU 18

Bottom-up Synthesis of Graphene Nanoribbon without Metal Catalyst

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Graphene nanoribbons have been shown to be produced and tailored on metal substrates via a bottom up approach from organic precursors which paves the way to their application in nanoelectronics after transfer to insulating substrates. Quantum confinement of the macromolecules leads to the creation of peculiar band structures, strongly influencing the topological characteristics of the ribbons. Therefore, it is important to be able to exactly engineer the ribbons, in order to precisely tune their electronic, optical and magnetic properties. Here, we present recent progress in achieving atomically precise bottom-up synthesis of nanoribbons without the presence of a metal catalyst by using fluorinated precursors to exploit cyclodehydrofluorination as reaction for surface-assisted synthesis [1,2], and/or by using the chemically stable environment inside carbon nanotubes as reaction environment [3]. We use resonance Raman spectroscopy as probe to analyse these nanoribbons via their spectral fingerprint.

[1]Amsharov, *Phys. Stat. Solidi B* 2016, 253, 2473.

[2]Kolmer et al., *Science* 2019, 363, 57-60.

[3]Kuzmany et al., *Phys. Status Solidi RRL* 2017, 11, 1700158.

THU 19

Lattice Opening Upon Bulk Reductive Covalent Functionalization of Black Phosphorus

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The chemical bulk reductive covalent functionalization of 2D black phosphorus (BP) using BP intercalation compounds has been developed. Through effective reductive activation, covalent functionalization of the charged BP is achieved by the use of organic alkyl halides. Functionalization was extensively demonstrated by means of several characterization techniques such as Raman Spectroscopy, TG-MS analysis, X-Ray Photoelectron Spectroscopy, ³¹P-MAS NMR Spectroscopy as well as by DFT calculations, showing higher functionalization degrees than the neutral routes.

THU 20

Revealing the interaction between Ag and Au nanoparticles in graphene-chitosan composites

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Graphene-nanoparticle composites (GNC) are designed to make graphene suitable for bioapplications. However, the low stability and high cytotoxicity of GNC from the lack of a bio-compatible organic matrix hamper their practical applications. Chitosan, has excel as an excellent biocompatible material with an advanced film-forming capacity, but much less is known about graphene-chitosan composites and their physical and structural properties that may help solve the biocompatibility issues in GNC.

We have stabilized gold and silver nanoparticles (NPs) to the graphene-chitosan composite surface by enhancing the catalytic activity of the NPs and graphene using cetyltrimethylammonium bromide (CTAB) while holding a biocompatible matrix using chitosan. We developed for the first time an absolute graphene-chitosan nanoparticle composite through an ex-situ approach. The samples were characterized with Raman and FTIR spectroscopy, atomic force and scanning electron microscopy revealing the interaction and presence of functionalization between chitosan and graphene plus a decoration with NPs. This new material could potentially be used in biological applications or as sensing nanomaterial.

THU 21**Dual Electrochemically-Gated Bilayer Transition Metal Dichalcogenides**

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New phenomena ranging from phase transitions to superconductivity are triggered in two-dimensional materials (2DMs) at high carrier densities/strong applied electrical fields. Currently the highest achievable carrier densities, 10^{15}cm^{-2} , were demonstrated using ionic liquid (IL) gating. Here we explore two regimes of dual electrochemically-gated 2DMs using independently-controlled ILs above and below the 2DM: 1) ultrahigh carrier density injection, 10^{15}cm^{-2} , and 2) creation of an ultra-strong perpendicular electric field, 10V/nm. Our I_{DS} vs V_g transport measurements indicate that the 2DM responds to both gates individually and simultaneously, and hints toward band structure changes as a function of perpendicular electric field strength due to controllable and reversible n-branch modification of a semiconducting bilayer 2DM. Additionally photoluminescence measurements of semiconducting bilayer 2DMs indicate a high carrier density regime determined by the emergence (removal) of a trion (neutral exciton) peak and an electric field regime determined by the emergence of a field-tunable peak that we attribute to the recombination of interlayer excitons.

THU 22**Exciton formation in monolayer MoS₂**

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Optical spectra of monolayer transition metal dichalcogenides such as MoS₂ are strongly dominated by excitonic peaks in the visible range. While the exciton, charge and spin relaxation dynamics in those materials have been studied extensively fewer studies consider the exciton formation dynamics [1,2].

We study the exciton formation dynamics in MoS₂ from first-principles by propagating the density matrix in time, including electron and hole correlations and time-dependent external fields [3]. When carriers are excited into the quasi-free electron-hole plasma far above the band gap, they first relax to the excitonic ground state via scattering by phonons, electrons or excitons. By inclusion of electron-phonon scattering matrix elements from first principles we elucidate the role of this scattering channel for the relaxation. Comparison with recent experiments yields detailed information on the relative importance of the different scattering processes.

- [1] F. Ceballos, DOI:10.1039/C6NR02516A
[2] C. Trovatiello, DOI:10.1364/CLEO_QELS.2018.FF1D.5
[3] A. Marini, DOI:10.1088/1742-6596/427/1/012003

THU 23

Assessing the Suitability of the Use of Nitrogen Within Graphene CVD

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Chemical vapour deposition (CVD) is now established as the foremost method for large scale production of large domain single layer graphene suitable for use within future electronic devices[1]. When considering the shift in CVD graphene manufacture from laboratory- to industrial-scale, the option to exchange the commonly used inert gas Ar for the cheaper option of N₂ should be highly attractive. However, until now, there has been no spectroscopic study of graphene grown using N₂ as the inert gas, to determine whether N₂ dissociates under the conditions used during graphene CVD, causing substitutional doping of the graphene lattice by atomic N. Such N-doping of the graphene lattice degrades charge carrier mobility[2]. We present a study of graphenes grown within Ar-, N₂- and periodically switched N₂-/Ar-buffered atmospheres. Results from Raman spectroscopy, X-Ray Photon Spectroscopy and Time-of-Flight Secondary Ion Mass Spectroscopy are presented to assess the possibility of nitrogen atom doping in graphene during graphene CVD.

1. Xin, H. & Li, W. Appl. Phys. Rev. (2018)

2. McManus, J. B. et al. Phys. Status Solidi Basic Res. (2017)

THU 24

Quantifying electron irradiation effects in transmission electron microscopy

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Evaluating the future possibilities of electron microscopy based atom manipulation [1] requires a precise physical understanding of the interactions of relativistic electrons with matter. Purely elastic knock-on damage cross sections in graphene can now be accurately predicted from first principles [2]. However, electron irradiation damage of other materials such as MoS₂ and hBN, or even graphene impurity sites [3], is either dominated or influenced by inelastic excitations.

Accurate measurements of electron irradiation damage at the level of single atoms in materials with varying dielectric properties at multiple and ever-lower electron energies are starting to emerge and will provide much needed experimental guidance for theory. Two-dimensional materials offer in our view the best chance for providing the experimental data needed for further model development, which can then be adapted to materials more generally to provide a truly general and quantitative understanding of structural changes caused by electron irradiation.

1 M. Tripathi et al., *Nano Lett.* 18, 5319 (2018)

2 T. Susi et al., *Nat. Commun.* 7, 13040 (2016)

3 T. Susi et al., *2D Materials* 4, 042004 (2017)

THU 25

Coulomb-blockade enhanced optomechanics

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A clean, suspended single wall carbon nanotube is the ultimate limit of a nanomechanical beam resonator, where the fundamental transversal vibration mode reaches resonance frequencies on the order of 100MHz – 1GHz and mechanical quality factors up to 10^6 . Placing a nanotube next to a coplanar resonator at cryogenic temperatures results in a microwave optomechanical system with dispersive coupling. This system, however, has a fundamentally new property: the nanotube is also a quantum dot, and strong interaction of motion and single electron tunneling dominates its behaviour.

We have implemented a transfer technique to integrate such a nanotube into a superconducting circuit, and present measurements on a combined device coupling a suspended quantum dot to a microwave resonator mode at millikelvin temperatures. The dispersively coupled optomechanical system is characterized via two-tone spectroscopy as well as optomechanically induced transparency (OMIT). The interaction of charge transport and vibration leads to a strongly enhanced optomechanical coupling.

THU 26

Direct observation of momentum-resolved Landau levels in strained single-layer graphene

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The quantum Hall effect belongs to the remarkable class of macroscopic quantum phenomena. But, while angle-resolved photoemission spectroscopy (ARPES) has been a powerful tool to investigate numerous quantum phases of matter, the traditional quantum Hall states have remained inaccessible. Such observations are hindered by the fact that ARPES measurements are incompatible with magnetic fields. Here, we circumvent this by using graphene's peculiar property of exhibiting large pseudomagnetic fields under particular strain patterns, to visualize the momentum-space structure of electrons in the quantum Hall regime. By measuring the unique energy spacing of the ensuing pseudo-Landau levels with ARPES, we extract a pseudomagnetic field strength of $B = 41$ T. This momentum-resolved study up to room temperature is made possible by exploiting shallow triangular nanoprisms in the SiC substrates that generate large, uniform pseudomagnetic fields, arising from strain, confirmed by STM and model calculations. Our work demonstrates the feasibility of exploiting strain-induced quantum phases in 2D Dirac materials on a wafer-scale size, opening the field to a range of new applications.

THU 27

Interaction dynamics of biomolecules on graphene surfaces probed by quartz crystal microbalance technique

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Graphene, with various chemical functionalities, is a versatile surface for bio-chemical interaction, for applications such as sensors and drug-delivery. But the dynamics of such interactions are poorly understood. Here, I will present two studies of bio-chemical interactions on graphene surfaces - (i) phospholipids and (ii) bovine serum albumin (BSA). The graphene surface studied are graphene oxide, and reduced graphene oxide of various reduction degrees, which allows precise control of the surface chemistry and wetting behaviour. The interaction dynamics are probed using the quartz crystal microbalance with dissipation monitoring technique (QCM-D). We correlate the graphene surface chemistry and wetting behaviour of the graphene surface correlates to the structure of phospholipid or BSA assembly kinetics and final structure. Phospholipids can be controlled to form self-assembled vesicles, monolayers or bi-layers. BSA can be controlled to form monolayer or multilayer assemblies with controlled orientation of BSA molecules. Furthermore, these molecules on graphene surfaces are shown to be active to binding to other compatible biomolecules, paving the way for biomedical applications.

THU 28**Time- and temperature-resolved in situ investigation of the metal-induced crystallization of amorphous carbon thin films**

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The graphitization of amorphous carbon in thin film stacks with Ni was investigated in situ as a function of the initial stacking order, temperature and time by Rutherford backscattering spectrometry and Raman spectroscopy. Four different bilayer and triple layer stacks were exposed to heating ramps up to 700 °C. The graphitization occurred simultaneously with a layer exchange (LE) and was completed during the applied heating ramp. The temperature-resolved measurements allowed the determination of the onset temperatures and transition rates for the respective stacking order. Finally, the activation energies for the graphitization of the amorphous carbon were estimated for both LE directions. In combination with thermodynamic calculations, this in situ study allowed to identify metal-induced crystallization with LE via wetting and diffusion along grain boundaries as mechanism responsible for the graphitization of amorphous carbon thin films in contact with Ni, instead of bulk dissolution/precipitation. The proposed model can potentially be used to estimate the catalytic transformation of group 14 elements in contact with transition metals.

THU 29**Orientalional order parameter of Multiwall Carbon nanotube sheets as aligning surfaces for liquid crystals**

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Carbon nanotubes (CNTs) have been studied for nearly two decades and their amazing properties continue to spur intense investigations and look for new applications such as liquid crystal displays (LCDs). Aligned multiwall CNT sheets from forests are multifunctional layers for LCDs working as transparent electrodes but also as aligning layers for LCs [1]. The good alignment of LCs directly relies on the degree of order of CNTs. Thus, keeping the uniformity and alignment of CNT sheets intact while depositing and improving their adhesion with the substrate is very important even if nontrivial. Here we report the degree of orientational order of the free-standing CNT sheets estimated from their optical dichroism and how it changes when realising CNT-based substrates for LCDs with different underlying surfaces [2]

and with transparent insulating over layers, useful for improving the electro-optic performance of LCs.

References

[1] T. Truong, J. H. Park, M. A. Rahman, M. Urbanski, E. S. Kim, G. Scalia, D. Suh, *Current Applied Physics* 19, 2, 162-167 (2019). [2] M. A. Rahman, H. Agha, T. K. Truong, J. H. Park, D. Suh, G. Scalia, *Journal of Molecular Liquids* 267, 363-366 (2018).

THU 30

Tip enhanced photoluminescence of CVD and exfoliated MoS₂ flakes

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2D materials are promising materials for using in diverse optoelectronics applications. However, the development of these materials requires an extensive characterization at nanoscale level. Tip enhanced spectroscopy techniques, like Raman spectroscopy (TERS) or photoluminescence (TEPL) should play a significant role to reach this goal. For example, the effect of transferring flakes from one substrate to another may be assessed by combination of these techniques. We investigated the gap-less TEPL of MoS₂ samples grown by chemical vapor deposition (CVD) on different substrates and treated under different conditions of oxygen plasma to evaluate the impact of defects and their distribution on the local PL of the flakes. Finally, we assess the effect of contamination on the TEPL signal in MoS₂ exfoliated layers.

THU 31

Atomic engineering of monolayer graphene: selective symmetry breaking and Kekulé bond order via lithium deposition

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The Kekulé distortion (KD) periodically alters the carbon-carbon hopping strengths in graphene, resulting in a $\sqrt{3} \times \sqrt{3}$ R30° superstructure and symmetry breaking

between three previously equivalent hexagonal plaquettes. Such a KD phase is induced in monolayer graphene by low-flux deposition of a small number of lithium adatoms and studied via angle-resolved photoemission spectroscopy (ARPES). In a regime where no charge-transfer doping by the lithium is apparent, the superstructure periodicity is observed in a sharp backfolding of the Dirac cones to the Γ point, as well as the appearance of corresponding peaks in low-energy electron diffraction (LEED). A gap opening ($2\Delta = 0.22 \pm 0.02$ eV) is observed at the Dirac point. Above ~ 30 K, the new features vanish, the gap closes, and neither is recovered upon subsequent cooling. A Monte Carlo toy model demonstrates that during low-flux deposition, adatoms prefer to occupy the same set of inequivalent plaquettes even when separated by many sites, producing a self-reinforcing, long-range order that is not observed at high flux.

THU 32

Cavity-control of bright and dark interlayer excitons in van der Waals heterostructures

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Monolayer transition metal dichalcogenides integrated in optical microcavities host exciton-polaritons as a hallmark of the strong light-matter coupling regime. Analogous concepts for hybrid light-matter systems employing spatially indirect excitons with a permanent electric dipole moment in heterobilayer crystals promise realizations of exciton-polariton gases and condensates with immanent dipolar interactions. Here, we identify optical signatures of spatially indirect interlayer excitons in vertical MoSe₂-WSe₂ heterostructures and implement cavity-control of both exciton manifolds. To this end we employ a tunable open-access cavity with one curved fiber-based mirror and one planar mirror with MoSe₂-WSe₂ heterobilayer flakes on top. The configuration of controlled intermirror spacing and lateral scanning capabilities is used to explore the light-matter coupling of excitons as a function of the cavity length at representative positions of heterobilayers selected by two-dimensional cavity imaging. Our experiments quantify the strength of interlayer excitons and demonstrate Purcell enhancement in cavity-modified photonic environments [1].

[1] Förg et al., arXiv:1710.00990(2017)

THU 33**Semiconductor-metal transition due to mechanical strain in MoS₂ monolayers on Au(111) substrate**

János Pető¹, Gergely Dobrik¹, Gergő Kukucska², Péter Vancsó¹, Ákos Hoffmann¹, Antal A. Koós¹, János Koltai², Péter Nemes-Incze¹, Levente Tapasztó¹

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Strained MoS₂ monolayers on Au(111) substrate show an interesting phenomenon. The unstrained regions of the MoS₂ display semiconductor behavior while the regions with 1-2 % or higher strain display metallic behavior which is caused by the shifting of the chemical potential towards the minimum of the conduction band. According to theoretical calculations strain is expected to move the chemical potential towards the minimum of the conduction band but in free-standing MoS₂ monolayers the required strain for transition is approximately 10 % which would tear the 2D crystal apart. The MoS₂/Au(111) system is needed to produce a strong n-doping which makes the transition possible at lower mechanical strain. We were able to observe this phenomenon via tunneling spectroscopy in MoS₂ nanobubbles which form at the MoS₂/Au(111) interface. This phenomenon could be a useful tool for strain engineering in the future. The creation of semiconductor-metal interfaces within the same monolayer could open up new possibilities for applications of this 2D crystal.

THU 34**In-situ spectromechano-electrochemistry of monolayer graphene**

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Sensitivity of 2D materials to external perturbations is a well-known issue as well as a potential route to further modification of their properties. However, a precise control of the external factors is imperative, alongside with the possibility to administer all of them simultaneously. We have therefore developed a micro-droplet spectromechano-electrochemical technique, which allows for concurrent deformation and electrochemical charging of supported 2D materials under in-situ monitoring with Raman microscope. The dimensions of the micro-droplet, which can be as small as few microns, enable directing the charge only to the basal plane or to the edges, and, without the reduction in the Raman or photoluminescence signal. We have employed this method to study the kinetics of redox reactions on monolayer graphene's surface under in-plane uniaxial loading up to 0.8% deformation. The utilization of

Raman spectroscopy is essential to quantify the real achieved strain. In addition, changes in the stress transfer from the polymer substrate caused by the local charging are observed, due to the manipulation of the interface between graphene and the substrate.

THU 35

Doping-induced many-body excitations in single-wall carbon nanotubes

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Quasi one-dimensional structure of single-wall carbon nanotubes causes the strong impact of the excitonic effect on their optical and electronic properties. Besides, doping of carbon nanotubes leads to activation of additional many-body energy levels commonly labeled as trions or localized excitons.

In the present work, we investigate the optical properties of single-wall carbon nanotubes doped by hydrochloric acid. We found that carbon nanotubes, doped in such a way, possess two additional energy levels, which we ascribe to the exciton, localized on a physisorbed H⁺ ion, and to the trion. As a result of pump-probe experiments, it was also found that the dynamics of the trion states matches the difference between the dynamics of the ordinary exciton and the localized exciton. Combining that with the results of photoluminescence and static absorption measurements, we concluded that the trion energy level is occupied via the relaxation from the energy level of localized excitons, but not via a direct optical excitation from the ground level of a carbon nanotube.

THU 36

REELS and Auger spectroscopy study of layers exchange in C/Ni-bilayer system

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New experimental methods for synthesis of low dimensional carbon structures still

attract considerable attention, many of them based on catalytically driven processes. In this contribution we present REELS and Auger spectroscopy study of Ni-induced layer exchange in Ni/C-bilayer thin film system. EELS spectroscopy in reflected mode (REELS) and Auger electron spectroscopy (AES) were employed to characterize the structure, homogeneity and quality of carbon and nickel film (each having thickness around 50 nm) and their interface between, before and after thermal annealing at 700 °C. AES mapping and depth profiling revealed a layer exchange between the layers after thermal annealing, accompanied by partial nickel diffusion into MgO substrate. REELS analysis showed successful structural transformation of initially amorphous carbon layer into compact graphitic one. The transformed carbon layer has a slightly rippled surface as confirmed by topological backscattered electron imaging.

THU 37

Infrared-to-violet tunable optical activity in atomic films of GaSe, InSe, and their heterostructures

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Two-dimensional semiconductors - atomic layers of materials with covalent intra-layer bonding and weak coupling between the layers – are a new class of materials with great potential for optoelectronic applications. Among them, a special position is now being taken by post-transition metal chalcogenides (PTMC), InSe and GaSe. It has recently been found [1] that the band gap in 2D crystals of InSe more than doubles in the monolayer compared to thick multilayer crystals.

Here, we use Raman and photoluminescence (PL) measurements of encapsulated few-layer samples prepared in a glovebox to reveal optical properties of atomically thin GaSe previously inaccessible due to oxidation. Overall, optical activity of these two almost lattice-matched PTMC films and their heterostructures densely cover the spectrum of photons from violet to infrared. We demonstrate the realisation of the latter opportunity by the observation of interlayer excitonic PL arising from Γ valleys of few-layer InSe/GaSe heterostructures.[1]

[1] Bandurin, D. A.; et al. Nat Nanotechnol, 3, 223-227 (2017)

[2] Terry, D. J.; et al. 2D Mater, 5, 041009 (2018)

THU 38**Electron-phonon coupling in highly strained suspended graphene**

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Magneto-Raman spectroscopy is a useful technique to investigate key mechanisms affecting the electronic properties of graphene, such as strain variations [1] or many-body effects [2]. Combining this method with control over strain in graphene would open the route to study pseudo-magnetic fields and advance the understanding of many-body effects and the electron-phonon coupling.

Here, we report on highly uniaxially strained, high-quality suspended graphene, which allows us to observe magneto-phonon resonances with non-degenerate G-mode phonons. We further study the electron-phonon coupling as a function of B -field and charge carrier density n . Strikingly, at $B = 0$ T we do not observe the expected strong renormalization of the G-mode energy [3], possibly due to a limited lifetime of the excited electron-hole pairs of approx. 5 fs, nearly independent of the laser power. Furthermore, we find an anomalous n -dependence of the G-modes in a B -field regime, which is expected to suppress the electron-phonon coupling [1].

[1] Neumann et al., Nat. Commun. 6, 8429 (2015)

[2] Sonntag et al., Phys. Rev. Lett. 120, 187701 (2018)

[3] Pisana et al., Nat. Mater. 6, 198-201 (2007)

THU 39**From Liquid to Solid State: preparation of highly homogeneous, smooth, transparent films of liquid-exfoliated WS₂ in the polymer matrix.**

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Since graphene discovery - a wonder material, scientists started looking for even more exciting 2-dimensional materials. Thanks to Liquid Phase Exfoliation access to 2D structures in a liquid form is no longer a challenge. One of uniquely defined 2D structures is Tungsten Disulfide.

Although in a liquid, WS₂ nanosheets exhibit a range of optical properties (i.e. PL) desirable for applications, there is a significant drawback associated with them being polydisperse size-wise and dispersed in a liquid. For many applications i.e. transistors, it is required that the material must be rich in monolayers and in a solid form. This is challenging without quenching the optical properties. Therefore, transfer from liquid to the solid became one of the hot topics in nowadays research.

The presented study discusses production of state of the art WS₂ dispersions, narrowing their size distribution (size selection), monolayer enrichment and finally:

preparation of highly homogenous, smooth and transparent WS₂ films with monolayer content of about 75% in the polymer matrix. The latest ones will surely be a new scope opening doors to fabrication of future electronic and optoelectronic devices.

THU 40

Interaction of multi-walled carbon nanotube aerogels with quasi-optical terahertz beams.

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Recently we have used a model of a regular wire medium consisting of conductors, equivalent to nanotubes, for the getting of effective parameters of MWCNT aerogels from polarizability measurements at 8-12 GHz. In this paper for the terahertz range (100 – 970 GHz) the reflection coefficient was used as the empirical parameter for the same aerogel model. The experimental study of MWCNT aerogel as well as modeling of an aerogel media equivalent wire medium, demonstrates that plane-parallel aerogel samples under a normal incidence of THz beam have a high reflection coefficient (0.6-0.9), while conductivity of effective media is markedly lower than that of metals (near 10^3 S/m). The reflection coefficient from the flat aerogel surface decreases with increasing of the incidence angle. Diffraction of quasi-optical beams on spherical aerogels differs significantly from the diffraction on metallic samples of the same diameter (the side scattering falls off quite rapidly with increasing frequency). The data obtained will be used to simulate the effective parameters of the 2D structure of the MWCNT aerogels in dielectric matrix. This work is supported by the RSF grant 17-73-20293

- 08:30 – 09:30 **TUTORIAL: A. Szameit, Rostock**
Non-hermitian topological photonics
- 09:30 – 10:00 **L. Golub, St.-Petersburg**
Photogalvanic effects in Weyl semimetals
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **H. Kim, Hamburg**
Design of Majorana Bound States in Engineered Atomic-Scale Superconductor-Magnet Hybrid systems
- 11:00 – 11:30 **R. Krupke, Karlsruhe**
Electroluminescence from carbon nanotubes: low temperature, tailored defects and short channels
- 11:30 – 12:00 **E. Alarcon Llado, Amsterdam**
The photonics of semiconductor nanostructures for new solar energy conversion concepts
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 17:30 **G. Kukucska, Budapest**
Simulation of Raman spectra based on first principles methods
- 17:30 – 18:00 **A. Setaro, Berlin**
Energy transfer in carbon nanotube-based hybrid systems
- 18:00 – 18:30 **SUMMARY: A. Jorio, Belo Horizonte**
Kirchberg 2019 - Conference Summary
- 18:30 – 20:00 **Break**
- 20:00 – 22:00 **Bauernbuffet – Farewell Dinner**

Friday, March 15th

Topological properties, applications

08:30

Non-hermitian topological photonics

Alexander Szameit¹

¹Institute for Physics, University of Rostock, Rostock

The recent development of topological insulator states for photons has led to an exciting new field of “topological photonics,” which has as a central goal the development of extremely robust photonic devices. Topological insulator physics has been studied extensively in condensed matter and cold atoms. However, photonic systems offer the possibility of non-Hermitian effects through the engineering of optical gain and loss, which opens an entire new field of physics. In this talk, we will discuss our recent experimental work on non-Hermitian topological phenomena in coupled lattice systems, in particular the first demonstration of non-hermitian PT-symmetric topological interface states.

09:30**Photogalvanic effects in Weyl semimetals**Leonid Golub¹¹Ioffe Institute, St.-Petersburg, Russia

Physics of Weyl semimetals is one of the most rapidly developing areas of the condensed matter science owing to their topological properties which manifest themselves in Fermi arcs and topological charges related with the chirality of the Weyl points in the momentum space. An excitation of Weyl semimetals with circularly polarized light leads to a photocurrent whose direction depends on the light helicity and is governed by the topological charges of the Weyl points. We demonstrate that the helicity-dependent photocurrent has a frequency dependence due to Coulomb interaction effects. For indirect intraband transitions, the helicity-dependent photocurrent generated within each Weyl node takes on a universal value determined by the fundamental constants. The magnetic-field induced photogalvanic effect, i.e. an appearance of a photocurrent under unpolarized excitation in a magnetic field, is also discussed. In quantized magnetic fields, the photocurrent is caused by optical transitions between the one-dimensional magnetic subbands.

L. E. Golub and E. L. Ivchenko, Phys. Rev. B 98, 075305 (2018).

10:30**Design of Majorana Bound States in Engineered Atomic-Scale Superconductor-Magnet Hybrid systems**Howon Kim¹, Roland Wiesendanger¹¹Department of Physics, University of Hamburg, Hamburg

Realizing Majorana bound states (MBS) in condensed matter systems is a key challenge on the way towards future topological quantum computing. As a promising platform, 1D magnetic chains and 2D magnetic islands on conventional s-wave superconductors were theoretically predicted to host MBS at the boundary. First, it will be introduced that a new approach to design topologically non-trivial superconducting 1D magnetic chains on a conventional s-wave superconductor using single-atom manipulation techniques based on a low-temperature scanning tunneling microscope. The artificially constructed atomic chains on a superconducting substrate exhibit non-collinear magnetic states and a remarkable enhancement of the zero-energy local density of states (LDOS) strongly localized at the ends of the chains. Second, we will address experimental and theoretical studies of monolayer topological superconductivity and chiral Majorana edge modes in model-type 2D magnetic islands on elemental superconductors. We demonstrate that interface engineering by an atomically thin oxide layer is crucial for driving the studied hybrid system into a topologically non-trivial state.

11:00**Electroluminescence from carbon nanotubes: low temperature, tailored defects and short channels**

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In the last years we have been developing carbon nanotube based on chip light sources integrated in optical waveguides that are electrically driven and which may provide a potential solution to a technological gap existing in silicon photonics [1]. The devices are CMOS compatible, scalable, have a response time below 100 ps and can be spectrally tailored by engineering the photonic environment. Moreover they can be operated as non-classical light sources at the verge of single photon emission, and have potential as electrically driven quantum emitters for on chip quantum information processing. Yet, the reproducibility of electrically-generated light emission is often limited by instabilities in current injection. Therefore we have been focusing on understanding and controlling the injection of carriers and the generation and recombination of excitons in pristine nanotubes and in nanotubes with tailored defects. Most importantly we acquired for the first time low-temperature electroluminescence excitation maps which help us to better understand the device physics and to identify regimes of stable excitonic and trionic emission.

[1] X. He et al., Nature Materials 17, 633 (2018).

11:30**The photonics of semiconductor nanostructures for new solar energy conversion concepts**Esther Alarcon Llado¹¹NWO-Institute Amolf, Amsterdam

Semiconductor nanostructures and in particular nanowires (NWs) are promising building blocks for next generation solar energy conversion at low cost. NW ensembles constitute a new class of metamaterial, where the optical properties of the array are tuned by the individual NW type, geometry and collective arrangement. Arising from the refractive index mismatch between NW and air and the sub-wavelength features, light propagation and distribution inside the nanostructure is strongly dependent on wavelength-geometry relation. While the photonic properties of small dielectric structures have been widely studied within the framework of Mie scattering, those of vertically standing nanowires cannot be explained with the same mathematical framework. In particular, coupling to poorly confined waveguided modes drives the absorption spectrum in NWs. The difficulty in obtaining III-V NWs on transparent substrates or self-standing, hampers the obtaining of their absorption properties experimentally. This work investigates how NWs interact with light from both theoretical and experimental methods. We will introduce scanning probe microscopy as an emerging tool for the characterization of nanoscale solar cells, as well as a new fabrication approach to create 3D nanostructures on demand. From these properties, we discuss a new variety of solar cell designs, that are not possible in the bulk form. We will discuss new photovoltaic and solar fuel conversion designs with efficient light trapping, coloured or optimized tandem structures.

17:00**Simulation of Raman spectra based on first principles methods**Gergő Kukucska¹¹Department of Biological Physics, Eötvös Loránd University, Budapest

Raman spectroscopy is undoubtedly one of the most widespread non-destructive optical method of our days. Despite its versatility from experimental point of view, theoretical modeling of Raman peak intensities can be hardly found in the literature. The available theoretical works usually utilize the Placzek approximation based on the response for a time independent electric field. This static approach is not only unapplicable for metallic systems, but also prevents comparison of excitation profiles with experimental results. Moreover, as the frequency dependent polarizability can be calculated including excitonic effects using the Bethe-Salpeter equation, thus many body effects can be captured in the excitation profile. In this talk I present our method to calculate Raman intensities, using the excitation energy dependent Placzek approximation and I show its applications for various systems [1,2].

[1] G. Kukucska and J. Koltai, Phys. Status Solidi (b), vol. 254, no. 11 (2017)

[2] G. Kukucska, V. Zólyomi and J. Koltai Phys. Rev. B 98, 075437 (2018)

17:30

Energy transfer in carbon nanotube-based hybrid systems

Mareen Glaeske¹, Sabrina Juergensen¹, Stephanie Reich¹, Antonio Setaro¹

¹Physics, Freie Universität Berlin, Berlin

While direct optical excitation of carbon nanotubes activates only the tube species strictly matching the excitation source, excitation transfer processes provides a single excitation channel for all the nanotubes species in a sample. Here we will discuss the performances of hybrid systems comprising nanotubes and small aromatic molecules, emphasizing the interplay between synthetic approach, physical parameters of the constituents and optical response of the final products.

Friday, March 15th

Topological properties, applications

18:00

Kirchberg 2019 - Summary

Ado Jorio¹

¹Physics, UFMG, Belo Horizonte

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