

Name

XXXIV<sup>th</sup>  
International Winterschool  
on Electronic Properties  
of Novel Materials

Molecular Nanostructures

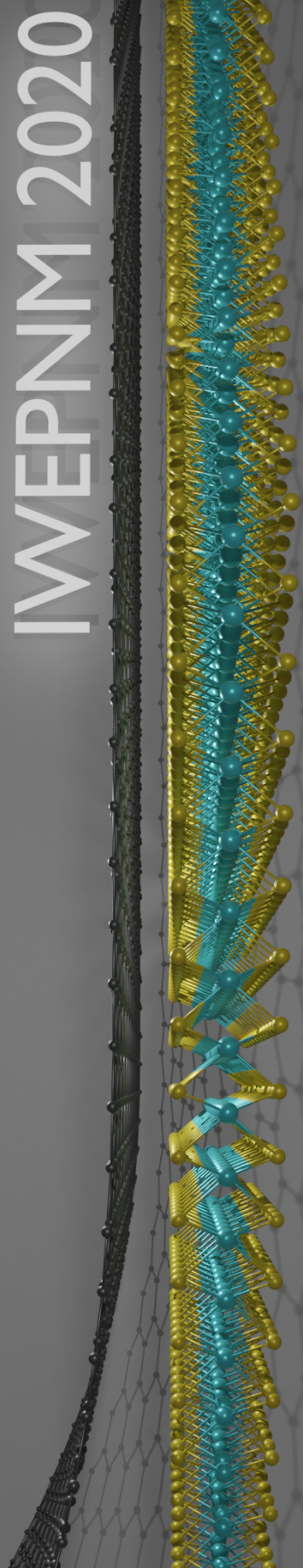
Program



Hotel Sonnalp  
Kirchberg/Tirol  
Austria

7 - 14 March, 2020

IWEPNM 2020





## SUPPORTERS

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

Verein zur Förderung der Internationalen Winterschulen in Kirchberg Austria

## PATRONAGE

Helmut Berger

Mayor of Kirchberg

## LAYOUT

María Machón, Felix Herziger

Logo designed by Stefan Wolff.

This year's Logo of the IWEPNM shows a schematic image of a graphene monolayer sheet which gets placed on top of a single layer of MoS<sub>2</sub>.

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Financial assistance from the sponsors and supporters is greatly acknowledged.





Dear Friend:

Welcome to the 34<sup>th</sup> International Winterschool on:

Electronic Properties of Novel Materials!

This Winterschool is a sequel of thirty-three 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
Kati Gharagozloo-Hubmann	accommodation finances
Laura Meingast	credit card maintenance
Roland Gillen	website
Sabrina Jürgensen	abstract booklet
Sandra Hinz	accommodation
Stefan Wolff	announcements, video transfer
Patryk Kusch	technical assistance, sponsoring
Georgy Gordeev	technical assistance, video transfer
Alphonse Fiebor	technical assistance
Gudrun May-Nasseri	visa applications, general assistance

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

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

Sincerely yours,  
Janina, Stephanie, Andreas, and Christoph

## Chairpersons

J. Maultzsch (Erlangen)

S. Reich (Berlin)

A. Hirsch (Erlangen)

C. Stampfer (Aachen)

## Program Committee

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H. Kuzmany (AT)	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 2020 starts on Saturday, 7 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, 14 March, breakfast. There will be a reception party on Saturday, 7 March, after dinner, and a farewell party including dinner on Friday, 13 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 2020 Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria

e-mail: [info@hotelsonnalp.info](mailto:info@hotelsonnalp.info), web: [www.hotelsonnalp.info](http://www.hotelsonnalp.info)

All questions concerning the IWEPNM 2020 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](mailto:iwepnm-info@physik.tu-berlin.de), web: [www.iwepnm.org](http://www.iwepnm.org)

### Participation

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

### Contributions

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

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

### Childcare

Childcare is provided by Michaela Kisch and her team ([michaela@kitzkids.com](mailto: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 IWEPNM 2020 are scheduled for publication as a special issue in *physica status solidi* (pss) (b). **Manuscript submission is due on April 24th.** 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 "IWEPNM: Electronic Properties of Novel Materials. If you intend to submit a "Rapid Research Letter", a "Feature Article" or a manuscript to *Advanced Electronic Materials*, please consult with the editors at [iwepm-publication@physik.fu-berlin.de](mailto:iwepm-publication@physik.fu-berlin.de).

IWEPNM 2020  
CHAIRPERSONS FOR THE ORAL SESSIONS

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

Sunday, 08.03.	morning morning, after coffee break evening	Stephanie Reich Claudia Backes Christoph Stampfer
Monday, 09.03.	morning morning, after coffee break evening	Viera Skakalova Stephane Berciaud Andreas Hirsch
Tuesday, 10.03.	morning morning, after coffee break evening	Anna Swan Shigeo Maruyama Ursula Wurstbauer
Wednesday, 11.03.	morning morning, after coffee break evening	Janina Maultzsch Alexander Högele Achim Hartschuh
Thursday, 12.03.	morning morning, after coffee break evening	Ralph Krupke Balazs Dora Sabine Maier
Friday, 13.03.	morning morning, after coffee break evening	Hans Kuzmany Christian Schönenberger Siegmar Roth

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 8		Monday, March 9	Tuesday, March 10	Wednesday, March 11	Thursday, March 12	Friday, March 13
Topics	Growth, synthesis; twisted 2L graphene	2D heterostructures, COFs	Excitons in CNT and 2D materials	Excitons, light-matter coupling in 2D materials	Transport in 2L graphene; applications	Molecules, transport in CNT, processing & growth
08:30	Growth and Optical Characterization of Various van der Waals Hetero-Nanotubes Based on SWCNTs MARUYAMA	TUTORIAL Superconductivity in atomically thin crystals and in materials with non-trivial topology GRIGORIEVA	TUTORIAL Spontaneous and intentional exciton trapping in carbon nanotubes VOISIN	TUTORIAL Classical and quantum transport of excitons in atomthin semiconductors GLAZOV	Gap Opening in Twisted Double Bilayer Graphene by Crystal fields ENSSLIN	Electron-beam manipulation of lattice impurities SUSI
09:00	Towards Rational Synthesis of Carbon Based Nanostructures on Insulating Surfaces AMSHAROV				Controlling optoelectronic properties of 2D semiconductors: band engineering and moiré superlattices GORBACHEV	Atomically Thin Confined Nanowires - the Final Orderable Structural Domain? SLOAN
09:30	On-surface synthesis: A versatile bottom-up strategy to low-dimensional carbon-based nanostructures MAIER	Dark and Bright excitons in heterostructures of 2D semiconductors FAUGERAS	Bright- and dark-exciton dynamics in carbon nanotubes KATO	Spatiotemporal exciton dynamics in atomically thin 2D materials MALIC	Topological valley transport in a folded bilayer graphene CAMPOS	Molecules in Carbon Nanotubes: Structure, Property and Reactivity KHLOBYSTOV
10:00 Coffee Break						
10:30	Sensing and manipulating electron spins in graphene nanostructures PASCUAL	Excitons in van der Waals heterostructures HÖGELE	Purified and Functionalized Carbon Nanotubes for Optical and Electronic Applications ZAUMSEIL	Interlayer interactions and the electronic and optical properties of 2D multilayer materials GILLEN	The optical response of transition metal dichalcogenides LIBISCH	Dynamically induced 0- $\pi$ transition in a carbon nanotube-based Josephson junction DEBLOCK
11:00	Following on-surface chemical reactions by atom manipulation KAISER	Condensation signatures and multi-valley physics of excitons in vdW hetero-bilayers WURSTBAUER	Toward a more reliable characterization of the chirality composition of sorted SWCNT samples FOREL	Phonon-limited transport in 2D materials SOHIER	Conductance quantization, supercurrent and multiple Andreev reflection in bilayer graphene quantum pointcontacts DANNEAU	Nanotube quantum dots: from microwave optomechanics to novel materials HÜTTEL
11:30	Mapping the twist-angle disorder and unconventional Landau levels in magic angle graphene ZELDOV (Video)	Charge carrier diffusion in hybrid halide perovskite thin films HARTSCHUH	The Dynamics of 2D Membranes VAN DER ZANT	Nonlinear polaritons in monolayer semiconductor coupled to optical bound states in the continuum IORSH	Strain-engineered graphene and one-dimensional edge states in few-layer WTe <sub>2</sub> SCHÖNENBERGER	Plasmonic nanoparticle crystals for deep strong light-matter coupling REICH

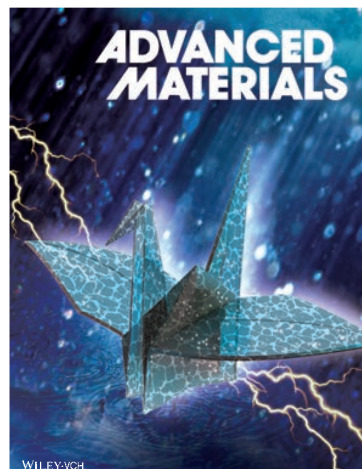
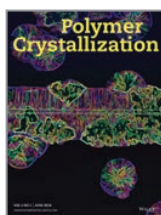
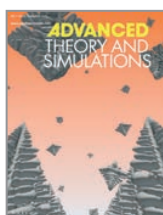
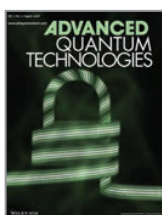
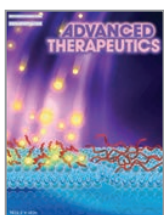


12:00 - 17:00	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops	Mini Workshops
17:00 - 18:30	Dinner					17:00 Lithographic bandgap engineering of graphene: the crucial role of edges BÖGGILD
18:30	Magic Angle Bilayer Graphene - Superconductors, Orbital Magnets, Correlated States and beyond EFETOV	Optoelectronic Processes in Covalent Organic Frameworks BEIN	Anisotropy controls phonon thermalization in photoexcited black phosphorus SEILER	TMDC nanophotonics for strong light-matter coupling SHEGAI	Atomristor: 2D Memory and Applications AKINWANDE	17:30 On the Fundamental Mechanisms that underpin CVD Technology for Atomically Thin 2D Films HOFMANN
19:00	Edge currents in monolayer and bilayer graphene TARASENKO	Unraveling the optical properties of triazine-based covalent organic frameworks from first principles GUERRINI	Unveiling valley lifetimes of free charge carriers in monolayer WSe <sub>2</sub> BESCHOTEN	Studying Exciton Polaritons in van der Waals Materials KUSCH	Inorganic - organic monolayer stacks DUSEBERG	18:00 Conference Summary JORIO
19:30		Towards an in-depth understanding of liquid exfoliation of layered crystals BACKES	Quantum simulation of the Hubbard model in a moiré superlattice MAK (Video)	Interaction-dominated transport in graphene: old mysteries and new regimes BANDURIN	Ångstrom-scale Capillaries: A Platform for investigating Confined flow BOYA	18:30 - 20:00 Break
20:00						
20:30		Poster I Monday	Poster II Tuesday	Poster IV Tuesday	Poster III Thursday	Bauernbuffet Farewell Dinner
Topics	Growth, synthesis; twisted 2L graphene	2D heterostructures, COFs	Excitons in CNT and 2D materials	Excitons, light-matter coupling in 2D materials	Transport in 2L graphene; applications	Molecules, transport in CNT, processing & growth
Sunday, March 8		Monday, March 9	Tuesday, March 10	Wednesday, March 11	Thursday, March 12	Friday, March 13

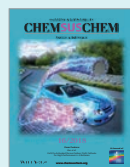
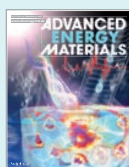
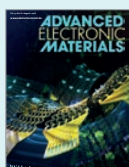
# Materials Science Matters

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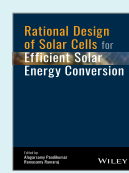
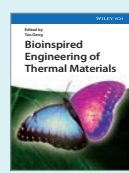
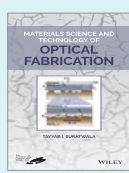
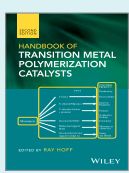
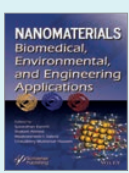
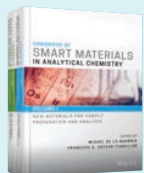


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**WILEY-VCH**

**ADVANCED  
SCIENCE NEWS**

**WILEY**

- 08:30 – 09:00 S. Maruyama, Tokyo**  
*Growth and Optical Characterization of Various van der Waals Hetero-Nanotubes Based on SWCNTs*
- 09:00 – 09:30 K. Amsharov , Halle**  
*Towards Rational Synthesis of Carbon Based Nanostructures on Insulating Surfaces*
- 09:30 – 10:00 S. Maier, Erlangen**  
*On-surface synthesis: A versatile bottom-up strategy to low-dimensional carbon-based nanostructures*
- 10:00 – 10:30 Coffee Break**
- 10:30 – 11:00 N. Pascual, San Sebastian**  
*Sensing and manipulating electron spins in graphene nanostructures*
- 11:00 – 11:30 C. Kastl, Munich**  
*Quantum optoelectronics in materials with topological order*
- 11:30 – 12:00 E. Zeldov, Rehovot**  
*Mapping the twist-angle disorder and unconventional Landau levels in magic angle graphene*
- 12:00 – 17:00 Mini Workshops**
- 17:00 – 18:30 Dinner**
- 18:30 – 19:00 D. Efetov, Barcelona**  
*Magic Angle Bilayer Graphene - Superconductors, Orbital Magnets, Correlated States and beyond*
- 19:00 – 19:30 S. Tarasenko, St. Petersburg**  
*Edge currents in monolayer and bilayer graphene*

Sunday, March 8th

CNT, nanomechanics, TEM

**08:30****Growth and Optical Characterization of Various van der Waals Hetero-Nanotubes Based on Single-Walled Carbon Nanotubes**Shigeo Maruyama<sup>1,2</sup><sup>1</sup>Department of Mechanical Engineering, The University of Tokyo, Tokyo<sup>2</sup>Energy NanoEngineering Lab., AIST, Tsukuba

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); SWCNT@BNNT [1]. We named these as one-dimensional van der Waals hetero-nanotubes, because we found no correlation between chiral angle of inner SWCNT and outer BNNT for the 'double-walled' SWCNT@BNNT. We have further developed the 1D coating CVD of transition metal dichalcogenide nanotubes (TMD-NT), such as MoS<sub>2</sub> nanotubes and WSe<sub>2</sub> nanotubes. We can grow MoS<sub>2</sub> nanotubes around relatively large diameter SWCNT or SWCNT@BNNT. These nanotubes can be labelled as SWCNT@TMD-NT or SWCNT@BNNT@TMD-NT. Because BNNT is thermally more stable than SWCNT, we can remove SWCNT from SWCNT@BNNT by the gentle oxidation process. Hence, we can produce BNNT with inner diameter determined by the original SWCNT. Then, the MoS<sub>2</sub> CVD can result BNNT@TMD-NT or TMD-NT@BNNT. These hetero-nanotubes are characterized by HR-TEM, STEM-EELS, and various optical spectroscopy.

[1] R. Xiang et al, Science (2020) in press.

**09:00**

**Towards Rational Synthesis of Carbon Based Nanostructures on Insulating Surfaces**

Konstantin Amsharov<sup>1</sup>

<sup>1</sup>Institut für Chemie - Organische Chemie, Martin-Luther-Universität, Halle

Nanographenes and carbon nanoribbons display outstanding electronic properties and are considered to be leading materials for future electronics. The possibility to fabricate such carbon-based nanostructures on metal surfaces by bottom-up approach has generated enormous expectations. However metallic substrates strongly limit the possible applications. The next challenge in this field is a controlled synthesis of these unique materials directly on insulating surfaces. We show that synthesis of such architectures can be realized effectively via cyclodehydrofluorination of specially fluorinated precursor molecules. Our finding opens up a venue towards rational synthesis of carbon based nanomaterial directly on insulating metal oxide surfaces.

**09:30****On-surface synthesis: A versatile bottom-up strategy to low-dimensional carbon-based nanostructures**Sabine Maier<sup>1</sup><sup>1</sup>Department of Physics, Friedrich-Alexander-University Erlangen-Nürnberg, Erlangen, Germany

On-surface synthesis has attracted significant attention in recent years due to its potential to fabricate novel low-dimensional carbon materials with atomic precision. In order to understand and control the synthesis of high-quality low-dimensional nanostructures, many efforts have been made to steer the reaction pathway by the design of smart precursors and by applying templating effects from the substrate. In my presentation, I will focus on recent high-resolution scanning probe microscopy experiments in combination with density-functional theory about the bottom-up fabrication and electronic properties of atomically precise one- and two-dimensional molecular nanostructures on metals. Thereby, the effect of functional groups, the flexibility and the symmetry of the precursor molecules on the structure formation of covalently-linked molecular structures will be discussed. In particular, I will outline how the use of debromination coupling reactions can fabricate well-ordered nanoporous 1D and 2D covalent molecular structures. We demonstrate how organo-metallic structures can act as a structural template for covalent structures.

**10:30**

**Sensing and manipulating electron spins in graphene nanostructures**

Nacho Pascual<sup>1</sup>, Niklas Friedrich<sup>1</sup>, Jingcheng Li<sup>1</sup>

<sup>1</sup>CIC nanoGUNE, San Sebastian (Spain)

Graphene can spontaneously develop intrinsic paramagnetism. Crucial examples are the magnetization of zig-zag edges in graphene, or the emergence of paramagnetism in open shell graphene nanostructures. I will show that graphene nanostructures fabricated with atomic precision on a metal surface exhibit fingerprints of  $\pi$ -paramagnetism, which can be detected and spatially localized using low temperature scanning tunneling.

Single electron spins emerge localized at certain zigzag sites of the carbon backbone. Their presence could be detected and mapped by spatially resolving the zero-energy resonance due to the Kondo effect. We found that near-by spins are coupled into a singlet ground state and quantify their exchange interaction via singlet-triplet inelastic electron excitations. Extra hydrogen atoms bound to radical sites quench their magnetic moment and switch the spin of the nanostructure in half-integer amounts.

Spin states can also be created on a ribbon simply by substitutional doping or by incorporating magnetic species into a ribbon using on-surface synthesis routes. We detected and characterized the spin states in two-terminal transport experiments, using the STM.



**11:00****Quantum optoelectronics in materials with topological order**Jonas Kiemle<sup>1,2</sup>, Paul Seifert<sup>1,2</sup>, Kehui Wu<sup>3</sup>, Yongqing Li<sup>3</sup>, Alexander Holleitner<sup>1,2</sup>, Christoph Kastl<sup>1,2</sup><sup>1</sup>Walter Schottky Institut, Technische Universität München, Garching<sup>2</sup>Munich Center for Quantum Science and Technology (MCQST), Munich, Germany<sup>3</sup>Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Crystals with symmetry-protected topological order, such as topological insulators or Weyl semimetals, promise coherent spin and charge transport even in the presence of disorder at room temperature. Here, we explore light-matter interactions in topological materials, and we probe the interplay of non-trivial spin-momentum textures, optical excitation, and non-equilibrium spin and charge carrier dynamics. In topological insulators, we apply the so-called Shockley-Ramo theorem to design an optoelectronic probe circuit for the gapless surface states, and we find a well-defined conductance quantization at  $1e^2/h$  within the experimental error without any external magnetic field. [1] The unprecedented response is a clear signature of local spin-polarized transport, it can be switched on and off via an electrostatic field effect. In Weyl semimetals, instead, the optoelectronic conductance is governed by non-zero Berry curvature, which results in an anomalous Hall-effect. [2] Our work elucidates fundamental light-matter interactions in topological materials.

[1] P. Seifert et al. Phys. Rev. Lett. 122, 146804 (2019).

[2] P. Seifert et al. Phys. Rev. B 99, 161403 (2019).

**11:30****Mapping the twist-angle disorder and unconventional Landau levels in magic angle graphene**Eli Zeldov<sup>1</sup><sup>1</sup>Department of Condensed Matter Physics, Weizmann Institute of Science, Israel

The emergence of flat bands and of strongly correlated and superconducting phases in twisted bilayer graphene crucially depends on the interlayer twist angle upon approaching the magic angle. Utilizing a scanning nanoSQUID-on-tip, we attain tomographic imaging of the Landau levels and derive nanoscale high precision maps of the twist-angle disorder in high quality hBN encapsulated devices, which reveal substantial twist-angle gradients and a network of jumps [1]. We show that the twist-angle gradients generate large gate tunable in-plane electric fields, unscreened even in the metallic regions, which drastically alter the quantum Hall state by forming edge channels in the bulk of the samples. The correlated states are found to be particularly fragile with respect to twist-angle disorder. We establish the twist-angle disorder as a fundamentally new kind of disorder, which alters the local band structure and may significantly affect the correlated and superconducting states.

[1] A. Uri, S. Grover, Y. Cao, J.A. Crosse, K. Bagani, D. Rodan-Legrain, Y. Myasoedov, K. Watanabe, T. Taniguchi, P. Moon, M. Koshino, P. Jarillo-Herrero, and E. Zeldov, arXiv:1908.04595 (Nature in press).

**18:30****Magic Angle Bilayer Graphene - Superconductors, Orbital Magnets, Correlated States and beyond**Dmitri Efetov<sup>1</sup><sup>1</sup>ICFO - The Institute of Photonic Sciences, Castelldefels (Barcelona)

When twisted close to a magic relative orientation angle near 1 degree, bilayer graphene has flat moire superlattice minibands that have emerged as a rich and highly tunable source of strong correlation physics, notably the appearance of superconductivity close to interaction-induced insulating states. Here we report on the fabrication of bilayer graphene devices with exceptionally uniform twist angles. We show that the reduction in twist angle disorder reveals insulating states at all integer occupancies of the four-fold spin/valley degenerate flat conduction and valence bands, i.e. at moire band filling factors  $\nu = 0, +(-) 1, +(-) 2, +(-) 3$ , and reveals new superconductivity regions below critical temperatures as high as 3 K close to  $\nu = 2$  filling. In addition we find novel orbital magnetic states with non-zero Chern numbers. Our study shows that symmetry-broken states, interaction driven insulators, and superconducting domes are common across the entire moire flat bands, including near charge neutrality. We further will discuss recent experiments including screened interactions, fragile topology and the first applications of this amazing new materials platform.

**19:00****Edge currents in monolayer and bilayer graphene**Sergey Tarasenko<sup>1</sup><sup>1</sup>Ioffe Institute, St. Petersburg

Driving charge carriers back and forth by ac electric field of laser radiation may generate a direct electric current in a system lacking the center of space inversion. Here, we discuss a class of such non-linear phenomena which occur at the edges of monolayer and bilayer graphene samples where the inversion symmetry is naturally broken. The current excited by linearly polarized radiation flows along the sample edge in a narrow channel of the mean free path width. It is caused by optical alignment of carrier momenta and the subsequent anisotropic relaxation of the alignment at the edge. The current direction is determined by the orientation of the ac electric field with respect to the edge and is opposite for n-type and p-type conductivities. Application of a strong perpendicular magnetic field leads to the quantum Hall effect. In this regime, the current is generated in topological chiral edge channels [1]. Its direction is solely determined by the magnetic field polarity while its magnitude is sensitive to the radiation polarization.

[1] H. Plank, M.V. Durnev, S. Candussio et al., 2D Materials 6, 011002 (2019).

- 08:30 – 09:30 **TUTORIAL: I. Grigorieva, Manchester**  
*Superconductivity in atomically thin crystals and in materials with non-trivial topology*
- 09:30 – 10:00 **C. Faugeras, Grenoble**  
*Dark and Bright excitons in heterostructures of 2D semiconductors*
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **A. Högele, Munich**  
*Excitons in van der Waals heterostructures*
- 11:00 – 11:30 **U. Wurstbauer, Münster**  
*Condensation signatures and multi-valley physics of excitons in vdW hetero-bilayers*
- 11:30 – 12:00 **A. Hartschuh, Munich**  
*Charge carrier diffusion in hybrid halide perovskite thin films*
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **T. Bein, Munich**  
*Optoelectronic Processes in Covalent Organic Frameworks*
- 19:00 – 19:30 **M. Guerrini, Berlin**  
*Unraveling the optical properties of triazine-based covalent organic frameworks from first principles*
- 19:30 – 20:00 **C. Backes, Heidelberg**  
*Towards an in-depth understanding of liquid exfoliation of layered crystals*
- 20:00 **Poster Session I**

Monday, March 9th

Heterostructures, nanooptics, perovskites

**08:30****Superconductivity in atomically thin crystals and in materials with non-trivial topology**Irina Grigorieva<sup>1</sup><sup>1</sup>University of Manchester, Manchester

Interest in ultrathin superconductors and the mechanisms responsible for the evolution of critical parameters for superconductivity with sample thickness has been revived recently due to the availability of atomically thin crystalline superconductors. I will briefly review relevant experimental observations, with a focus on recent studies of atomically thin intrinsic superconductors, such as NbSe<sub>2</sub> and TaS<sub>2</sub>. As the thickness of a superconductor is reduced to just a few atomic layers, the transition temperature  $T_c$  typically goes down. However, an opposite and still puzzling trend – an increase of  $T_c$  with decreasing thickness – has been found recently for TaS<sub>2</sub>. I will discuss our experimental findings for these two materials and the various factors that contribute to the evolution of their  $T_c$ 's with decreasing thickness. Another group of superconductors under intense current scrutiny are materials with non-trivial topology. I will present and discuss our observations of unusual features in surface magnetization of an intrinsic non-symmorphic 3D superconductor, which we interpret as signatures of topological surface states.

**09:30****Quantum simulation of the Hubbard model in a moiré superlattice**Kin Fai Mak<sup>1</sup><sup>1</sup>Cornell University, Ithaca

The Hubbard model, first formulated by physicist John Hubbard in the 1960s, is a simple theoretical model of interacting quantum particles in a lattice. The model is thought to capture the essential physics of high-temperature superconductors, magnetic insulators, and other complex emergent quantum many-body ground states. Although the Hubbard model is greatly simplified as a representation of most real materials, it has nevertheless proved difficult to solve accurately except in the one-dimensional case. Physical realizations of the Hubbard model in two or three dimensions, which can act as quantum simulators, therefore have a vital role to play in solving the strong-correlation puzzle. In this talk, I will discuss a recent experimental realization of the two-dimensional triangular lattice Hubbard model in angle-aligned WSe<sub>2</sub>-WS<sub>2</sub> bilayers, which form moiré superlattices because of the difference in lattice constant between the two 2D materials. We obtain a quantum phase diagram of the two-dimensional triangular lattice Hubbard model near the half filling by probing both the charge and magnetic order of the system. Implications for future studies will also be discussed.



**10:30**

**Excitons in van der Waals heterostructures**

Alexander Högele<sup>1</sup>

<sup>1</sup>Fakultät für Physik, Munich Quantum Center and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Munich, Germany

Van der Waals crystals of transition metal dichalcogenide (TMD) semiconductors have evolved as an increasingly significant material platform for condensed matter research. The crystals can be routinely exfoliated down to the monolayer limit and subsequently assembled into rationally designed van der Waals heterostructures. In analogy to their monolayer counterparts, TMD heterostructures exhibit remarkable optical properties associated with spin-valley polarized excitons. I will present our recent studies of interlayer excitons in TMD heterobilayers and heterotrilayers, and discuss the signatures of layer number, atomic registry and external magnetic field in cryogenic optical spectroscopy of van der Waals heterostructures.

**11:00****Condensation signatures and multi-valley physics of excitons in vdW hetero-bilayers**Lukas Sigl<sup>1</sup>, Florian Sigger<sup>1</sup>, Fabian Kronowetter<sup>1</sup>, Jonas Kiemle<sup>1</sup>, Alexander Holleitner<sup>1,2</sup>, Ursula Wurstbauer<sup>3</sup><sup>1</sup>Walter Schottky Institute and Physics Department, TU Munich, Germany<sup>2</sup>Munich Center for Quantum Science and Technology (MCQST), Germany<sup>3</sup>Institute of Physics, Westfälische Wilhelms-Universität Münster, Germany

Increasing the interaction strength between quasiparticles can cause strong correlations, collective phenomena and transition to emergent quantum phases. VdW heterobilayers are ideal systems for the realization of exciton condensation because of large exciton binding energies [1], long lifetimes [2] and a permanent dipole allowing for the manipulation of the exciton ensembles via electric fields [3]. In photo-generated exciton ensembles hosted in MoSe<sub>2</sub>–WSe<sub>2</sub> hetero-bilayers, we observe several criticalities with respect to photoluminescence intensity, linewidth, and temporal coherence. The phenomena survive above 10 Kelvin, consistent with the predicted critical condensation temperature of a Bose-Einstein condensate. We observe strong condensation signatures at elevated temperatures of MoSe<sub>2</sub>-WSe<sub>2</sub> hetero-bilayers and map the many-body phase diagram of the interlayer excitons.

We acknowledge supported by DFG via projects WU 637/4- 1 and HO 3324/9-1.

[1] J. Klein et al, Appl. Phys. Lett. 115, 261603 (2019).

[2] B. Miller, et al., Nano Lett. 17(9), 5229–5237 (2017).

[3] J. Kiemle et al. arXiv:1901.01042 (2019).

**11:30****Charge carrier diffusion in hybrid halide perovskite thin films**Achim Hartschuh<sup>1</sup>, Alexander Biewald<sup>1</sup>, Richard Ciesielski<sup>1</sup>, Nadja Giesbrecht<sup>1</sup>, Thomas Bein<sup>1</sup>, Pablo Docampo<sup>1</sup><sup>1</sup>Department of Chemistry and CeNS, LMU Munich, Munich, Germany<sup>2</sup>School of Electrical and Electronic Engineering, Newcastle University, Newcastle upon Tyne, UK

Perovskite-based thin-film solar cells today reach power conversion efficiencies of more than 22%. Methylammonium lead iodide (MAPI) is prototypical for this material class and at the focal point of interest for a growing community in research and engineering. We investigate the ambipolar diffusion of charge carriers in MAPI thin films using time-resolved photoluminescence (PL) microscopy. We first visualize the diffusion of charge carriers and measure the diffusion constant in large grains. We then determine its temperature dependence, which can be described by a power law indicating scattering at optical phonons and lattice fluctuations as the main processes limiting carrier transport [1]. We find that grain boundaries in these films act as solid walls restricting diffusion, but that they do not lead to significant quenching [2]. Local disorder, which occurs at the transition between two crystal phases, interrupts carrier diffusion in MAPI thin films, which indicates the sensitivity of carrier transport to structural perturbations.

[1] A. Biewald et al., ACS Appl. Mater. Interfaces 11, 20838 (2019). [2] R. Ciesielski et al., ACS Appl. Mater. Interfaces 10, 7974 (2018).

**18:30****Optoelectronic Processes in Covalent Organic Frameworks**Thomas Bein<sup>1</sup><sup>1</sup>Department of Chemistry, University of Munich (LMU), Munich, Germany

Photoactive molecular building blocks can be spatially integrated into the crystalline lattice of covalent organic frameworks (COFs), allowing us to create highly ordered organic optoelectronic systems. We will discuss different strategies aimed at creating electroactive networks capable of light-induced charge transfer. For example, we have developed COFs containing stacked light-harvesting building blocks acting as electron donors, which showed light-induced charge transfer to an intercalated fullerene acceptor phase. On the other hand, a COF integrated heterojunction consisting of alternating columns of stacked donor and acceptor molecules promotes the photo-induced generation of mobile charge carriers inside the COF network. Moreover, COFs integrating extended chromophores capable of efficiently harvesting visible and near infrared light have been created. Employing a solvent-stable oriented photoabsorber film structure, we have recently established COF-based photoelectrochemical water splitting. The great structural diversity and morphological precision that can be achieved with COFs makes them intriguing model systems for organic optoelectronic materials.

**19:00****Unraveling the optical properties of triazine-based covalent organic frameworks from first principles**Michele Guerrini<sup>1</sup>, Caterina Cocchi<sup>1</sup><sup>1</sup>Institut für Physik and IRIS Adlershof, Humboldt Universität zu Berlin, Berlin

In the field of reticular chemistry, Covalent organic frameworks (COFs) are novel nanomaterials, consisting of a porous network of covalently bonded organic units.[1] In spite of the extended research on synthesis and characterization of COFs, an in-depth microscopic understanding of their electronic and optical properties is currently missing. Due to their complex crystalline structure, COFs are challenging to be treated from first principles. On the other hand, the periodic nature of the network permits to deduce the properties of the COFs from those of its building blocks. In this way, we investigate the electronic and optical properties of triazine-based COFs and of their amino-functionalized counterpart in aqueous solution from time-dependent DFT within the polarizable continuum model. Our results show that nitrogen protonation in solution is the leading mechanisms ruling the electronic structure and the optical properties of these COFs. In particular, it is responsible for the spectral shifts observed in the experiments, as demonstrated by our analysis of the optical excitations in protonated and unprotonated species.

[1] X. Liu et al., Chem. Soc. Rev., 2019, 48, 5266

**19:30****Towards an in-depth understanding of liquid exfoliation of layered crystals**Claudia Backes<sup>1</sup>, Beata M. Szydłowska<sup>1</sup>, Nicola Marzari<sup>2</sup>, Jonathan Coleman<sup>3</sup>, Hai Wang<sup>4</sup><sup>1</sup>Applied Physical Chemistry, Heidelberg University, Germany<sup>2</sup>Theory and Simulation of Materials, EPFL Lausanne, Switzerland<sup>3</sup>School of Physics, Trinity College Dublin, Ireland<sup>4</sup>Molecular Spectroscopy, Max Planck Institute for Polymer Research, Mainz, Germany

Liquid phase exfoliation has become an important top down production technique giving access to large quantities of nanosheets in colloidal dispersion. Importantly, this is a highly versatile technique that can be applied to numerous layered materials from graphite to transition metal dichalcogenides, h-BN, III-VI semiconductors, hydroxides etc. All materials can be exfoliated in a similar way using aqueous surfactant or suitable solvents as stabilisers. Nanosheets in dispersion are extremely polydisperse with broad lateral size and thickness distributions. To narrow size and thickness distributions, liquid cascade centrifugation has proven to be a powerful tool for efficient size selection yielding nanosheet dispersions with well-defined dimensions. In spite of this progress, we have not reached a fundamental understanding of the process. In which way is the yield, nanosheet size and layer number dependent on the liquid medium? What is a good descriptor for the exfoliation efficiency and what does it depend on? What is the role of defects? In this talk, these fundamental questions will be addressed and a picture of the current understanding will be drawn.

**MON 1****Response of a few-layer graphene to high shear stress**

Mingzhi Yuan<sup>1</sup>, Shujia Li<sup>1</sup>, Bin Chen<sup>1</sup>, Alexander V. Soldatov<sup>1,2</sup>

<sup>1</sup>Center for High Pressure Science and Technology Advanced Research, Shanghai, People's Republic of China

<sup>2</sup>Department of Engineering Sciences and Mathematics, Lulea University of Technology, Lulea, Sweden

Graphene has been in the focus of materials research over a decade due to the superior physical properties it exhibits. Yet its behavior under high pressure and shear stress still not well understood. We conducted an in-situ Raman study of a few-layer graphene in powder form under high pressure and shear stress in a rotational diamond anvil cell. The recovered from high pressure samples were characterized by HRTEM and multi-wavelength Raman. Spectral mapping revealed high inhomogeneity of the Raman spectra across the sample: a minor change in the spectra in the center vs very high increase of defect concentration (D-band intensity) on the sample periphery. Remarkably, the graphene structure was totally ruined in between, where certain combination of shear- and normal stress was reached. We interpret the data in terms of specificity of shear stress distribution in the pre-compressed sample. Our results provide deeper insight into the structural transformation of graphene exposed to different type of stress and demonstrate that shear stress at certain level may become the factor limiting performance (or even causing damage) of the stress sensors based on this strongest material.

**MON 2****Single-electron double quantum dots in bilayer graphene**

Luca Banszerus<sup>1,2</sup>, Samuel Möller<sup>1</sup>, Eike Icking<sup>1,2</sup>, Takashi Taniguchi<sup>3</sup>, Kenji Watanabe<sup>3</sup>, Christian Volk<sup>1</sup>, Christoph Stampfer<sup>1,2</sup>

<sup>1</sup>2nd Institute of Physics, RWTH Aachen University, Aachen, Germany

<sup>2</sup>Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, Jülich, Germany,

<sup>3</sup>National Institute for Materials Science, Tsukuba, Japan

Bilayer graphene (BLG) offers a compelling platform for spin-qubit-based quantum computation, as long spin coherence times are expected thanks to its low spin-orbit and hyperfine interaction. The possibility to open up a band gap in BLG allows for electrostatic confinement of charge carriers. We present transport measurements through an electrostatically defined BLG double quantum dot in the single- and few-electron regime. With the help of a back gate, two split gates and two finger gates we are able to control the number of charge carriers on two gate-defined quantum dots independently between zero and five. The high tunability of the device meets requirements to make such a device a suitable building block for spin-qubits. In the single electron regime, we determine interdot tunnel rates around 2 GHz. Both, the interdot tunnel coupling, as well as the capacitive interdot coupling increase with dot occupation, leading to the transition to a single quantum dot. Finite bias

magneto-spectroscopy measurements allow to resolve the excited state spectra of the first electron in the double quantum dot; being in agreement with spin and valley conserving interdot tunneling processes.

### MON 3

#### **Colloidal synthesis and characterization of the heavy Pnictogens Antimony and Bismuth**

Christian Dolle<sup>1</sup>, Víctor Oestreicher<sup>1</sup>, Marta Alcaraz<sup>1</sup>, Roger Sanchis Gual<sup>1</sup>, Jose Alberto Carrasco<sup>1</sup>, María Varela<sup>2</sup>, Gonzalo Abellán<sup>1</sup>

<sup>1</sup>Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, Spain

<sup>2</sup>Departamento de Física de Materiales, Universidad Complutense de Madrid, Spain

Pnictogens (group-15 elements) are a new member in the fascinating world of post-graphene elemental 2D materials. Since exceptionally strong interlayer forces challenge their physical exfoliation, we will present a bottom-up approach for the wet chemical synthesis of Antimony and Bismuth based on colloidal chemistry as valuable alternative.

For in-depth characterization we employed Raman spectroscopy, coupled TG-GC-MS, PXRD and aberration corrected high resolution STEM (HRSTEM), which enabled us to reveal the perfect atomic order of the stable crystallites. Despite the obtained materials being commonly prone to oxidative decomposition, a native oxygen layer conserves the structural integrity in solid state against disintegration after prolonged exposure to ambient conditions.

By tuning the experimental conditions, we can control shape and size of the obtained materials, giving access to structures from nm-sized spherical particles to extended hexagons with thickness control.

This will allow to build a platform for a thorough study of the exciting properties of these novel 2D materials.

### MON 4

#### **Predicting graphene transport properties using Raman 2D peak-splits: experiment and simulation**

Anna K. Swan<sup>1,2,3</sup>, Zhuofa Chen<sup>1</sup>, Nathan Ullberg<sup>3</sup>, Mounika Vutukuru<sup>1</sup>, David Barton<sup>1</sup>

<sup>1</sup>Electrical and Computer Engineering, Boston University, Boston

<sup>2</sup>Photonics Center, Boston University

<sup>3</sup>Physics, Boston University

Avoiding charge density variations and impurities in graphene is vital for high-quality graphene devices. Electrical transport measurements reveal the degree of scattering centers and charge puddling in the sample, but require labor-intensive and time-consuming device fabrication. Raman spectroscopy using the graphene G and 2D phonon modes is sensitive to charge, but only for doping levels higher than  $\sim 10^{12} \text{ cm}^{-2}$ . We use the asymmetry of the 2D peak that appears at low charge,



here quantified as two peaks, ( $2D_1$  and  $2D_2$ ) of varying spectral separation  $\omega_{2D}$  and total intensity, to determine charge levels and charge variations within the optical spot for  $n \sim 1\text{-}50 \cdot 10^{10} \text{ cm}^{-2}$ . Raman maps of fabricated transport devices can easily identify if the device has high or low mobility and its degree of charge puddling as extracted by two-terminal transport data. To quantitatively determine charge and charge puddling from the Raman data, we use gated Raman measurements as well as simulations of the Raman spectra from charge puddles within in the optical spot. The results demonstrate how local charge variation predictably alters the 2D peak behavior.

## MON 5

### **Air stable FeCl<sub>3</sub>-intercalated collapsed CNT fibers. Towards the creation of light cables.**

Cristina Madrona Maqueda<sup>1</sup>, María Vila Santos<sup>1</sup>, Juan José Vilatela<sup>1</sup>

<sup>1</sup>IMDEA Materials, Madrid, Spain

Fibers of collapsed (or 'dog bone') carbon nanotubes have been intercalated with ferric chloride (FeCl<sub>3</sub>) as a means of increasing their conductivity for their potential use as light cables. Ferric chloride tends to form layered structures. Thus, the use of fibers made of collapsed CNT bundles is considered an interesting choice due to the combination of the planar graphite-like contact surfaces between collapsed tubes (where the intercalant is introduced) with the properties of the CNT fiber. Furthermore, in the widely studied graphite intercalation compounds (GICs), some mechanisms have been observed to stabilize FeCl<sub>3</sub>-GICs against intercalant desorption. Our intercalation compound remains stable even after four months exposure to ambient air due to the spontaneous creation of a passivating layer that forbids both the insertion of further air and the desorption of intercalant. This system, until now unexplored, has been characterized by transmission electron microscopy (TEM), electron diffraction (ED), wide-angle x-ray scattering (WAXS), Raman spectroscopy, x-ray photoelectron spectroscopy (XPS), and four-point probe resistivity measurements.

## MON 6

### **Intertube excitons and phonons in single chirality carbon nanotubes thin films**

Georgy Gordeev<sup>1</sup>, Anna Wróblewska<sup>2</sup>, Oisín Garrity<sup>1</sup>, Mariusz Zdrojek<sup>2</sup>, Li Han<sup>3</sup>, Benjamin Flavel<sup>3,4</sup>, Stephanie Reich<sup>1</sup>

<sup>1</sup>Department of Physics, Freie Universität Berlin, Berlin, Germany

<sup>2</sup>Faculty of Physics, Warsaw University of Technology, Warsaw, Poland

<sup>3</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

<sup>4</sup>Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

In single walled carbon nanotubes the exciton wave functions extend over the nanotube surface. For two tubes in close proximity the excitons in different tubes can

interact and form extended states. Only an averaged response is achieved in mixed chirality bundles, but single chirality films provide an ideal platform for studying intertube exciton coupling. We study (6,5) nanotube films by optical spectroscopy (resonance Raman, UV-Vis, Photoluminescence). A typical fingerprint of strong coupling is the splitting of free excitons into bonding and antibonding states. We observe this as up to 20 meV difference between absorbance and emission energies (anti-Stokes shift). A two-dimensional change in confinement of nanotubes inside a homogenous film also alters their vibrational properties. An additional low energy mode that represents a breathing of an entire bundle occurs. The high-energy modes (G modes) are accompanied by the E phonon in the film, whereas in the individual nanotubes this phonon is forbidden. These findings unveil intriguing possibilities for physics and applications of spatially separated (momentum indirect) excitons in nanotube ensembles.

## MON 7

### Ultrafast microscopy and spectroscopy of graphene

Achim Hartschuh<sup>1</sup>, Lucas Lange<sup>1</sup>, Konrad Birkmaier<sup>1</sup>, Veit Giegold<sup>1</sup>

<sup>1</sup>Department of Chemistry and CeNS, LMU Munich, Germany

We investigate the ultrafast response of graphene using transient reflection and non-linear Raman techniques. High electronic temperatures reached for pulsed laser excitation cause a partial Pauli-blocking of optical transitions. This leads to reduced transient absorption and hence enhanced reflection. Importantly, the transient reflectivity signal detected at different time delay and energy detuning between pump and probe pulse can be used to investigate spatial inhomogeneities in as prepared single-layer graphene, such as grain boundaries and wrinkles. We discuss the decay dynamics of this transient response based on complementary Raman spectra. In addition, the hot electronic temperatures reached upon pulsed excitation are found to cause a partial Pauli blocking of interfering quantum pathways contributing to resonant Raman scattering in graphene. As a consequence, the signal intensities of the two dominant Raman bands G and 2D together with their ratio strongly depend on the laser intensity and result in a super-linear and sub-linear power dependence of the G band and 2D band intensity, respectively.

## MON 8

### Topological band representations in layered structures

Ivanka Milosevic<sup>1</sup>, Zoran Popovic<sup>1</sup>, Bozidar Nikolic<sup>1</sup>, Milan Damnjanovic<sup>1</sup>

<sup>1</sup>Faculty of Physics, University of Belgrade, Belgrade

Layer groups (LGs) can be seen as subgroups of space groups. However, this correspondence is not unique and it is difficult to extract relevant data for particular layered structure from the existing space group data base of elementary band representations (EBRs). Two-dimensionality of the irreducible domain (ID) of the Brillouin zone of the LGs make the calculations less expensive and in most cases, in order

the calculations to be tractable it is not required to circumvent any part of ID, not even the generic stratum.

We use program POLSym [1] in which we have incorporated subroutines which are based on topological quantum chemistry [2] which establishes symmetry relations between localized and extended crystal states. POLSym outputs complete set of irreducible representations and EBRs for LGs, including Double-LGs, Gray-LGs and Double-Gray-LGs. EBRs are graphically presented and specified by orbital, Wyckoff position, symmetry and topology. Obstructed atomic limits are found.

[1] M. Damnjanovic, I. Milosevic, Physics Reports 581, 1-43 (2015)

[2] B. Bradlyn, L. Elcoro, J. Cano, M.G. Vergniory, Z. Wang, C. Felser, M.I. Aroyo, B.A. Bernevig, Nature 547, 298-305 (2017)

## MON 9

### Novel 2D Gd-Pt surface alloy on Pt(111): electronic and structural properties

Marta Przychodnia<sup>1</sup>, Michał Hermanowicz<sup>1</sup>, Emil Sierda<sup>2</sup>, Micha Elsebach<sup>2</sup>, Roland Wiesendanger<sup>2</sup>, Maciej Bazarnik<sup>1,2</sup>

<sup>1</sup>Institute of Physics, Poznan University of Technology, Poznan

<sup>2</sup>Department of Physics, University of Hamburg, Hamburg

A new class of 2D materials has been recently discovered, namely rare earth (RE) metals – transition metals (TM) surface alloys. Their specific properties mean that they can be used in a wide range of potential applications. Limiting the dimensionality of such a system to 2D (so-called surface alloys) influences their properties. Apart of interesting electronic properties they also exhibit impressive magnetic properties defined by indirect interactions between RE atoms via the TM lattice which changes when dimensions are reduced, for example, a GdAu<sub>2</sub> surface alloy is ferromagnetic while in bulk this alloy is antiferromagnetic. Here, I will present the Gd-Pt surface alloy grown on Pt(111). The atomic-scale electronic properties of the three distinct, different surface alloys were investigated by means of scanning tunneling spectroscopy (STS) and density functional theory (DFT) calculations. Further, I will analyze their structural properties in atomic scale deduced out of scanning tunneling microscopy (STM) studies.

## MON 10

### Crystalline and amorphous graphene from aromatic precursors

K. G.-Hubmann<sup>1</sup>, T. Lehnert<sup>2</sup>, N. Mueller<sup>1</sup>, P. Kusch<sup>1</sup>, U. Kaiser<sup>2</sup>, S. Reich<sup>1</sup>

<sup>1</sup>Department of Physics, Freie Universität Berlin, Berlin

<sup>2</sup>Ulm University, Central Facility of Electron Microscopy Electron Microscopy, Ulm

We study the growth of graphene from large (poly)aromatic precursors that react on a substrate while preserving their sp<sup>2</sup> structure. These precursors require lower growth temperatures, produce specific types of defects and are self-limited to a monolayer. As the growth temperature (500°C) is far below the typical growth tem-

perature (900°C) from the gaseous precursors, the structure of the aromatic  $C_6H_6$  unit is preserved in the grown layer. Raman spectra verified the high quality of the obtained graphene domains. With transmission electron microscopy, we show that the synthesized domains consist of crystalline and amorphous parts. For determining the defect density, we systematically studied the Raman D and G bands. The domain boundaries of the grown graphene are compared to the edges of exfoliated graphene by characterizing their D/G ratio.

## MON 11

### Visualization and precharacterization of as-grown suspended CNTs for fabrication of CNFETs

Miroslav Haluska<sup>1</sup>, Keno Ky Studer<sup>1</sup>, Marcel Staudenmann<sup>1</sup>, Seoho Jung<sup>1</sup>, Christofer Hierold<sup>1</sup>

<sup>1</sup>Micro and Nanosystems D-MAVT, ETH Zurich, Zurich, Switzerland

Localization and characterization of as-grown suspended single walled carbon nanotubes (SWCNTs) is required for effective fabrication of devices based on dry-transferred individual CNTs [1]. Optical microscopy (OM) of suspended CNTs temporally decorated by micrometer large particles of easy volatile material [2] can be used for visualization of CNTs. OM offers quick information about CNTs occurrence, position, length and orientation on the growth substrates. To visualize suspended CNTs we used p-nitrobenzoic acid (pNBA) [2]. Optically detectable particles or even “layers” were formed on CNTs in about 1 minute of pNBA deposition for  $T_{evap} = 110 - 120^\circ\text{C}$  and  $N_2$  flow rate 400-500 sccm. The pNBA deposit can be easily removed from CNTs at about  $120^\circ\text{C}$  in  $N_2$  flow after short image collection by OM. Further, Raman spectroscopy can be used to characterize pre-localized individual CNTs. No changes in Raman signal have been detected comparing CNT spectra prior to pNBA deposition and after its evaporation from CNTs.

[1] M. Muoth, C. Hierold, IEEE MEMS 2012, Paris, pp 1352-1355 (2012).

[2] G. Zeevi et al., Nature Communications, 7, 12153 (2016).

## MON 12

### Highly Efficient and Reversible Covalent Patterning of Graphene: 2D Management of Chemical Information

Tao Wei<sup>1</sup>, Malte Kohring<sup>1</sup>, Heiko B Weber<sup>1</sup>, Frank Hauke<sup>1</sup>, Andreas Hirsch<sup>1</sup>

<sup>1</sup>Organische Chemie II, Friedrich-Alexander-Universität, Erlangen

A very efficient approach for spatially resolved graphene patterning by covalent functionalization is reported. The facile addend binding to monolayer graphene relies on reductive activation of the carbon lattice, antaratopic quenching by a noninert substrate and classical lithography. Two types of covalent patterning functionalizations were performed and the resulting structured graphene sheets were unambiguously characterized by statistical Raman spectroscopy in combination with SEM/EDS.

Reversible defunctionalization upon recovery of intact graphene was monitored by temperature dependent Raman spectroscopy. This allowed for the accurate modulation of the functionalization degree by controlled annealing. Our discovery provides the basis for management of chemical information by establishing of complete write/store/erase cycles.

### **MON 13**

#### **Novel Covalent Approaches to Control the Doping Level within Carbon Nanotubes**

Antonio Setaro<sup>1</sup>, Alphonse Fiebor<sup>1</sup>, Mohsen Adeli<sup>2</sup>, Stephanie Reich<sup>1</sup>

<sup>1</sup>Physics, Freie Universität Berlin, Berlin

<sup>2</sup>Chemistry, Freie Universität Berlin, Berlin

Achieving precise and controlled charge management of carbon nanotubes is a key element towards their technological applications. Here we will discuss how the covalent method through a triazine-based cycloaddition we recently developed is beneficial not only in preserving and regenerating the pi-conjugation of the tubes but also in allowing electronic communication between the functional groups and the nanotubes themselves. We will discuss different groups that up- or downshift the position of the Fermi level within the tubes and highlight the consequences onto the phenomenology of their optical response.

### **MON 14**

#### **Programmable photodoping in van der Waals heterostructure**

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Two-dimensional (2D) transition-metal dichalcogenide (TMD) based electronic and optoelectronic devices have been extensively explored toward the post-Moore era. Huge efforts have been devoted to modulating the doping profile of TMDs to achieve 2D logic units and memory devices. Here, we report a programmable photodoping technique in 2D TMDs based on a van der Waals heterostructure of TMDs and hexagonal boron nitride (hBN). Taking 2D MoTe<sub>2</sub> as an example, the electron transport property in the MoTe<sub>2</sub> device can be precisely controlled by modulating the photodoping gate. Through tuning the polarity of the photodoping gate, such a doping effect can be programmed with excellent repeatability, and is retained for over 14 days. By spatially controlling the photodoping region, the photoresist-free logic units, including p–n junction and inverter in the MoTe<sub>2</sub> homo-structure are achieved with outstanding performance. In addition to 2D logic units, a multibit nonvolatile optoelectronic memory based on a heterostructure of WSe<sub>2</sub> and hBN has also been realized, with over 128 distinct storage states.

**MON 15****Ghost Anti-Crossing caused by Umklapp Scattering in 2D Heterostructures**Matthew Hamer<sup>1,2</sup>, Abigale Graham<sup>3</sup>, Roman Gorbachev<sup>1,2</sup>, Neil Wilson<sup>3</sup><sup>1</sup>Department of Physics and Engineering, University of Manchester, Manchester<sup>2</sup>National Graphene Institute, University of Manchester, Manchester<sup>3</sup>Department of Physics, University of Warwick, Coventry

Two-dimensional materials characteristically have weak van der Waals interactions between layers allowing 2D heterostructures to be designed by stacking 2D crystals. Generally, the electronic structures of individual 2D layers are retained in the heterostructure, with weak coupling between layers. However, these weak inter-layer interactions can lead to dramatic twist-angle dependent effects, such as transforming normally metallic graphene into a superconductor by a “magic angle” moiré superlattice potential [1]. This has led to the new field of twistronics, engineering electronic structure and properties through twist-angle dependent interactions.

Here we report a new twistronic effect whereby it is possible to engineering strong interlayer coupling at defined energy and momenta in otherwise weakly coupled systems. This result, observed in ARPES, is measured in heterostructures of graphene combined with semiconducting post transition metal chalcogenides and can be explained by Umklapp scattering. This effect is important as it provides a new tool for controlling charge transport between layers of 2D materials.

[1] Nature 556, 43–50 (2018)

**MON 16****Filtering the photoluminescence spectra of atomically thin semiconductors with graphene**Etienne Lorchat, Luis E. Parra Lopez, Cédric Robert<sup>1</sup>, Delphine Lagarde<sup>1</sup>, Guillaume Froehlicher, Takashi Taniguchi<sup>2</sup>, Kenji Watanabe<sup>2</sup>, Xavier Marie<sup>1</sup>, Stéphane Berciaud<sup>1</sup>Université de Toulouse, INSA-CNRS-UPS, LPCNO, Toulouse, France<sup>2</sup>National Institute for Materials Science, Tsukuba, Ibaraki, Japan

Atomically thin semiconductors made from transition metal dichalcogenides (TMDs) are model systems for investigations of strong light-matter interactions and applications in nanophotonics, opto-electronics and valley-tronics. However, the photoluminescence spectra of TMD monolayers display a large number of features that are challenging to decipher. On a practical level, monochromatic TMD-based emitters would be beneficial for low-dimensional devices but no solution has yet been found to meet this challenge. Here, using a counter-intuitive strategy that consists in interfacing TMD monolayers with graphene, a system known as an efficient luminescence quencher, we demonstrate bright, single and narrow-line photoluminescence arising solely from TMD neutral excitons. This observation stems from two effects:

(i) complete neutralization of the TMD by the adjacent graphene leading to the absence of optical features from charged excitons (ii) selective non-radiative transfer of TMD excitons to graphene, that is sufficiently rapid to quench radiative recombination of long-lived excitonic species without significantly affecting bright excitons.

Reference: <https://arxiv.org/abs/1908.10690>

## MON 17

### **Optical and magnetic properties of graphene nanoribbons with embedded Co atoms synthesized inside SWCNTs**

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Graphene nanoribbons (GNRs) are a promising 1D carbon-based nanomaterial that has a great potential for nanoelectronics and optics. The band structure of GNRs is influenced by the width of the ribbon or atoms that are placed on the edges. Along with that the fine tuning of the properties can be achieved by incorporation of various atoms inside the ribbon [1]. Modification of the GNR structure or external environment leads to the changes of the material optical properties [2]. In this work we study the formation of narrow GNRs with dopant Co atoms inside the single-walled carbon nanotubes. The synthesis approach allows to form ultralong and narrow (around 1 nm in width) GNRs. In order to probe the magnetic properties in thin samples of GNRs we excited the samples at a wavelength corresponding to the Co-related absorption band and probed the response via transverse magneto-optic Kerr effect (TMOKE). Comparison with the SQUID measurements has been performed.

The work was supported by RFBR grant 18-02-01099.

[1] Senkovskiy, B. V.; Usachev, D. Yu.; et al. ACS Nano 2018, 12 (8), 7571-7582.

[2] Chernov, A. I.; Fedotov, P. V.; et al. Nanoscale 2018, 10 (6), 2936-2943.

## MON 18

### **Optical Properties of MoS<sub>2</sub>, WS<sub>2</sub> and Graphene Deposited from Gas Phase**

Elena D. Obraztsova<sup>1,2</sup>, Pavel V. Fedotov<sup>1,2</sup>, Pavel Vinokurov<sup>3</sup>, Ekaterina A. Obraztsova<sup>1,4</sup>, Vera Islamova<sup>1,2</sup>, Maxim Rybin<sup>1,2</sup>, Svetlana Smagulova<sup>3</sup>

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MoS<sub>2</sub> and WS<sub>2</sub> are interesting examples of 2D materials. Bulk crystals of MoS<sub>2</sub> and WS<sub>2</sub> are semiconductors with the indirect gaps of 1.2 eV and 1.3 eV, correspondingly. With the layer number decrease the indirect-gap semiconductors transform into the direct-gap ones with the increased gap value. The direct gap provides an efficient generation of electron-hole pairs upon photoexcitation being promising for optoelectronics. Chemical vapor deposition (CVD) technique provides the extended samples of high quality. In this work the films of MoS<sub>2</sub>, WS<sub>2</sub> and graphene were grown by CVD technique. Transition from islands (of 80 mkm on SiO<sub>2</sub> and 250 mkm on sapphire) to the continuous film were controlled by deposition time [1]. The Raman and Photoluminescence studies were performed [1,2]. The Raman spectra (and especially their low-frequency part) were very informative for the layer number estimation. The properties of heterostructures MoS<sub>2</sub>-graphene and WS<sub>2</sub>-graphene were investigated.

The work was supported by RFBR project 18-29-19113 and RSF project 20-42-08004.

[1] S.A. Smagulova, et al., Semiconductors (2020) (in press).

[2] E.A. Obraztsova, et al., Phys. Stat. Sol. B 245(2008)2055.

## MON 19

### Infrared luminescence of bulk Black Phosphorus at low temperature

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Atomic layers of Black Phosphorus (BP) have been recently isolated, ten years after graphene. Among 2D materials, BP presents unique properties: atomic layers have a direct bandgap which can be tuned by the layer number. They interact with light in a wide range of wavelengths from visible (monolayer) to mid-infrared (bulk). Despite many investigations on atomic layers, the optical properties of the bulk crystals remain poorly known.

In order to get reference data, we investigate photoluminescence (PL) of bulk BP at 2K. Two intense peaks are evidenced at 0.275 eV and 0.26 eV. Highest energy narrow peak is the first identification of the bulk exciton in PL corroborating previous reflectance measurements (Morita, Appl. Phys., 1986). However its existence is fragile and is shown to be cut down due to crystal inhomogeneity, ageing process or simply exfoliation. The lower energy peak, formerly observed at higher temperature



(Chen et al., Nano Lett., 2019) could be defect-related. Its thickness dependence is studied from bulk to thin layers, showing an unexpected behavior that will be discussed.

## MON 20

### Hybrid Superconducting-magnetic orders in a single layer of (BETS)<sub>2</sub>GaCl<sub>4</sub>

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Magnetic order is known to be antagonistic to conventional superconductors due to its interference with the pairing mechanism. We present scanning tunneling microscopy and spectroscopy to study the interplay between superconductivity and magnetism in a single layer of organic d-wave superconductors (BETS)<sub>2</sub>GaCl<sub>4</sub> on Ag(111). Antiferromagnetic molecular chains of GaCl<sub>4</sub> are spontaneously formed within the (BETS)<sub>2</sub>GaCl<sub>4</sub> superconducting layer due to shortage of BETS dimers. Below transition temperature of 7K, the superconducting order masks the antiferromagnetic order and dominates the electronic properties showing a ubiquitous gap over the entire island with proximity effect across the island/Ag(111) interface. These features gradually decay with the raise in temperature giving way to an abrupt emergence of Kondo dip and vibronic features on GaCl<sub>4</sub> the stripes respectively. The concurrent absence of these signals below T<sub>c</sub> may be related to a renormalization process where both phonon and antiferromagnetic fluctuation exhibit a cooperative existence to mediated superconductivity in d-wave superconductors.

A. Hassanien, Adv. Electron. Mater. 5(1):1800247( 2019).

## MON 21

### Electron and exciton phonon interaction in gate tunable transition metal dichalcogenide layers

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Atomically thin two-dimensional layered materials receive great interest because of their unique properties. Particularly, monolayers of semiconducting transition metal dichalcogenides (SC-TMDCs) excel due to their strong exciton dominated light matter interaction as well as their valley- and spin properties. Key to the interest in SC-TMDC is the possibility to tune and engineer their properties on demand and on-chip by external stimuli. We report on a distinct increase of the degree of valley polarization of up to 60% even at elevated temperatures of more than 220 K by increasing the charge carrier concentration [1]. Phonons are a significant mechanism for valley depolarization at elevated temperatures. We observe a significant

coupling between the long-range oscillating electric field induced by the LO phonon. This Fröhlich exciton LO-phonon interaction [1] is suppressed by doping and correlates with the distinct increase of the degree of valley polarization. We study the electrical and optical response of gate tunable TMDC flakes by combined spectroscopic imaging ellipsometry, PL and Raman measurements.

[1] B. Miller et al., Comm. 10, 807 (2019).

## MON 22

### 2D nanomagnets – exfoliation of layered crystals with intrinsic magnetism

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Magnetism in 2D materials is not only of fundamental scientific interest but also shows promise for numerous applications. However, the magnetic properties of many materials are arising from extrinsic effects like defects or dopants. Layered metal phosphorus trisulfides show intrinsic magnetic properties in bulk solid but are instable when being exfoliated. Thus very little is known about the intrinsic magnetic ordering of the corresponding nanoparticles. It is known that the properties of other 2D crystals are drastically changing from bulk to few- and monolayer sheets and even vary for different sizes of the same thickness. This makes control over the sheet dimensions extremely important. Different centrifugation-based size selection techniques have been developed in this regard.

In this contribution, we show progress in producing nanosheet dispersions of 3 different magnetic crystals of metal phosphorus trisulfides ( $MPS_3$ ;  $M = Mo, Fe, Ni$ ) by liquid phase exfoliation in inert gas atmosphere. We provide new insights in the degradation kinetics and thermodynamics of these intrinsic 2D magnets by ensemble measurements on well-defined nanosheet size distributions.

## MON 23

### Structural Characterization of PtSe<sub>2</sub> Films Grown by One Zone Selenization

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Platinum diselenide (PtSe<sub>2</sub>) has attracted interest due to its semi-metallic electronic structure, high optoelectronic performance, and enhanced photocatalytic activities. Moreover, thin PtSe<sub>2</sub> films show a metal to semiconductor transition upon thinning. Several methods have been reported for the growth of monolayer or few-layer PtSe<sub>2</sub> films (CVD growth, thermally assisted conversion). In most cases, films are poly-

crystalline with many randomly orientated domains and domain boundaries. Thus epitaxial films prepared on a single-crystal substrate such as sapphire or GaN are more favorable.

Here, we present the fabrication of epitaxially aligned  $\text{PtSe}_2$  thin films on a c-plane sapphire substrate using one zone selenization of magnetron sputtered platinum layers. We studied the influence of synthesis conditions and an initial Pt thickness on the alignment and properties of as-prepared  $\text{PtSe}_2$  films.

## MON 24

### Thermochemical adsorption as effective method to adjust electronic structure of CVD graphene

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Here we present the CVD-synthesis of graphene on copper foils, its transfer onto dielectric substrate, and the study of the electronic, optical and thermoelectric properties. The result of the work is a demonstration of the possibility of changing the electronic structure of the initial graphene by functionalizing the surface of the material with ferric chloride crystals or cobaltocene crystals to obtain hole or electron conductivity in graphene, respectively. Using Raman spectroscopy, the obtained samples were analyzed and the shift of the main G-peak in graphene allows us to conclude that its electronic structure changes. Also, these changes are confirmed by optical absorption spectroscopy. The type of conductivity and the quantitative value of the doping effect were achieved using electrophysical measurements of surface resistance and measurements of the Seebeck effect.

## MON 25

### Investigation of dark plasmons in oligomers by spatial modulation spectroscopy

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We realized to excite dark plasmons directly via spatial modulation spectroscopy with structured light. Dark plasmons are plasmons that have a vanishing total dipole moment, they are so interesting because they have stronger near fields and a longer lifetime than the well-known plasmonic bright modes. [1] To excite the dark plasmons we used light with different spatial polarization profiles, such as linear light with angular momentum, azimuthal or radial polarized light. In combination with the spatial modulation setup we were able to measure the extinction (absorption + scattering) of gold nano-oligomers (dimers and tetramers), which were produced by electron beam lithography.

[1] D. E. Gómez et al., Nano Letters 13 (8), 3722-3728 (2013)

**MON 26****Electromechanic properties of graphene aerogels**

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Graphene aerogel is a three-dimensional porous form of graphene with a high surface-to-volume ratio. Graphene aerogels have attracted a significant amount of interest in recent years due to their unique mechanical and electrical properties that show great potential for numerous applications in engineering, electrochemistry, and biology. These unique properties are originating from a clever arrangement of two-dimensional graphene sheets in a three-dimensional porous monolith structure containing air-filled pores. Here we investigate the structure, mechanical and charge transport properties of graphene aerogels prepared via hydrothermal reduction of graphene oxide. The graphene aerogels demonstrate superelastic compressibility up to GPa pressure, yet they are highly sensitive to small pressures in their electrical response. Our findings provide new insights into the relationship between charge transport and mechanical deformation of graphene aerogels.

**MON 27****Local spectroscopic investigation of strongly interacting TMDC-metal heterostructure**

Matěj Velický<sup>1,2</sup>, Alvaro Rodriguez<sup>3</sup>, Milan Bouša<sup>3</sup>, Martin Kalbáč<sup>3</sup>, Martin Vondráček<sup>4</sup>, Jan Honolka<sup>4</sup>, Andrey Krayev<sup>5</sup>, Mahdi Ahmadi<sup>1</sup>, Gavin Donnelly<sup>6</sup>, Fumin Huang<sup>6</sup>, Héctor D. Abruña<sup>1</sup>, Kostya S. Novoselov<sup>2</sup>, Otakar Frank<sup>3</sup>

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The recently introduced method for exfoliation of TMDCs on freshly deposited gold yields extremely high monolayer coverage [1-3]. However, the exact nature of the strong interaction between the two components of the heterostructure still remains to be described in detail. In the present work, we have undertaken a comprehensive study of MoS<sub>2</sub> exfoliated on gold deposited by e-beam evaporation, magnetron sputtering, and thermal evaporation with thickness varying from 3 to 50 nm. The interaction between Au and MoS<sub>2</sub> with different number of layers (1, 2, 3 and bulk) has been studied by AFM, Raman microspectroscopy as well as TERS, microXPS and microARPES. The results clearly evidence a heterogeneity of the interface, depending on the substrate roughness and its exposure to air. While the microscale characterization methods (Raman, XPS, ARPES) show broadening and splitting of

the respective bands, the observations at nanoscale (AFM, TERS) reveal distinct features, related to the local variations of the strength of interaction between Au and MoS<sub>2</sub>.

[1] Velický et al. Acs Nano 12, 10463, 2018.

[2] Desai et al. Adv Mater 28, 4053, 2016.

[3] Magda et al. Sci Rep 5, 14714, 2015.

## MON 28

### The properties of MoS<sub>2</sub> films tailored by sulfurization of annealed molybdenum layers

Peter Hutár<sup>1</sup>, Ivan Kundrata<sup>1</sup>, Michaela Sojková<sup>1</sup>, Lenka Pribusová Slušná<sup>1</sup>, Karol Végső<sup>2</sup>, Peter Šiffalovič<sup>2</sup>, Edmund Dobročka<sup>1</sup>, Martin Hulman<sup>1</sup>

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Two-dimensional MoS<sub>2</sub> still attract a research interest due to its electronic properties and facile fabrication of thin films by sulfurization. Structural properties of MoS<sub>2</sub> thin films reflect the details of a sulfurization method used as well as properties of pre-deposited molybdenum layers. Here, we present fabrication of MoS<sub>2</sub> thin films by one-zone sulfurization of molybdenum oxide layers. First, thin Mo films were annealed in O<sub>2</sub> atmosphere under different conditions (temperature, O<sub>2</sub> pressure, etc.). Depending on the parameters, annealing provides thin layers of either MoO<sub>2</sub> or MoO<sub>3</sub>. These layers were subsequently sulfurized in sulfur vapors. The crystal structure and chemical composition of molybdenum oxide layers and MoS<sub>2</sub> films were characterized by X-ray diffraction methods, Raman and optical spectroscopy and X-ray photoelectron spectroscopy. We show that properties of as-prepared MoS<sub>2</sub> films depend sensitively on the oxidation state of the initial molybdenum oxide layers.

## MON 29

### Resonance Raman, Photoluminescence Spectroscopy and Imaging Investigation of Monolayer MoS<sub>2</sub> Grown by Chemical Vapor Deposition

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MoS<sub>2</sub> has attracted significant interest because of special electronic and optoelec-

tronic properties in the monolayer and few-layer forms that are different from those manifested by the bulk form.

These intriguing properties prompted substantial research to discover the means of fabrication and the physical characteristics of two-dimensional crystals to produce integrated electronics. Here we report on the varying optical properties of CVD grown  $MoS_2$  monolayer flakes with different shapes using  $MoS_2$  powder as a precursor.

Detailed investigations of the spatial distribution of the photoluminescence energy reveal that depending on the shape of the  $MoS_2$  flakes, the width of the strain field is different. Thus, our results help to elucidate the fundamental mechanisms responsible for the differences in photoluminescence and Raman signals between the perimeter region and the center region of monolayer  $MoS_2$  and suggest that the induced strain plays an important role in the growth of monolayer material.

### MON 30

#### Tip-Enhanced Raman Spectroscopy in Graphene

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Here we present experimental and theoretical tip-enhanced Raman Spectroscopy (TERS) in graphene, a spatially delocalized two-dimensional sample, addressing different aspects: resolution and interference effects on defect characterization, interference of substrate of TERS response, resolution beyond the tip-apex dimensions. The the later is due to the field configuration resulting from the coupled tip-sample-substrate system, exhibiting a non-trivial spatial surface distribution. The field distribution and the symmetry selection rules are different for different TERS geometries, influencing on the overall enhancement, which depends on the Raman mode symmetry and substrate structure, impacting the nanometrology of two-dimensional systems based on nano-optics.

### MON 31

#### Spatially Resolved Bottom-Side Fluorination of Graphene by 2D-Substrate Patterning

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Patterned functionalization, which can on the one hand open the bandgap of graphene and on the other hand program demanding designs on graphene, is essential for graphene-based nano-architectures. Here, a new and highly efficient method was applied to obtain patterned functionalization on graphene by the mild fluorination with spatially arranged AgF arrays on the structured substrate, which was directly demonstrated by Scanning Raman Spectroscopy (SRS) and Scanning Electron Microscopy coupled with Energy-dispersive X-ray Spectroscopy (SEM-EDS). For the first time, chemical patterning on the bottom-side of graphene was realized. The chemical nature of the patterned functionalization is established to be the ditopic scenario with F-atoms occupying the bottom-side and hydroxy groups or H-atoms binding on the top-side, which further discloses the mechanism of the fluorination process. Our novel strategy can be conceptually extended to pattern other functionalities by using other reactants and this bottom-side patterned functionalization releases lots of possibilities on the top-side, enabling great potentials for graphene-based devices.

## MON 32

### **Electron-donating groups onto single-walled carbon nanotubes via non-destructive and covalent functionalization by [2+1] cycloaddition**

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The need to develop new functionalization of carbon nanotubes techniques grows due to its unique and outstanding properties. These properties have been utilized in electronics, optics, biosensing, bioimaging, chemotherapy, etc. Previous works [1, 2] by our group were effective in developing a non-destructive and covalent functionalization of single-walled carbon nanotubes by a cycloaddition reaction. Encouraged by the results obtained, we seek to synthesize di- and mono-substituted aniline derivatives with electron-donating functional groups using a nitrene backbone. These compounds will further be converted into azido derivatives and conjugated onto the single-walled carbon nanotube via the azido linker. We report the structural properties and degree of functionalization of the resulting functionalized carbon nanotubes with di- and mono-substituted derivatives.

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

[2] Setaro, A. *Condens. Matter. J. Phys.*, 2017, 29, 423003.

**MON 33****Deciphering the origin of anharmonicity in  $\text{CH}_3\text{NHPbI}_3$  using low frequency polarized Raman**

Rituraj Sharma<sup>1</sup>, Matan Menahem<sup>1</sup>, Zhenbang Dai<sup>2</sup>, Thomas Brenner<sup>1</sup>, Lingyuan Gao<sup>2</sup>, Andrew M. Rappe<sup>2</sup>, Omer Yaffe<sup>1</sup>

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Methylammonium lead iodide (MAPI) has emerged as an outstanding photovoltaic absorber material. Recent experimental and theoretical evidences indicate that the electronic and structural dynamics in MAPI are strongly coupled. Therefore, understanding the nature of the anharmonic lattice motions in MAPI is crucial. We employ low frequency Raman measurements using polarized light at 1.16 eV excitation to assign the symmetries of all the observed Raman-active modes in the orthorhombic phase of MAPI. Subsequently, we investigate the microscopic mechanisms leading to structural anharmonicity that persists through the high temperature phases. Our study provides a tool to assign the vibrational modes in halide perovskites simultaneously delineating the origin of their anharmonic structural dynamics.

**MON 34****Can electron-electron collisions activate two-dimensional plasmons?**

Dmitry Aleksandrovich Svintsov<sup>1</sup>

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The main effort in solid-state plasmonics is concentrated on increasing the plasmon lifetime. This generally requires suppression of electron scattering. Here, we show that electron-electron (e-e) scattering can have very non-trivial effect on plasmon lifetime in 2d electron systems [1]. Counter-intuitively, strong e-e collisions can even 'activate' 2d plasmons in the presence of direct current. More precisely, we reveal several mechanisms of current-driven plasmon instabilities that are possible in hydrodynamic transport regime (dictated by strong e-e collisions) [2,3] and impossible in collisionless one [4]. We show that e-e collisions can renormalize the plasmon spectrum in a dissipationless manner by reducing the plasmon phase velocity [1]. This enables phase synchronism between drifting electrons and emitted waves, resulting in possible Cerenkov-type plasmon emission.

[1] D. Svintsov, Phys. Rev. B vol. 97, 121405(R) (2018)

[2] D. Svintsov, Phys. Rev. B vol. 100, 195428 (2019)

[3] D. Svintsov, arXiv:1910.01190

[4] D. Svintsov and V. Ryzhii, Phys. Rev. Lett. vol. 123, 219401 (2019)



**MON 35****The excitonic luminescence of 7-A graphene nanoribbons**

Pavel V. Fedotov<sup>1,2</sup>, Alexander Chernov<sup>2</sup>, Ekaterina A. Obratsova<sup>1</sup>,  
Elena D. Obratsova<sup>1,2</sup>

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The graphene nanoribbons (GNRs) are narrow stripes of graphene exhibiting strong quantum confinement effects. The electrons and phonons properties of GNRs are defined by the width and the edge type of a nanoribbon. Atomically precise armchair GNRs (AGNRs) can have a variable optical bandgap depending on the nanoribbon family type and width. 7-AGNRs belong to 3N+1 family and have one of the largest bandgaps. To produce atomically smooth GNRs one can apply a bottom-up approach. In this work we report the modified CVD method based on a bottom-up approach to scale up synthesis of 7-AGNRs. The obtained nanoribbon films exhibit typical for 7-AGNRs Raman features. The conducted multi-wavelength Raman study confirms high quality of produced GNRs. We also demonstrate that suspending nanoribbons in organic solvents facilitates the registration of a bright excitonic luminescence of GNRs. The observed features in UV-Vis-IR optical absorption and photoluminescence spectra are in good agreement with previous reports of 7-AGNRs.

The work was funded by RFBR project 19-32-60006.

**MON 36****Temperature dependent transport measurements of thin PtSe<sub>2</sub> layers: weak localization or strong electron-electron interaction?**

Martin Hulman<sup>1</sup>, M. Sojková<sup>1</sup>, M. Moško<sup>1</sup>, V. Štrbík<sup>1</sup>, N. Gál<sup>1</sup>, L. Pribusová-Slušná<sup>1</sup>,  
E. Dobročka<sup>1</sup>

<sup>1</sup>Institute of Electrical Engineering SAS, Bratislava, Slovakia

Electronic structure of PtSe<sub>2</sub> is complex with the valence and conduction bands intersecting and the material is classified as a Weyl semimetal. A complete switching from a metal to a semiconductor in atomically thin PtSe<sub>2</sub> was observed as the layer thickness is reduced. We present measurements of electrical conductivity of thin PtSe<sub>2</sub> layers grown by selenising platinum films 0.5 - 5 nm thick. The temperature dependence of the conductivity critically depends on the layer thickness: for the thinnest layers, the conductivity increases in the whole temperature range between 5 K and room temperature. On the other hand, the conductivity decrease with increasing temperature for the thickest samples. For the PtSe<sub>2</sub> samples about 5-6 nm thick, both regimes were observed. In particular, the conductivity scales as  $\ln T$  at low temperatures which indicates either a weak localization or strong electron-electron interaction. The transport measurements were complemented by measuring optical conductivity in the visible and infrared ranges. The optical conductivity has a minimum in the infrared and increases as the frequency approaches zero.

**MON 37****The Anomalous Raman Response for 6-Armchair Graphene Nanoribbons (6AGNR)**Hans Kuzmany<sup>1</sup>, Lei Shi<sup>2</sup>, T. Pichler<sup>1</sup>, T. Saito<sup>3</sup><sup>1</sup>Elektronische Materialeigenschaften, Universität Wien, Fakultät für Physik, Wien, Austria<sup>2</sup>State Key Laboratory of Optoelectronic Materials and Technologies, Nanotechnology Research Center, School of Material Science and Engineering, Sun Yat-sen University, Guangzhou, Guangdong, China<sup>3</sup>Nat. Inst. of Advanced Industrial Science and Technology (AIST), Nanomaterials Research Institute, Tsukuba, Japan

Recently we characterized and identified several graphene nanoribbons grown from ferrocene molecules inside single-walled carbon nanotubes [1]. Evidence was obtained for 6AGNR and 7AGNR but indications were also observed for 5AGNR and 8AGNR. Evidence for the ribbons came from high resolution TEM, Raman scattering and high level quantum chemical calculations. Raman scattering experiments were in quantitative agreement with the provided calculations except for the CH in plane bent mode of the 6AGNR at  $1244\text{ cm}^{-1}$ . The Raman response for this mode was far too strong compared to the calculations which were carried out for free molecules. In this poster we provide evidence for an influence of environment (diameter of hosting tube) and transformation process (transformation temperature) on the anomalous enhancement of this line. This is in turn an indication for an extrinsic influence on the anomalous Raman response of this mode.

[1] H. Kuzmany et al., Geometrical and Electronic Structure of High Quality Sub-Nanometer Graphene Ribbons, unpublished

**MON 38****Anharmonicity and Symmetry Breaking in 2D Hybrid Halide Perovskites**Matan Menahem<sup>1</sup>, Omer Yaffe<sup>1</sup><sup>1</sup>Materials and Interfaces, Weizmann Institute of Science, Rehovot

2D hybrid halide perovskites have been the focus of extensive study due to their easy tuneability and potential in optoelectronic applications such as solar cells and LEDs. It has been established that the electronic properties of halide perovskites are largely affected by thermal fluctuations (electron-phonon interaction). Yet, the phonons in 2D perovskites were not thoroughly studied and were mainly analyzed in the context of  $\text{PbI}_2$  lattice fluctuations.

In order to directly probe the dominant lattice vibrations and their influence on the electronic properties of 2D perovskites, we measured low frequency polarized Raman of prototypical 2D perovskite  $(\text{C}_4\text{H}_9\text{NH}_3)_2\text{PbI}_4$  as a function of temperature. Raman scattering results indicate a large anharmonic structural dynamic even at cryogenic temperature. Spectral broadening and loss of polarization dependence

with increasing temperature suggest symmetry breaking and phonon-phonon scattering, which govern electron-phonon interaction.

### MON 39

#### The equilibration dynamics of spin-polarized quantum Hall edges at graphene p-n junction

Arup Kumar Paul<sup>1</sup>, Chandan Kumar<sup>1</sup>, Manas Ranjan Sahu<sup>1</sup>, Kenji Watanabe<sup>2</sup>, Takashi Taniguchi<sup>2</sup>, Anindya Das<sup>1</sup>

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<sup>2</sup>National Institute for Materials Science, Ibaraki, Japan

The equilibration dynamics between quantum Hall (QH) edge states play a central role in realizing an electron interferometer. Recently graphene  $p-n$  junction (PNJ) with co-propagating, spin-valley polarized QH edges have been demonstrated as a promising platform for an electron interferometer. However, the interplay of different inter-channel scattering mechanisms in equilibration of polarized QH edges along a PNJ remain unexplored. In this work, we have carried out the conductance together with shot noise measurements to unravel the equilibration dynamics, in a dual graphite gated hexagonal boron nitride ( $hBN$ ) encapsulated graphene device. Our shot noise results as a function of filling factors of both  $p$  and  $n$  sides reveal that the inter-channel scattering mechanisms at the PNJ is fully tunable from the incoherent to complete coherent regime with the variation of the participating polarized QH edges at the PNJ. This is in sharp contrast with the previous shot noise studies, showing only incoherent processes as the dominant scattering mechanism. Thus our results will pave the way towards a more complete understanding of equilibration at graphene PNJ.

### MON 40

#### Conductive Atomic Force Microscopy of Atomic Reconstructions in Twisted Bilayers of Transition Metal Dichalcogenides

Astrid Weston<sup>1,2</sup>, Alex Summerfield<sup>1,2</sup>, Vladimir Enaldiev<sup>1,2,3</sup>, Viktor Zolyomi<sup>1,2</sup>, Samuel Magorrian<sup>1,2</sup>, Zohanna Zoltak<sup>1,2</sup>, Peter H. Beton<sup>4</sup>, Roman Gorbachev<sup>1,2,5</sup>

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<sup>3</sup>Kotelnikov Institute of Radio-engineering and Electronics, Russian Academy of Sciences, Moscow, Russia

<sup>4</sup>School of Physics and Astronomy, University of Nottingham, Nottingham, UK

<sup>5</sup>Henry Royce Institute for Advanced Materials, University of Manchester, Manchester, UK

Recent investigations of very low-twist angle graphene bilayers (BLs) have reported a range of exotic behaviours such as superconductivity, Mott insulator-like states and networks of topological edge states.

We show, for the first time, using conductive atomic force microscopy (cAFM) the domain structure formed by low-twist angle BL transition metal dichalcogenide (TMDC) devices of either  $\text{MoS}_2$  or  $\text{WS}_2$ . The cAFM measurements reveal a highly uniform triangular network of alternating high and low conductivity corresponding to 3R stacking in agreement with atomic-resolution scanning transmission electron microscopy (STEM) measurements [1]. These reconstructions are observable over a range of tip-surface biases for both 3R BLs and, additionally, a hexagonal reconstruction is observed in anti-parallel aligned TMDC BLs exhibiting 2H stacking.

Due to the lack of inversion symmetry, these structures offer a broader diversity of physical properties than graphene BLs such as electrical tuning of novel optical devices and the presence of strong pseudo-magnetic fields.

[1] Weston, A., Zou, Y., Enaldiev, V., Summerfield, A., Clark, N., et al., submitted, (2020)

## MON 41

### Solving the Thermoelectric Trade-Off Problem with Metallic Carbon Nanotubes

Yota Ichinose<sup>1</sup>, Akari Yoshida<sup>1</sup>, Kanako Horiuchi<sup>1</sup>, Kengo Fukuhara<sup>1</sup>, Natsumi Komatsu<sup>2</sup>, Weilu Gao<sup>2</sup>, Yohei Yomogida<sup>1</sup>, Manaho Matsubara<sup>3</sup>, Takahiro Yamamoto<sup>3</sup>, Junichiro Kono<sup>2,4,5</sup>, Kazuhiro Yanagi<sup>1</sup>

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<sup>2</sup>Department of Electrical and Computer Engineering, Rice University

<sup>3</sup>Department of Liberal Arts, Tokyo University of Science

<sup>4</sup>Department of Physics and Astronomy, Rice University

<sup>5</sup>Department of Material Science and NanoEngineering, Rice University

Semiconductors are generally considered far superior to metals as thermoelectric materials because of their large Seebeck coefficients  $S$ . However, a maximum  $S$  in a semiconductor is normally accompanied by small electrical conductivity, and hence, the power factor  $P$  remains small. However, an attempt to increase conductivity by increasing the Fermi energy (EF) decreases  $S$ . This trade-off between  $S$  and conductivity is a well-known dilemma in developing high-performance thermoelectric devices based on semiconductors. Here, we show using metallic carbon nanotubes (CNTs) with tunable EF solves this long-standing problem. We studied the EF dependence of  $S$ , conductivity, and  $P$  in a series of CNT films with systematically varied metallic CNT contents. In metallic CNTs, both  $S$  and conductivity monotonically increased with EF, continuously boosting  $P$  with increasing EF. Particularly, in an aligned metallic CNT film, the maximum  $P$  was 5 times larger than that in the high-purity (99%) semiconducting CNT film. We attribute these superior thermoelectric properties of metallic CNTs to the simultaneously enhanced  $S$  and conductivity of the first van Hove singularity.

**MON 42****DIAMOND NANOSTRUCTURES FOR PHOTONICS**

Marián Varga<sup>1</sup>, Lukáš Ondič<sup>1</sup>, Jan Fait<sup>1</sup>, Karel Hruška<sup>1</sup>, Alexander Kromka<sup>1</sup>

<sup>1</sup>Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

Diamond has outstanding optical properties such as large optical transmission window and possibility to host a variety of optically-active color centers. Diamond can be fabricated as a single-crystal plate or polycrystalline diamond film.

2D photonic structures (PhC) with periodicity spanning in the horizontal plane, typically composed of columns or air holes are designed to control the light propagation. Their unique properties, such as inhibition of spontaneous emission or enhancement of optical gain, motivate the search for technological approaches enabling fabrication of PhCs with high structural and optical quality.

Here, we demonstrate 3 different approaches for fabrication of diamond PhCs based on: i) etching of continuous diamond film, ii) diamond growth on periodically structured quartz substrates and iii) combined dry&wet etching for fabrication of suspended PhCs. We investigate the influence of the dimensions and structural quality of the PhCs on the (out)coupling of the light. We also show an easy way how to spectrally overlap the optical modes of the structures with the emission of Si-V color centers.

This work was supported by the GAČR 19-14523S.

**MON 43****Annealing effect on different layer in bilayer graphene**

Jinglan Liu<sup>1</sup>, Xuwei Zhang<sup>1</sup>, Pei Zhao<sup>1</sup>

<sup>1</sup>School of Aerospace, Zhejiang University, Zhejiang University, Hangzhou

Thermal annealing is a necessary step in the standard fabrication process of graphene for the removal of Polymethyl Methacrylate (PMMA). Its influence on monolayer graphene (MLG) has been intensively studied previously, whereas such effect on bilayer graphene (BLG) that is more complex remains unclear. Using designed BLG samples in which each graphene layer is formed by different carbon isotopes, we differentiate their Raman peaks of the two layers so that the shift in each spectrum affected by the annealing process can be probed. Results show that for both layers of BLG their Raman G peak blue shifts are smaller than that of MLG, and such blue shift for the adlayer of twisted BLG is larger than that for the adlayer of AB-BLG. We believe that our work can provide more understanding for the post-treatment of graphene on substrates as well as the characterization of their layers.



**HÜBNER Photonics**  
Coherence Matters.



- 08:30 – 09:30 **TUTORIAL: C. Voisin, Paris**  
*Spontaneous and intentional exciton trapping in carbon nanotubes*
- 09:30 – 10:00 **Y. K. Kato, Tokyo**  
*Bright- and dark-exciton dynamics in carbon nanotubes*
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **J. Zaumseil, Heidelberg**  
*Purified and Functionalized Carbon Nanotubes for Optical and Electronic Applications*
- 11:00 – 11:30 **S. Forel, Antwerp**  
*Toward a more reliable characterization of the chirality composition of sorted SWCNT samples*
- 11:30 – 12:00 **H. van der Zant, Delft**  
*The Dynamics of 2D Membranes*
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **H. Seiler, Berlin**  
*Anisotropy controls phonon thermalization in photoexcited black phosphorus*
- 19:00 – 19:30 **B. Beschoten, Aachen**  
*Unveiling valley lifetimes of free charge carriers in monolayer WSe<sub>2</sub>*
- 19:30 – 20:00 **K. F. Mak, Ithaca**  
*Quantum simulation of the Hubbard model in a moiré superlattice*
- 20:00 **Poster Session II**





**8:30**

**Spontaneous and intentional exciton trapping in carbon nanotubes**

Christophe Raynaud<sup>1</sup>, Antoine Borel<sup>1</sup>, Jana Zaumseil<sup>2</sup>, Yannick Chassagneux<sup>1</sup>,  
Christophe Voisin<sup>1</sup>

<sup>1</sup>Ecole Normale Supérieure, Paris, France

<sup>2</sup>Heidelberg University, Germany

Exciton localization in carbon nanotubes plays a key role towards the control of their light emission properties for quantum optics applications, including single photon generation. Here, we used a combination of hyperspectral super-localization microscopy and quasi-resonant excitation photoluminescence spectroscopy techniques to study the localization of one-dimensional excitons in pristine and functionalized single wall carbon nanotubes at low and room temperature [1]. Using numerical simulations, we interpreted the nearly resonant excitation spectra either in terms of excited trapped states selectively coupled to a single localized ground state or, at higher energy, in terms of delocalized one dimensional excitonic states providing uniform excitation of all the localized ground states along the nanotube axis.

[1] C. Raynaud et al., Nanoletters 19, 7210 (2019)

**09:30****Bright- and dark-exciton dynamics in carbon nanotubes**Y. K. Kato<sup>1,2</sup><sup>1</sup>Quantum Optoelectronics Research Team, RIKEN Center for Advanced Photonics, Japan<sup>2</sup>Nanoscale Quantum Photonics Laboratory, RIKEN Cluster for Pioneering Research, Japan

Electron-hole pairs form tightly-bound excitons in carbon nanotubes due to limited screening of the Coulomb interaction, and these mobile excitons exhibit long diffusion lengths. In combination with the increased scaling due to one-dimensionality, efficient exciton-exciton annihilation leads to antibunching at room temperature [Phys. Rev. Applied 8, 054039 (2017)]. There exist excitonic fine structures within the large binding energy, many of which are dark states with optical transitions forbidden by spin, momentum, and parity selection rules. By studying the dynamics and diffusion properties of the bright excitons and the parity-even dark excitons, we find that more than half of the dark excitons can be transformed into the bright excitons [Phys. Rev. X 9, 041048 (2019)]. The conversion efficiency is significantly enhanced by adsorbed air molecules on the surface of the nanotubes, demonstrating the potential for engineering the dark-to-bright conversion process by using surface interactions.

Work supported in part by MIC (SCOPE 191503001), JSPS (KAKENHI JP16H05962), and MEXT (Nanotechnology Platform). We thank the Advanced Manufacturing Support Team for technical assistance.

**10:30****Purified and Functionalized Carbon Nanotubes for Optical and Electronic Applications**Jana Zaumseil<sup>1</sup><sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, Heidelberg

Polymer-sorted semiconducting single-walled carbon nanotubes (SWNTs) are available in large amounts and can be used for a wide range of optoelectronic devices. Here, we report on the investigation of charge transport properties of dense semiconducting nanotube films in field-effect transistors using temperature and carrier density dependent mobility and Seebeck coefficient measurements as well as charge modulation spectroscopy. The impact of diameter and mixing ratios of SWNTs with different bandgaps gives insights into the role of inter- and intranantube transport in networks. Furthermore, we show how both the emissive and charge transport properties of SWNTs can be tuned by light-switchable functional groups of the wrapping polymer and selected lattice defects introduced via diazonium and aryl halide chemistry in organic solvents. We show that the dominant type of defect and hence the red-shifted defect emission wavelength can be tuned by the reaction conditions.

**11:00****Toward a more reliable characterization of the chirality composition of sorted SWCNT samples**Salomé Forel<sup>1</sup>, Alice Castan<sup>1</sup>, Frédéric Fossard<sup>1</sup>, Joeri Defiliet<sup>1</sup>, Dmitry Levshov<sup>1</sup>, Wim Wenseleers<sup>1</sup>, Annick Loiseau<sup>1</sup>, Sofie Cambré<sup>1</sup><sup>1</sup>Experimental Condensed Matter Physics Laboratory, University of Antwerp, Antwerp, Belgium

Recent progress in sorting and/or selective synthesis of specific single-wall carbon nanotube (SWCNT) chiralities, with increasing chiral purity, demands an optimized characterization methodology. Often, optical spectroscopy such as optical absorption spectroscopy (OAS) or fluorescence-excitation (PLE) spectroscopy, combined with resonant Raman spectroscopy (RRS) at a few distinct laser excitation wavelengths, is used to assess the chirality distribution, but absorption and Raman cross-sections and PL quantum efficiencies not only depend on the SWCNT chirality, but are also highly influenced by other factors such as SWCNT specific internal and external environment. In this work, we systematically compare the intensity chirality distribution obtained from three different optical spectroscopic techniques, i.e. OAS, PLE and wavelength-dependent RSS, with the chirality distribution obtained from high-resolution transmission electron microscopy for sorted and unsorted HiPco SWCNTs. This combined approach allows for identifying the discrepancies between the techniques and demonstrates that a combined approach is essential for a reliable characterization of SWCNT chirality distributions.

**11:30****The Dynamics of 2D Membranes**Herre van der Zant<sup>1</sup><sup>1</sup>Delft University of Technology, Delft, Netherlands

Atomically thin membranes are ideal building blocks of nano-electrical-mechanical systems (NEMS) because of their unique mechanical properties and their low mass. We make suspended membranes by transferring thin vanderWaals materials on top of silicon oxide substrates pre-patterned with (circular) holes, thereby forming 'drums' with (sub)micron diameters. The suspended parts form the membranes that are characterized by atomic force microscopy to determine their static mechanical properties (Young's modulus, pre-stress) and with a laser interferometer set-up that gives access to information on the dynamics in the frequency- and time-domain. The interferometer setup has also been equipped with a moveable x-y stage so that the membrane motion can be visualized with a displacement resolution of  $11 \text{ fm}/\sqrt{\text{Hz}}$ ; additionally, the nonlinear response of the motion can be used to extract the mechanical parameters such as the Young's modulus. In this talk I will introduce the technique and discuss two applications of these nanodrums: (i) the fabrication of different types of pressure sensors and (ii) the probing of (magnetic) phase transitions by purely mechanical means.

**18:30****Anisotropy controls phonon thermalization in photoexcited black phosphorus**

Hélène Seiler<sup>1</sup>, Daniela Zahn<sup>1</sup>, Marios Zacharias<sup>2,3</sup>, Patrick Hildebrandt<sup>1</sup>, Thomas Vasileiadis<sup>1</sup>, Will Windsor<sup>1</sup>, YingPeng Qi<sup>1</sup>, Christian Carbogno<sup>2</sup>, Claudia Draxl<sup>4</sup>, Fabio Caruso<sup>4</sup>, Ralph Ernstorfer<sup>1</sup>

<sup>1</sup>Physical Chemistry, Fritz-Haber-Institut der Max-Planck Gesellschaft, Berlin

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<sup>3</sup>Department of Mechanical and Materials Science Engineering, Cyprus University of Technology, Limassol

<sup>4</sup>Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin

Anisotropic structure in materials gives rise to a variety of anisotropic macroscopic properties, such as thermal and electrical conductivities, thermoelectric figure of merit, as well as optical properties. Recently, significant efforts have been geared toward exploiting these anisotropic properties in device applications. All of the proposed applications operate either in quasi-equilibrium, or strongly non-equilibrium conditions. It is thus desirable to gain a microscopic understanding of non-equilibrium states. Here we investigate electron-phonon and phonon-phonon interactions in photoexcited black phosphorus. Femtosecond electron diffuse scattering experiments combined with first principle computations reveal profoundly anisotropic electron-phonon and phonon-phonon thermalization dynamics. The transient anisotropy is reproduced using a minimal non-thermal lattice model derived from mode-resolved computations of electron-phonon and phonon-phonon coupling terms.

**19:00****Unveiling valley lifetimes of free charge carriers in monolayer WSe<sub>2</sub>**Bernd Beschoten<sup>1</sup><sup>1</sup>2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Aachen

Two-dimensional transition metal dichalcogenides offer the possibility to address the electron's valley degree of freedom making them interesting for valleytronics. The device performance of potential applications largely depends on the valley lifetimes of free charge carriers. Here, we report on nanosecond long, gate-dependent valley lifetimes of free charge carriers in WSe<sub>2</sub>, unambiguously identified by the combination of time-resolved Kerr rotation and electrical transport measurements. While the valley polarization increases when tuning the Fermi level into the conduction or valence band, there is a strong decrease of the respective valley lifetime consistent with both electron-phonon and spin-orbit scattering. The longest lifetimes are seen for spin-polarized bound excitons in the band gap region. We explain our findings via two distinct, Fermi level-dependent scattering channels of optically excited, valley polarized bright trions either via dark or bound states. By electrostatic gating we demonstrate that WSe<sub>2</sub> can be tuned to be either an ideal host for long-lived localized spin states or allow for nanosecond valley lifetimes of free charge carriers (> 10 ns).



**TUE 1****2D MoS<sub>2</sub> coated flexible graphite-polymer film for wearable energy storage**Kalyan Ghosh<sup>1</sup>, Cameron Jellett<sup>2</sup>, Martin Pumera<sup>1,2</sup><sup>1</sup>Central European Institute of Technology, Brno University of Technology, Brno, Czech Republic<sup>2</sup>Center for Advanced Functional Nanorobots, Department of Inorganic Chemistry, Faculty of Chemical Technology, University of Chemistry and Technology in Prague, Prague, Czech Republic

Flexible electronics have become a center of attention due to their vast application in multimedia devices, medical diagnosis, military defense, and sports. Flexible supercapacitors can be used as energy storage systems to power these electronics. However, facile fabrication of a thin, lightweight and flexible supercapacitor is still limited. Herein, to develop the supercapacitor, a graphite-poly(lactic acid (PLA) - based flexible conductive film was fabricated first, followed by electrodeposition of 2D MoS<sub>2</sub> on top of it. A solid-state flexible supercapacitor was then developed using the prepared MoS<sub>2</sub>/graphite-PLA film as electrode materials and polyvinyl alcohol (PVA)/H<sub>3</sub>PO<sub>4</sub> as gel electrolyte. This fabrication route eliminates the use of external current collectors such as Cu foil or Ni foam, and a separator building an ultra-thin device. The MoS<sub>2</sub> coating on graphite-PLA film facilitates the reversible charge storage mechanisms ensuring a high specific capacitance. The supercapacitor showed a high areal capacitance of 33 mF cm<sup>-2</sup> at a current density of 0.1 mA cm<sup>-2</sup>, which can power up wearable devices such as a smartwatch, the Internet of Things and healthcare monitoring systems.

**TUE 2****K<sup>+</sup> incorporation into methylammonium-based bromide rich mixed halide perovskites**Mehmet Derya Özeren<sup>1</sup>, Bea Botka<sup>1</sup>, Áron Pekker<sup>1</sup>, Katalin Kamarás<sup>1</sup>, Márton Kolár<sup>2</sup>, Endre Horváth<sup>2</sup>, László Forró<sup>2</sup><sup>1</sup>Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Budapest<sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Perovskite solar cells based on lead halides with organic cations exhibit over 20% certified efficiency. Iodide-based perovskites are prone to vacancy mediated halide migration upon illumination.[1] Recently it was suggested that potassium (K<sup>+</sup>) addition can be an effective way to eliminate the phase segregation although the underlying processes have not been clarified yet.[2] We studied the effect of K<sup>+</sup> addition in bromide rich wide band gap MAPb(Br<sub>x</sub> I<sub>1-x</sub>)<sub>3</sub> perovskites under illumination using photoluminescence and infrared spectroscopy. The phase segregation involves three different steps: initial, intermediate (iodide rich complex), and fully separated (degraded). Preliminary results suggest that the initial segregation behaviour, which occurs rapidly even upon low intensity illumination, is not affected by the alkali cation

addition. However, the stability of the intermediate phase under high intensity UV illumination is clearly enhanced.

[1] E. T. Hoke et al., Chem. Sci. 6, 613, (2015)

[2] M. Abdi-Jalebi et al., Nature, 555, 497, (2018)

### **TUE 3**

#### **Resolving few layer Antimonene/Graphene Heterostructures**

Tushar Gupta<sup>1</sup>, Kenan Elibol<sup>2</sup>, Stefan Hummel<sup>2,3</sup>, Michael Stöger-Pollach<sup>4</sup>, Clemens Mangler<sup>2</sup>, Gerlinde Habler<sup>5</sup>, Jannik C. Meyer<sup>2</sup>, Dominik Eder<sup>1</sup>, Bernhard C. Bayer<sup>1,2</sup>

<sup>1</sup>Institute of Materials Chemistry, Vienna University of Technology (TU Wien), Vienna, Austria.

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<sup>3</sup>GETec Microscopy GmbH, Vienna, Austria

<sup>4</sup>USTEM, Vienna University of Technology (TU Wien), Vienna, Austria

<sup>5</sup>Department of Lithospheric Research, University of Vienna, Vienna, Austria

Two-dimensional (2D) antimony (Sb, “antimonene”) recently attracted interest due to its peculiar electronic properties and its suitability as anode material in next generation batteries. Sb however exhibits a large polymorphic structural diversity, which is also influenced by the Sb’s support. Thus understanding of Sb heterostructure formation is key in 2D Sb integration. 2D Sb/graphene interfaces are of prime importance as contacts in electronics and electrodes in batteries. We thus here study few-layered 2D Sb/graphene heterostructures by atomic-resolution (scanning) transmission electron microscopy ((S)TEM). In our heterostructures we find the co-existence of the thermodynamically predicted layered 2D beta Sb phase but also of a metastable cubic Sb phase. Both Sb phases show rotational Van-der-Waals epitaxy with the graphene support and both Sb phases are well resilient against environmental oxidation. Exact Sb growth results are sensitive on employed processing and substrate properties incl., notably, the nature of support type underneath the direct graphene support. Our work provides insights into the rich phase and epitaxy landscape in 2D Sb & 2D Sb/graphene heterostructures

### **TUE 4**

#### **Temperature-dependent Raman studies of a natural van der Waals heterostructure**

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Van der Waals heterostructures (vdWH) formed of two-dimensional (2D) materials offer means to obtain materials by design with unique electronic properties. Research on 2D vdWH has so far been focused on fabricating such heterostructures by stacking individual 2D crystals, which leads to stacks with the presence of fabrication defects. Franckeite (Fr) is a naturally occurring vdWH comprised of two different alternately stacked semiconducting layers, that enables the study of a complex layered system where the crystal orientation between layers has been preserved. Unlike other layered sulfide-based materials, Fr is a grained- textured rock composed of few-millimeter flakes in random orientation. In consequence, the exfoliation of uniform thin flakes is especially challenging. By precise manipulation of the starting flake in combination with different substrates, we were able to increase the quality of exfoliation and obtain few-layer Franckeite flakes with uniform surface areas of approximately 5 microns. Here we present results on the developed exfoliation technique and the evolution of Raman peaks of Fr with increasing temperature.

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## **TUE 5**

### **Field-effect in gapless carbon nanotube based devices**

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As the dimensions of the elementary electronic devices decrease due to advances in technology role of the contact phenomena becomes crucial for their performance. The first CNT based field effect transistor (CNFET) was demonstrated more than twenty years ago and ever since effects of contact configuration on the performance of such devices has been studied intensely.

Conventional wisdom regarding CNFET operation is that the tunability of the current through the channel formed by a CNT originates primarily from existence of a band gap in the charge carriers' spectrum. For a truly metallic CNT free of defects conductance of the channel should be independent of the gate voltage at least at high enough temperatures. In this work we demonstrate that even in such a case contact phenomena lead to a notable field-effect: we observe a suppression of conductance when the Fermi level is around the charge neutrality point (CNP) with the "ON-OFF" ratio about two. This value appears to be insensitive to the temperature within a

range from 10 to 300 K. We explain observed behaviour by the modifications of the CNT band structure under the metal, caused by the CNT deformation.

## TUE 6

### Visualizing Poiseuille flow of hydrodynamic electrons

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Hydrodynamics, which generally describes the flow of a fluid, is expected to hold even for fundamental particles such as electrons when inter-particle interactions dominate. Although various aspects of electron hydrodynamics have been revealed in recent experiments, the fundamental spatial structure of hydrodynamic electrons - the Poiseuille flow profile - has remained elusive. Here we provide direct imaging of the Poiseuille flow of an electronic fluid, as well as a visualization of its evolution from ballistic flow. Using a scanning carbon nanotube single-electron transistor, we image the Hall voltage of electronic flow through channels of high-mobility graphene. We image the transition from flat, ballistic field profiles at low temperatures into parabolic field profiles at elevated temperatures, which is the hallmark of Poiseuille flow. The curvature of the imaged profiles is qualitatively reproduced by Boltzmann calculations, which allow us to create a 'phase diagram' that characterizes the electron flow regimes. Our results provide direct confirmation of Poiseuille flow in the solid state, and enable exploration of the rich physics of interacting electrons in real space.

## TUE 7

### Better in Vacuum - how high vacuum improves conductive Atomic Force Microscopy on 2D materials

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In the recent years, downscaling in the semiconductor industry lead to an increasing interest for 2D-materials. Among them, transition metal dichalcogenides (TMDs) exhibit promising electrical characteristics, such as an inherent band gap and a high

charge carrier mobility. However, the desired electrical properties are often confined to single grains or islands.

Conductive atomic force microscopy (C-AFM) can resolve the morphology and local heterogeneities in the electrical conductivity of 2D materials at the same time. Here, we used CAFM to map the conductivity of MoS<sub>2</sub> layers grown onto sapphire substrates with varying thicknesses. In particular, we investigated the effect of water on CAFM data on MoS<sub>2</sub> by comparing measurements in air and in high vacuum of down to  $1 \times 10^{-5}$  T using a Park Systems Hivac AFM. Water contaminations naturally present on surfaces in ambient conditions can reduce the conductivity of MoS<sub>2</sub> by p-doping of the material. Results showed an overall increase in the local conductivity from air to vacuum and, moreover, conductivity maps in vacuum showed a higher sensitivity, resolving the local decrease of conductivity at the position of grain walls.

## TUE 8

### Graphene nanoribbons encapsulated in carbon nanotubes prepared from coronene precursors

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We investigated the optical properties of graphene nanoribbons prepared by annealing coronene-filled single walled carbon nanotubes at various temperatures. The carbon nanotubes were filled at low temperature using supercritical CO<sub>2</sub> as solvent. [1] The advantage of this filling method is that it provides high filling ratio, while preventing undesired polymerised byproduct formation on the outer surface of the carbon nanotubes. [2] The graphene nanoribbon formation inside the carbon nanotubes was monitored via Raman and photoluminescence spectroscopy. We compared the graphene nanoribbons encapsulated into the carbon nanotubes with literature data of stand-alone graphene nanoribbons.

[1] B. Botka, M. E. Füstös, Gy. Klupp, D. Kocsis, E. Székely, M. Utczás, B. Simándi, Á. Botos, R. Hackl, and K. Kamarás, *Physica Status Solidi (b)* 249, 2432 (2012)

[2] B. Botka, M. E. Füstös, H. M. Tóháti, K. Németh, Gy. Klupp, Zs. Szekrényes, D. Kocsis, M. Utczás, E. Székely, T. Vácz, Gy. Tarczay, R. Hackl, T. W. Chamberlain, A. N. Khlobystov and K. Kamarás, *Small* 10, 1369 (2014)

**TUE 9****Enhancement of second- and third- order nonlinear optical processes on metal nanostructures and WS<sub>2</sub>**

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Nonlinear optical processes on a surface are interesting for nanoscale sensing applications and frequency conversion. Moreover, nonlinear optical processes can also be used to probe the electronic properties of novel materials.

In this work we study the enhancement of second- and third- harmonic generation (SHG, THG), sum-frequency generation (SFG) and four-wave mixing (FWM) using two spatially and temporally overlapped femtosecond laser pulses with different frequencies. This enhancement is explored on a nanostructured gold surface and a monolayer WS<sub>2</sub> flake.

For the nanostructures on gold we find enhancement factors of more than three orders of magnitude highly depending on their geometric parameters. We show that the nonlinear optical enhancement is due to the generation of plasmons in the nanostructure.

For isolated WS<sub>2</sub> flakes, despite being only a few atomic layers thick, we observe various nonlinear optical effects with a higher efficiency than a semi-infinite gold surface. We show a nonlinear exciton excitation in the monolayer WS<sub>2</sub> and a resonant behaviour of the SHG near the exciton wavelength.

**TUE 10****Visible graphene plasmons enhanced Raman scattering on heavily nanocorrugated graphene**

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Ever since the discovery of plasmonic excitations in graphene, the quest for visible graphene plasmons has actively been pursued. Besides their fundamental importance, the main driving force stems from envisaged applications, given that our most efficient optical techniques are available for visible light. A route to tune up the graphene plasmon frequencies from their native THz values to the visible range is the lateral confinement into graphene structures below 10 nm. An intrinsic limitation of this approach is the detrimental effect of edges, drastically damping plasmon resonances. Here we demonstrate the realization of visible graphene plasmons through their edge-free lateral confinement into sub-5 nm graphene corrugations. The strong near-fields of localized visible graphene plasmons enable a particularly

strong enhancement of Raman scattering and emission from specific molecules adsorbed on heavily nanocorrugated graphene sheets. The new mechanism of the graphene mediated visible light - matter interaction enhancement can be exploited in fluorescence-free and biocompatible graphene SERS substrates, as well as efficient quantum emitters.

## TUE 11

### **Flat Visible-Light Absorption Properties of Nano-Granular Ag-Fe-O Thin Films Prepared by Pulsed Laser Deposition**

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Black insulative thin films have attracted much attention as coating materials for touch-panel displays. For those applications, not only a flat and large absorption coefficient in the visible range but also an electrically insulative property is required; however, it is difficult to achieve these properties simultaneously in single phase because they are basically trade-off relation. Nano-sized metal particles dispersed into an insulator matrix is focused on in this study, in which the coexistence of Drude absorption of metal and inter-band absorption of insulator is expected. Ag-Fe<sub>2</sub>O<sub>3</sub> is selected because it can be stable in wide range of temperature and pressure. The Ag-Fe-O thin films were prepared by pulsed laser deposition. The films deposited using the 60mol%Ag-FeO target shows large and flat absorption in visible range and large sheet resistance. The ADF-STEM and XRD indicate that metallic Ag, spinel iron oxide and amorphous Ag-Fe-O phase coexist. In the thin film, Ag phase was separated by the insulator matrix partially having Ag and large resistance. This microstructure seems to be responsible for the electrically insulative property even for high Ag content.

## TUE 12

### **High frequency contactless characterization of 2D materials: graphene, WS<sub>2</sub>**

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The electrical conductivity of two-dimensional materials without any electrical contact could be obtained using two different methods: using the TeraHertz-Time Domain Spectroscopy (TH-TDS) method, in the range from MHz up to 2 THz [1]. Or using a Rutile Dielectric Resonator (RDR), in which case we are obtaining the conductivity at the resonant frequency of the device, close to 9.0 GHz [2]. Using TH-TDS by transmission we focus on the sample directly. In the last case (RDR), the sample is placed inside the resonant cavity working at TE<sub>011</sub> mode and has to have

exactly the same surface size as the cavity, 12x12 mm in our device. From the Q factor variation of the resonant cavity due to the sample, we can extract its surface resistance. In order to check the results and also to enlarge the frequency range, we performed FTIR spectroscopy on the same samples. We realized those measurements on different two-dimensional materials: graphene and WS<sub>2</sub>. We analyzed and compared both methods, obtaining good agreement.

[1] D. Arcos, D. Gabriel, D. Dumcenco, A. Kis, N. Ferrer-Anglada; pss (b), 2017.

[2] P. Krkotić, A. Aguasca, J. M. O'Callaghan; EuMC, Madrid, 2018.

## TUE 13

### **From 1D carbyne to hybrid 2D sp-sp<sup>2</sup> carbon-based nanostructures: a density functional theory investigation of structural, electronic and vibrational properties**

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Carbon-atom wires are linear molecules displaying tunable structural, electronic and optical properties and whose limit is 1D carbyne [1,2]. Similarly, 2D sp-sp<sup>2</sup> carbon nanostructures (such as graphdiynes-GDY) show structure-dependent properties and a fundamental issue regards how they can be modulated by controlling  $\pi$ -electron conjugation. Here, DFT calculations are used to predict the structure, the band gap, and the Raman/IR response of GDY structures based on previous studies on carbynes. First, the band structure and the spectra of 2D-GDY are analyzed to shed light on topological effects. Second, GDY nanoribbons (NR) are simulated to reveal confinement effects on the gap and on the vibrational response as a function of width and edge-type [3]. The gap modulation in armchair and zigzag GDYNR is discussed while Raman/IR spectra reveal marker bands dependent on the edge-type or the NR width. Guidelines are given for the characterization and design of 2D sp-sp<sup>2</sup> carbon nanostructures, where topology plays a major role in tuning the final response.

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

[2] C.S. Casari, A. Milani, MRS Comm 2018, 8, 207

[3] P. Serafini et al submitted

## TUE 14

### **Impact of disorder and imperfections on the optical properties of TMDCs**

Julian Klein<sup>1</sup>, Hendrik Lambers<sup>2</sup>, Florian Sigger<sup>1</sup>, Margaux Lassaunière<sup>2</sup>, David O. Tiede<sup>2</sup>, Alexander Holleitner<sup>1</sup>, Ursula Wurstbauer<sup>2</sup>

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Interfacial imperfections induced by substrate and environment are known to potentially reduce the electronic and optical properties of semiconducting transition metal dichalcogenides [1]. On the other hand, deterministically induced point defects induced by focused ion beams are promising candidates to serve as quantum emitters with well controlled energies that can be positioned with nm resolution [2,3]. Here, we investigate signature of disorder, imperfections and lattice defects on the properties of semiconducting 2D materials by a combination of scanning probe methods, optical and Raman spectroscopy.

Work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – EXC 2089/1 – 390776260 and projects WU 637/4- 1 and HO 3324/9-1.

[1] J. Klein et al. Appl. Phys. Lett. 115, 261603 (2019).

[2] J. Klein et al 2D Materials 5, 11007 (2018).

[3] J. Klein et al. Nature Commun. 10, 10, 2755 (2019).

## TUE 15

### Direct growth of monolayer MoS<sub>2</sub> at Au-SiO<sub>2</sub> interface

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While numerous methods have been developed to realize large area growth of high quality transition metal dichalcogenide sheets, the materials synthesized are, however, succumbed to various threats when stored under ambient conditions or used during device fabrication, causing rapid degradation, damages or contamination. Herein, by using alkali halide-assisted CVD technique, we demonstrate a novel growth of monolayer MoS<sub>2</sub> directly at the interface between Au and SiO<sub>2</sub> substrate. Monolayer MoS<sub>2</sub> grains were found to nucleate progressively beneath the pre-deposited gold from the boundary edges via an interface diffusion mechanism. Continuous growth and fusion forms the connected MoS<sub>2</sub> network as reaction proceeds. The sample grown was observed using cross-sectional TEM. Its identity was confirmed using Raman and PL spectroscopy. The mapping results suggested a high uniformity in crystal and optical qualities comparable to that exfoliated one. In this way, the growth can be manipulated over the desired location by programming the Au pattern, and functional FET devices can also be created at ease.

**TUE 16****Atomic structure and electronic properties of graphene sheets with extreme nanoscale corrugation**Gergely Dobrik<sup>1</sup>, Péter Süle<sup>1</sup>, Miklós Menyhárd<sup>1</sup>, Levente Tapasztó<sup>1</sup><sup>1</sup>Centre for Energy Research, Institute of Technical Physics and Materials Science, Budapest, Hungary

We have strain-engineered unprecedentedly strong nanoscale corrugations into graphene sheets by a cyclic thermal annealing process. The RMS value characterizing the surface roughness of such graphene sheets is about 0.5 nm, which is almost the double of the RMS value measured in graphene on SiO<sub>2</sub>. The characteristic aspect ratio (hmax/R) of 0.5 is much higher than the aspect ratios of graphene nanobubbles holding pressures of several MPa, clearly highlighting the extreme nature of the corrugation in our graphene sheets. The atomic structure of such sheets have been investigated the STM and AFM measurements. The heavy graphene nanocorrugations induce significant changes in the electronic properties. Tunneling spectroscopy and theoretical calculation (DFT) reveal clear signatures of charge carrier confinement in individual graphene nanocorrugations with high aspect ratios. From the tunneling spectra we can estimate the confinement area to be of about 3-4 nm. EELS reveal a strong quenching of the Pi graphene plasmon peak near 6 eV, clearly confirming the significant change induced in the atomic and electronic structure by the extreme nanoscale deformations of the graphene sheet.

**TUE 17****Ni-mediated reactions in nanocrystalline diamond on Si substrate: the role of the oxide barrier**Viera Skakalova<sup>1,2</sup>, Semir Tulic<sup>1</sup>, Thomas Waitz<sup>1</sup>, Maria Caplovicova<sup>3</sup>, Viliam Vretnar<sup>3</sup>, Marian Varga<sup>4</sup>, Alexander Kromka<sup>4</sup>, Oleksandr Romanjuk<sup>4</sup>, Bohuslav Rezek<sup>4</sup><sup>1</sup>Physics of Nanostructured Materials, University of Vienna, Austria<sup>2</sup>Institute for Advanced Studies, University of Cergy-Pontoise, France<sup>3</sup>Centre for nanodiagnostics, Slovak University of Technology, Bratislava, Slovakia<sup>4</sup>Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

Nanocrystalline diamond (NCD) films grown on Si substrates by microwave plasma enhanced CVD were subjected to Ni-mediated graphitization to cover them with a conductive layer. Results of TEM including EELS of cross-sectional samples demonstrate that the oxide layer on Si substrates (5 nm native SiO<sub>2</sub>) has been damaged by microwave plasma during the early stage of NCD growth. During the heat treatment for graphitizing the NCD layer, the permeability or absence of the oxide barrier allow Ni nanoparticles to diffuse into the Si substrate and cause additional solid-state reactions producing pyramidal crystals of NiSi<sub>2</sub> and SiC nanocrystals. The latter are found impinged into the NiSi<sub>2</sub> pyramids but only when the interfacial oxide layer is absent, replaced by amorphous SiC. The complex phase morphology of the samples is also reflected in the temperature dependence of electrical conduc-

tivity, where multiple pathways of the electronic transport dominate in different temperature regions. We present models explaining the observed cascade of solid-state reactions and resulting electronic transport properties of such heterostructures.

## TUE 18

### Surface plasmon in doped one-dimensional system

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In this work, we discuss the surface plasmon (SP) in doped single-wall carbon nanotube (SWCNT) and doped graphene ribbon (GR), which we refer to as quasi-one-dimensional systems. SP is a collective oscillation of electron density that couples with incident light. The SP in SWCNT has been observed by Yanagi et al, in which the intersubband SP absorption peak appears when the polarization of the incident light is perpendicular to the tube axis. Here, we investigate the dependence of SP energy on diameter ( $d$ ) and the Fermi energy ( $E_F$ ) of SWCNT. We show here the calculated SP energy using random phase approximation as a function of  $d$  and  $E_F$  for many combinations of chiralities.

The accumulated charges near the edge of GR can also oscillate collectively and form so-called edge-plasmon. In this work, we discuss the edge-plasmon in GR with finite width. In particular, we found that the electric field of edge-plasmon on the surface of graphene rotates near the edge that induces rotating surface current. The in-plane rotation of the electric field corresponds to the out-of-plane spin angular momentum of light and the spin direction depends on the position on the ribbon.

## TUE 19

### Towards plasmonic tunnel gaps for nanoscale photoemission currents by on-chip laser ablation

Philipp Zimmermann<sup>1,2</sup>, Alexander Hötger<sup>1</sup>, Noelia Fernandez<sup>1</sup>, Anna Nolinder<sup>1</sup>, Kai Müller<sup>1</sup>, Jonathan Finley<sup>1,2</sup>, Alexander Holleitner<sup>1,2</sup>

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<sup>2</sup>Nanosystems Initiative Munich (NIM), Munich

We demonstrate that prestructured metal plasmonic nanogaps can be shaped on-chip to below 10 nm by femtosecond laser ablation [1]. We explore the plasmonic properties and the nonlinear photocurrent characteristics of such formed tunnel junctions. The photocurrent can be tuned from multiphoton absorption toward the laser-induced strong-field tunneling regime in the nanogaps, and gives rise to a field emission of ballistic hot electrons propagating across the nanoscale junctions. We show that a unipolar current of hot electrons is achieved by designing the plasmonic enhancement factors in the junctions to be asymmetric, which allows ultrafast electronics on the nanometer scale. We particularly demonstrate that femtosecond

optical pulses in the near-infrared (NIR) applied to such nanogaps can drive electronic circuits with a prospective bandwidth of up to 10 THz [2].

We thank the DFG for funding via the Cluster of Excellence e-conversion.

[1] Philipp Zimmermann, et al. Nano Let. 2019 19 (2), 1172-1178.

[2] Christoph Karnetzky, et al. Nature Comm. 2018 9 2471.

## TUE 20

### **Negative differential resistance in the single-atom(molecule) structure**

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We theoretically analyzed electron transport through the impurity (molecular) complex with strong Coulomb correlations between localized electrons by means of the generalized Keldysh diagram technique. We revealed that the presence of strong Coulomb correlations in the asymmetric tunneling contact (coupling strength between the impurity (molecular) complex and metallic contacts strongly differ) leads to the formation of multiple well pronounced regions with negative tunneling conductivity in the I-V curves. This finding is very promising in the sense of dopant atoms (individual molecules) application as basic elements in modern nanoelectronic circuits. We also applied proposed theoretical model for the explanation of the experimentally measured I-V curves, which demonstrate well resolved areas with negative differential resistance both at low and room temperatures. Simulations based on the theoretical model of the device reproduce all the essential features of the measured transport characteristics. The use of unconventional dopants in silicon, such as potassium, is a major step forward towards the implementation of room-temperature single-atom electronics.

## TUE 21

### **Experimental study of diamond with high density of nitrogen-vacancy centers**

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Diamonds with a high density of nitrogen-vacancy centers are promising candidates for room temperature magnetometers with outstanding sensitivity. We report the preparation of nitrogen-vacancy centers in diamond in a high concentration. We find that electron spin resonance is a powerful tool to determine the concentration of such defects in contrast to optical methods. We investigate both neutron and electron irradiated samples. During the production, we determine the number of NV centers based on electron spin resonance spectra. The spin polarization effect caused by the illumination of the samples during ESR measurement enables us to enhance the sensitivity by two orders of magnitude. In addition, we show optically detected magnetic resonance measurements on NV centers that give an insight into the dynamics of the excited states.

## **TUE 22**

### **The Kibble-Zurek scaling at exceptional points**

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Exceptional points (EPs) are ubiquitous in non-hermitian systems, and represent the complex counterpart of critical points. By driving a system through a critical point at finite rate induces defects, described by the Kibble-Zurek mechanism, which finds applications in diverse fields of physics. Here we generalize this to a ramp across an EP. We find that adiabatic time evolution brings the system into an eigenstate of the final non-hermitian Hamiltonian and demonstrate that for a variety of drives through an EP, the defect density satisfies a universal scaling form in terms of the usual critical exponents and the speed of the drive. Defect production is suppressed compared to the conventional hermitian case as the defect state can decay back to the ground state close to the EP. We provide a physical picture for the studied dynamics through a mapping onto a Lindblad master equation with an additionally imposed continuous measurement.

## **TUE 23**

### **Flat band induced long-range out-of-plane behavior of LDOS in strained graphene**

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The strain induced deformation of the Dirac cone (DC) determines many unique and exceptional electronic properties of graphene and topological insulators, and its energy spectrum. Here, we show, the emergence of an anomalous long-range behaviour in the LDOS of strongly strained graphene. No such out-of-plane LDOS tail can be seen in equilibrium graphene. In particular, a long range diffuse tail in the LDOS perpendicular to the graphene sheet has been calculated by accurate peri-

odic plane wave DFT codes. The revealed phenomenon has been found in various strained graphene systems such as nanodomes, deformed plane graphene or in magic-angle twisted bilayer graphene which display flat bands (FBs) in their energy spectra. The FBs could emerge due to several strain induced phenomena such as minigap opening or pseudo-Landau level quantization (PLLQ). The increase in electron repulsion in FBs could lead to the enhancement of LDOS diffusivity above the sheet and could be a general phenomenon in strained 2D materials. Related LDOS maps are also shown and a specific complex pattern has been revealed which is attributed to the spatial distribution of the pseudo-magnetic field when PLLQ occurs.

## TUE 24

### Process Integration of Few-Layer MoS<sub>2</sub> into a-Si:H Heterojunction pin-Photodiodes for extended Infrared Detection

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Photodiodes play a significant role in optical communication or sensor applications. One emerging field are wavelength-selective detection systems. Starting point of this work are well-established amorphous silicon (a-Si) pin-diodes being sensitive in the visible range (VIS). Such diodes are based on a mature thin-film technology and prone for tandem vertical stack integration. To enhance their detection range, we succeeded in the reproducible, scalable integration of large-area few-layer molybdenum disulfide (MoS<sub>2</sub>), a 2D transition metal dichalcogenide (TMDC) with tailored optical properties in the IR regime. The TMDC was successfully integrated on a cm-scale utilizing conventional deposition processes. Despite of MoS<sub>2</sub> having a bandgap of 1.4 eV, the resulting hybrid vertically integrated a-Si/MoS<sub>2</sub> sensor arrays yield a broad absorption from 400 nm to at least 2120 nm, probably due to indirect optical transitions at the material interface. Moreover, their sensitivity can be tuned from the VIS to the IR range depending on the applied bias voltage. Furthermore, the a-Si passivates the MoS<sub>2</sub> and ensures a long-term device stability.

Bablich et al., ACS Photonics 6 (2019) 1372-1378

**TUE 25****Ultralong spin lifetime in graphene doped with light alkali metals**

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We report ultralong (3-27 ns) spin relaxation time in few layer graphene (FLG) doped with light alkali metals (Li and Na) utilizing liquid ammonia synthesis. The emergence of Fano lineshapes in the G-line Raman spectral region as an indicative of strong electron-phonon coupling, attest the high level of doping for both lithium and sodium. We find that Na dopes solely the monolayer graphene as it is known to be inert against graphitic carbon. Alkali doping allows us to access the intrinsic spin-relaxation time of doped FLG via electron spin resonance (ESR). The spin-relaxation time indicates a lifetime which is superior compared to that found in mono or few layer graphene using transport methods. Moreover, a 1.1 eV shift of the Fermi energy was found from the Pauli spin-susceptibility for both alkalis, which is comparable to that in LiC<sub>6</sub> GIC. Our study paves the way to explain spin-relaxation properties of graphene and to advance its use in spintronics devices. In addition, our synthesis method opens the possibility for an efficient Li/Na intercalation of graphene for the purpose of improved energy storage.

**TUE 26****Time and temperature resolved in situ investigation of the metal-induced crystallization of amorphous carbon thin films**

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The metal-induced crystallization of amorphous carbon in thin film stacks with Ni

was investigated in situ as a function of 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. Formation of turbostratic carbon occurred simultaneously with a layer exchange (LE) and was completed during the applied heating ramp up to 700 °C. The temperature resolved measurements allowed the determination of the onset temperatures and transition rates as a function of the annealing temperature and the stacking order. Finally, the activation energy for both LE directions was estimated. In combination with thermodynamic calculations [1], this in situ study allows to identify metal-induced crystallization via wetting and diffusion along grain boundaries as the responsible mechanism for crystallization of amorphous carbon with layer exchange in contact with Ni.

[1] D. Janke et al., Carbon 2019, DOI: 10.1016/j.carbon.2019.12.006

## **TUE 27**

### **How can one measure the entropy of a mesoscopic system?**

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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 Coulomb-blockaded mesoscopic system from transport measurements. We prove analytically and demonstrate numerically the applicability of the method to such 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 of the experimentally observed finite thermoelectric response at the apparent particle-hole symmetric point.

## **TUE 28**

### **Anisotropic Electron-Photon-Phonon Coupling in Layered MoS<sub>2</sub>**

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Transition metal dichalcogenide, especially MoS<sub>2</sub> has attracted lot of attention recently owing to its tunable visible range band gap and anisotropic electronic and transport properties. Here, we report a comprehensive inelastic light scattering measurements on CVD grown (horizontally and vertically aligned flakes) as well



as single crystal flakes of  $\text{MoS}_2$ , probing the anisotropic optical response via studying the polarization dependence intensity of the Raman active phonon modes as a function of different incident photon energy and flake thickness. Our polarization dependent Raman studies intriguingly revealed strong anisotropic behavior reflected in the anomalous renormalization of the modes intensity as a function of flake thickness, phonons and photon energy. Our observations reflects the strong anisotropic light-matter interaction in this high crystalline symmetric layered  $\text{MoS}_2$  system especially for the in-plane vibrations, which is crucial for understanding as well application of these materials for future application such as optoelectronic applications.

## TUE 29

### **Freestanding and permeable nanoporous gold membranes for surface-enhanced Raman scattering**

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Surface-enhanced Raman spectroscopy (SERS) demands reliable, high enhancement substrates in order to be used in different fields of application. Permeable, freestanding SERS active membranes are particularly beneficial as they enable pressure-controlled high-throughput screening of gaseous and liquid analytes. Here, we introduce freestanding porous gold membranes (PAuM) as easy to produce, scalable and effective SERS substrates. We fabricate large-scale sub-30 nm thick PAuM, that form freestanding membranes with varying morphologies depending on the nominal gold thickness. These PAuM are mechanically stable for pressures up to  $> 3$  bar, and exhibit surface-enhanced Raman scattering with local enhancement factors of  $10^4$  to  $10^5$ , which we demonstrate by wavelength-dependent and spatially resolved Raman measurements using graphene as a local Raman probe. Numerical simulations reveal that the enhancement arises from individual, nanoscale pores in the membrane acting as optical slot antennas. Our PAuM are mechanically stable, provide robust SERS enhancement for excitation power densities up to  $10^6 \text{ W cm}^{-2}$ , and will in the future enable the creation of flow-through SERS sensors.

**TUE 30****Two-dimensional antimony oxide**

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Two-dimensional (2D) antimony, so-called antimonene, is one of the promising novel elemental 2D materials. However, it can form antimony oxide, when exposed to air. This may even be beneficial for the stability of the material and at the same time result in interesting electronic properties. We present different types of 2D antimony single- and few-layer oxide structures, based on density functional theory (DFT) calculations. Depending on stoichiometry and bonding type, these novel antimony oxide layers have different structural stability and electronic properties, ranging from topological insulators to semiconductors with direct and indirect band gaps between 2.0 eV and 4.9 eV. Furthermore, we discuss their vibrational properties and predict Raman spectra, which allow experimental identification of the different structures. Our theoretical results are in good agreement with recent experimental findings. Additionally, oxidized few-layer antimonene can form heterostructures consisting of semiconducting antimony oxide and semimetallic few-layer antimonene.

**TUE 31****Interband Junctions in Twisted Double Bilayer Graphene**

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When two layers of graphene are twisted by a small angle, a Moiré pattern appears. The coupling between the layers depends on the twist angle. With twisted double bilayer graphene, similar effects hold while a band gap can be opened in each bilayer by an out-of-plane electric field. Using local gates in devices with different twist angles we define junctions between electrons and/or holes in different bands. We then define cavities leading to Fabry-Pérot oscillations. For low enough twist angles, we reach the characteristic Van Hove singularity [1],[2]. This allows us to probe junctions and cavities between gamma-electrons (holes) and kappa-electrons (holes). We furthermore engineer regions in which one of the bilayers is gapped,

thus leading to the definition of interlayer junctions. At some gating configurations, we observe gaps due to correlations or due to crystal field effects [3].

- [1] Y. Cao . . P. Jarillo-Herrero, Nature 556, 43 (2018)
- [2] Y. Cao . . . P. Jarillo-Herrero, Nature 556, 80 (2018)
- [3] P. Rickhaus, J. Lado, G. Zheng . . T. Ihn and K. Ensslin, Nano Lett. (2019)

## TUE 32

### Site-selectively generated photon emitters in monolayer MoS<sub>2</sub>

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We demonstrate the site-selective generation of optically active defect emitters in a monolayer MoS<sub>2</sub> van der Waals heterostructure [1]. Irradiation of monolayer MoS<sub>2</sub> on standard SiO<sub>2</sub>/Si substrates by helium ions manifests in spectrally broad (about 40 meV) defect emission [2]. Full encapsulation of the defective MoS<sub>2</sub> with hBN before irradiation reveals narrow spectral lines (about 1-6 meV) that are typically  $\Delta E = 100\text{-}220$  meV below the neutral 2D exciton [1]. Through several cool-down cycles, the emission energy distribution can be reduced, while the emitters stay active at the treated sites [3]. Our results pave the way towards scalable single optically active defects with high spectral homogeneity and nanometer spatial positioning in two-dimensional semiconductors.

- [1] J. Klein et al., Nature Comm. 10, 2755 (2019)
- [2] J. Klein et al., 2D Mater. 5, 1 (2017)
- [3] K. Barthelmi et al., in preparation (2020)

## TUE 33

### Non-catalytic Epitaxial Growth of Hexagonal Boron Nitride Single-crystals on Graphite

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Graphene has been considered as promising materials due to excellent proper-

ties. However, the properties of graphene are degraded by environment. h-BN has been used as a protective material to achieve ideal properties. Graphene encapsulated by h-BN showed higher mobility than on Si/SiO<sub>2</sub>. Most works on the properties of graphene on h-BN used exfoliation, which is uncontrollable. Another way is transferring of CVD-grown graphene and h-BN, but the transfer leads to impurities. Controlled and impurity-free methods are highly desired. In this work, we perform non-catalytic growth of h-BN on graphite from NH<sub>3</sub>BH<sub>3</sub> by chemical vapor deposition. The uniformity of the alignment of h-BN confirmed that h-BN was epitaxially grown. The characterization by Raman, XPS, and AES confirmed high quality. Nucleation density was tuned by hydrogen pressure and baking condition to remove tape residue. With optimized condition, the largest size of single-crystals reached 1  $\mu$ m. We also show that the insight obtained in two-dimensional growth can be applied to the growth of single-walled carbon nanotubes encapsulated by boron nitride nanotubes, which is recently reported new class of material.

## TUE 34

### In-plane magnetic coupling in in MoS<sub>2</sub>/Graphene/Co interface

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A two-dimensional crystal of molybdenum disulfide (MoS<sub>2</sub>) monolayer is a direct gap semiconductor. Due to the strong spin-orbit coupling and symmetry breaking it has two fully out of plane spin polarized valley on the top of valence band in K and K' points in the Brillouin zone. This makes MoS<sub>2</sub> monolayer a very promising for spintronics[1]. Here we propose MBE growth of MoS<sub>2</sub> monolayer on graphene/Co interface.

Via XPS and LEED techniques we prove that we indeed have a quasi freestanding orientated monolayer of MoS<sub>2</sub>, using ARPES we show its valence band electronic structure and finally Spin resolved ARPES provides the prove that in-plane magnetic field induced in Co thin film modifies in-plane spin structure of MoS<sub>2</sub> in Gamma and K points.

The fact that MoS<sub>2</sub> in this system is freestanding is fascinating because such MoS<sub>2</sub> system can be used in optical devices [2] (MoS<sub>2</sub> on metal substrates can't be used for such purpose because any excited states would relax through the metal substrate). By this work we show the opportunity to magnetically control MoS<sub>2</sub> spin structure and thereby its optical properties.

[1] Cao et al., 10.1038/ncomms(2018)

[2] N. Ehlen et al 2019 2D Mater. 6 011006

**TUE 35****Measurement of spin – orbit interaction strength in bilayer graphene/TMD heterostructures**

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To study the short-range van der Waals proximity effects in graphene based devices the bilayer graphene is ideal as by applying perpendicular electric displacement field (D) it will become a layer polarized insulator and the electronic states in it are strongly localized [1].

Here we investigate bilayer Graphene/WSe<sub>2</sub> heterostructures encapsulated in hBN. In such devices the WSe<sub>2</sub> enhance layer selectively the spin–orbit coupling (SOC) in graphene with proximity effect which was shown with weak antilocalization measurements [2] and spin valve measurements [3]. To study the SOC quantitatively quantum hall effect (QHE) measurements offers a novel way [4,5]. We have studied the QHE at different fixed magnetic fields as a function of D and n, using dual gated devices. We observed Landau level crossings at different D from which the SOC parameters can be extracted.

[1] McCann et al. Rep. Prog. Phys. 76, 056503 (2013)

[2] Wang et al. Phys. Rev. X 6, 041020 (2016)

[3] Avsar, A. et al. Nat Commun 5, 4875 (2014)

[4] Levitov et al. Phys. Rev. B 98, 115307 (2018)

[5] Island, J.O et al. Nature 571, 85–89 (2019)

**TUE 36****Hysteresis free carbon nanotubes transistors embedded in boron nitride / polytetrafluorethylene heterolayers**

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Carbon nanotube field effect transistors fabricated on silicon wafers with thermal oxide often suffer from large gate voltage hysteresis, induced by charge trapping sites in SiO<sub>2</sub>, surface OH-groups, and the presence of water molecules. Surface functionalization and passivation, vacuum annealing and reduced operating tem-

perature have shown to diminish or even eliminate hysteresis. In this work we demonstrate fabrication of hysteresis-free transistors on Si/SiO<sub>2</sub> by embedding carbon nanotubes and the connecting electrodes in a hexagonal boron nitride (hBN) bottom layer and a polytetrafluorethylene (PTFE) top layer. We discuss the conditions at which catalyst-free synthesis of hBN on SiO<sub>2</sub>/Si with Borazine is obtained, and the subsequent liquid phase deposition of PTFE. Device transfer curves were measured before and after PTFE deposition. We find that the hysteresis is reduced after PTFE deposition, but disappears completely only after a waiting period of several days. Simultaneously the on state current increases with time. The results give evidence for the absence of trap states in hBN/PTFE heterolayers and a high break through field strength in those wafer scalable materials.

## TUE 37

### Twistronics in van der Waals Material Heterostructures: from Spin-Orbit Coupling to Superconductivity

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We study spin-orbit coupling (SOC) in bilayer graphene/few-layer WSe<sub>2</sub> heterostructure devices. In our high mobility devices, we measure the quantum Hall effect versus doping and perpendicular displacement field. The Landau level (LL) crossing points and measured inter-LL gaps yield both the Ising and Rashba spin orbit coupling. We find the Ising SOC  $\approx 2.2$  meV, while the Rashba SOC is  $\approx 15$  meV. The observed sign of the Ising SOC is consistent with theory predicting a dependence of the SOC on twist angle.

Moreover, we will discuss recent measurements of twisted bilayer graphene (tBLG), on a device with a twist angle of  $0.93^\circ$ , below the magic angle. We find in addition to Mott-like insulator and superconducting states near half filling, evidence for a novel correlated state at five electrons/moiré unit cell. Our results reveal that the magic range of tBLG is in fact larger than what is previously expected, and provide a wealth of new information to help decipher the strongly correlated phenomena observed in tBLG.

**TUE 38****Ethanol Sensing with Surface-Mounted Metal-Organic-Framework Functionalized Graphene Transistors**

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Surface-mounted metal-organic frameworks (SURMOFs) are crystalline nanoporous layers constituting of metal cation nodes and organic linker molecules, providing precisely controlled nano-environments for various applications. [1] The affinity of the host framework towards specific guest molecules can be tailored by selecting the appropriate SURMOF building blocks. In this work we followed the idea of combining a graphene field effect transistor (GFET) sensitive to environmental changes, with a SURMOF which provides the required selectivity for sensing applications. We have grown Cu (BDC) SURMOF-2 (BDC = Benzene-1,4-dicarboxylate) on top of CVD-graphene on Si/SiO<sub>2</sub>(300nm) based on liquid phase epitaxy process. The SGFET devices show shifts in the Dirac voltage under exposure to ethanol molecules but remain insensitive against other gases (H<sub>2</sub>O, CO<sub>2</sub> etc.) and alcohols (IPA, methanol). The response times of the SGFETs are on the order of tens of seconds and resetting occurs at similar timescales by current annealing. Simulations are undergoing to reproduce the experimental observations.

[1] L. Heinke and C. Wöll, Adv. Mater. (2019), 31, 1806324.

**TUE 39****Graphene nanoribbons from sulfur-containing precursors**

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Sulfur-containing compounds have been used for graphene nanoribbon production [1,2]. Here, we study the nanoribbon formation process from tetrathiotetracene, and sexithiophene encapsulated in the inner cavity of single-walled carbon nanotubes. For the encapsulation, we use vapour-phase [2] and supercritical carbon dioxide. With the latter technique, we can perform low-temperature encapsulation, avoiding the polymerisation of the molecules on the outside part of the tube. Afterwards, using the appropriate solvents, we washed out the molecules from the outer walls of

the carbon nanotubes. Samples prepared at various annealing temperatures were analysed by Raman spectroscopy with various excitation energy lasers. We show a comparison between the filling methods and the annealing temperature, observing how the polymerisation proceeds, from the dimers to the nanoribbons.

- [1] A. Chuvilin, E. Bichoutskaia, M. C.Gimenez-Lopez, T. W. Chamberlain, G. A. Rance, N. Kuganathan, and A. N. Khlobystov, *Nature Materials*, 10, 687, (2011)
- [2] M. Kalbáč, L. Kavan, S. Gorantla, T. Gemming, and L. Dunsch, *Chemistry-A European Journal*, 16, 11753, (2010)

## **TUE 40**

### **Yu-Shiba-Rusinov states in a break junction**

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A magnetic field is known to suppress superconductivity by pair breaking. A single localized spin in a superconductor in a similar manner results in Yu-Shiba-Rusinov subgap states by this same pair breaking effect. Here we present an experimental finding of Yu-Shiba-Rusinov states in electromigrated Au break junctions with proximity induced superconductivity induced by a layer of NbTiN. By tuning the local back-gate voltage at the junction, signatures of a quantum dot in the form of Coulomb blockade and a charge resonance were found. When the quantum dot is tuned to be resonant with the electrodes, subgap peaks appear in the differential conductance that disperse with gate voltage. Theoretical modelling of the Yu-Shiba-Rusinov states using the zero bandwidth limit of the single impurity Anderson model have been performed. Efforts are under way to extend the zero bandwidth limit approach and to study Yu-Shiba-Rusinov states in graphene nanoribbons.

## **TUE 41**

### **Crested two-dimensional transistors**

Tao Liu<sup>1</sup>

<sup>1</sup>Chemistry, National University of Singapore, Singapore

Two-dimensional transition metal dichalcogenides (TMD), albeit promising candidates for applications in electronics and optoelectronics, are still limited by their low electrical mobility under ambient conditions. Here we report a large increase in the performance of TMD field-effect transistors operating under ambient conditions, achieved by engineering the substrate's surface morphology. For MoS<sub>2</sub> transistors fabricated on crested substrates, we observed an almost two orders of magnitude increase in carrier mobility compared to standard devices, as well as very high saturation currents. With comprehensive investigation of different dielectric environments and morphologies, we demonstrate that the substrate's increased corrugation, with its resulting strain field, is the dominant factor driving performance enhancement. This strategy is universally valid for both p-doped and n-doped semiconducting TMD



materials, opening them up for applications in heterogeneous integrated electronics. We also show that the mechanical strain can effectively alter the magneto-transport properties of  $\text{MoS}_2$  at low temperature.

## TUE 42

### Platinum Diselenide - accessing semiconducting properties and its superior sensing abilities via LPE

Beata M. Szydłowska<sup>1,2</sup>, Key Lee<sup>2</sup>, Bartłomiej Tywoniuk<sup>2</sup>, Niall McEvoy<sup>4</sup>, Zdenek Sofer<sup>3</sup>, Georg S. Duesberg<sup>2</sup>, Claudia Backes<sup>1</sup>

<sup>1</sup>Physical Chemistry, Heidelberg Universität, Heidelberg, Germany

<sup>2</sup>Institute of Physics, EIT 2, Universität der Bundeswehr München, München, Germany

<sup>3</sup>Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

<sup>4</sup>School of Chemistry and CRANN, Trinity College Dublin, Dublin, Ireland

Platinum diselenide ( $\text{PtSe}_2$ ), a recent member of TMDC group 10, according to DFT undergo a transition from semi-metal to semi-conductor as gets thinned down to monolayer. It is expected to exhibit bandgap of 1.2 eV, 0.21 eV and no bandgap for mono-, bi-, and tri- layer/bulk respectively. By now only few efforts were taken by the community in order to access predicted monolayer semiconducting properties and due to the structure resulting in extremely strong interlayer bonding, only a fewlayer  $\text{PtSe}_2$  were reported to be so far isolated. Here for the first time, we report successful isolation of bi- and mono-layered  $\text{PtSe}_2$  sheets via Liquid Exfoliation method both in the water and solvent environment. Nanosheets of a different number of layers were extensively characterised by microscopic and spectroscopic techniques revealing the extremely high quality of LPE  $\text{PtSe}_2$  while compared to TAC or CVD and other methods what is reflected for instance in much narrower Raman  $\text{Eg1}$  and  $\text{A1g}$  modes. Moreover,  $\text{PtSe}_2$  poses exceptional ambient conditions stability and based on first tests exhibits outstanding enhanced sensitivity and very short recovery times making it perfect gas sensing material.

## TUE 43

### Raman spectroscopy of chemically functionalized $\text{MoS}_2$

Narine Moses Badlyan<sup>1</sup>, Nina Pettinger<sup>1</sup>, Xin Chen<sup>2</sup>, Wanzheng Zhang<sup>2</sup>, Kathrin Knirsch<sup>2</sup>, Andreas Hirsch<sup>2</sup>, Janina Maultzsch<sup>1</sup>

<sup>1</sup>Lehrstuhl für Experimentalphysik, FAU Erlangen-Nürnberg, Erlangen, Germany

<sup>2</sup>Lehrstuhl für Organische Chemie II, FAU Erlangen-Nürnberg, Erlangen, Germany

2D materials, such as molybdenum disulfide ( $\text{MoS}_2$ ), qualify as candidates for novel applications in various fields, including electronics and flexible optoelectronics. The electronic and optical properties of chemically and mechanically exfoliated  $\text{MoS}_2$  can be further tuned by covalent or non-covalent functionalization.

Here, we present a spectroscopic study of functionalized  $\text{MoS}_2$  flakes. They are

prepared by mechanical exfoliation from MoS<sub>2</sub> crystals and by chemical exfoliation from MoS<sub>2</sub> powder and are subsequently covalently functionalized with various organic molecules. We discuss the temperature dependence of the Raman spectra of the functionalized MoS<sub>2</sub> powder samples. Furthermore, we show for multilayer chemically functionalized MoS<sub>2</sub> flakes evidence for a transition to the 1T' phase.



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FT-IR

- 08:30 – 09:30 **TUTORIAL: M. Glazov, St. Petersburg**  
*Classical and quantum transport of excitons in atom-thin semiconductors*
- 09:30 – 10:00 **E. Malic, Gothenburg**  
*Spatiotemporal exciton dynamics in atomically thin 2D materials*
- 10:00 – 10:30 **Coffee Break**
- 10:30 – 11:00 **R. Gillen, Erlangen**  
*Interlayer interactions and the electronic and optical properties of 2D multilayer materials*
- 11:00 – 11:30 **T. Sohler, Lausanne**  
*Phonon-limited transport in 2D materials*
- 11:30 – 12:00 **I. Iorsh, St. Petersburg**  
*Nonlinear polaritons in monolayer semiconductor coupled to optical bound states in the continuum*
- 12:00 – 17:00 **Mini Workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **T. Shegai, Göteborg**  
*Anisotropy controls phonon thermalization in photoexcited black phosphorus*
- 19:00 – 19:30 **P. Kusch, Berlin**  
*Studying Exciton Polaritons in van der Waals Materials*
- 19:30 – 20:00 **D. Bandurin, Cambridge**  
*Interaction-dominated transport in graphene: old mysteries and new regimes*
- 20:00 **Poster Session IV**



**08:30**

**Classical and quantum transport of excitons in atom-thin semiconductors**

Mikhail Glazov<sup>1</sup>

<sup>1</sup>Sector of Quantum Coherent Phenomena, Ioffe Physical-Technical Institute of the RAS, St. Petersburg

We present the theory of the exciton transport phenomena in atom-thin semiconductors based on the transition metal dichalcogenides. We highlight novel aspects resulting from the reduced dimensionality and enhanced coupling of excitons with phonons, on the one hand, and from the multivalley bandstructure of the monolayers. We demonstrate that non-equilibrium phonons can drag excitons resulting in the enhancement of their diffusion and halo formation. We also show that the strong exciton-acoustic phonon scattering leads to significant quantum corrections to the exciton diffusion coefficient. Finally, we address the spin transport of excitons and exciton valley-Hall effect in transition metal dichalcogenide monolayers.

The work is partially supported by the RSF project # 19-12-00051.

**09:30****Spatiotemporal exciton dynamics in atomically thin 2D materials**Ermin Malic<sup>1</sup><sup>1</sup>Chalmers University of Technology, Gothenburg, Sweden

Monolayer transition metal dichalcogenides (TMDs) exhibit a remarkable excitonic landscape including bright exciton states, but also a variety of momentum- and spin-dark excitons. Solving 2D material Bloch equations for excitons, phonons and photons, we obtain a microscopic access to the spatiotemporal dynamics in TMDs. In particular, we shed light on the interplay of optics, ultrafast dynamics and diffusion processes of excitons. In joint theory-experiment studies, we reveal formation, thermalization, and photoemission of bright and dark intra- and interlayer excitons in TMD monolayers and related van der Waals heterostructures. We show pronounced low-temperature signatures of momentum-dark excitons in PL spectra. Finally, we demonstrate exciton propagation and formation of spatial exciton rings (halos) due to the emission of hot phonons giving rise to strong spatial temperature gradients and additional thermal drifts. The gained microscopic insights into the spatiotemporal exciton dynamics are crucial for understanding, predicting, and controlling exciton optics, dynamics and transport in the technologically promising 2D materials.

**10:30****Interlayer interactions and the electronic and optical properties of 2D multilayer materials**Roland Gillen<sup>1</sup>, Janina Maultzsch<sup>1</sup><sup>1</sup>FAU Erlangen

Despite largely non-covalent interlayer interactions, the electronic and optical properties of stacked homo- and hetero-multilayers of 2D materials can show an interesting variation with the twist angle due to differences in the crystal potential and symmetry breaking. In principle, this offers the possibility of a tailoring of the physical properties of interest of composite materials through variation of the relative alignment of the constituting materials. In this talk, I will explore the effect of stacking order for two bilayer materials: For MoSe<sub>2</sub>/WSe<sub>2</sub> heterobilayers, the local stacking order leads to small variations in the hybridization between the MoSe<sub>2</sub> and WSe<sub>2</sub> bands and has a decisive effect on the polarization dependence of the momentum-direct interlayer excitonic absorption, while the interlayer exciton binding energies are only weakly affected [1]. For stacked homo-bilayers of Antimonene, I will show that the interlayer interaction has a significant covalent contribution [2]. The residual bonding effects result in a closing of the indirect electronic band gap for AB stacking and small twist angles, which can be lifted for larger twist angles.

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

[2] Gibaja et al., Angewandte Chemie Int. Ed. 55, 14345 (2016)



**11:00****Phonon-limited transport in 2D materials**Thibault Sohler<sup>1,2</sup>, Marco Gibertini<sup>2</sup>, Davide Campi<sup>2</sup>, Nicola Marzari<sup>2</sup><sup>1</sup>Nanomat/QMAT/CESAM, Université de Liège, Belgium<sup>2</sup>THEOS and MARVEL, École Polytechnique Fédérale de Lausanne, Switzerland

Recently, some of us identified close to 2000 exfoliable 2D materials from first-principles calculations. We are now characterizing the scattering of electrons by phonons in this database, with the objective of finding electrostatically-doped 2D semiconductors with superior intrinsic transport properties.

This work relies on three developments: i) density functional perturbation theory to compute electron-phonon interactions with 2D periodic boundary conditions and gates to induce doping; ii) a high-accuracy workflow to compute phonon-limited mobilities automatically; iii) a more approximate workflow to estimate transport performances at reduced cost.

The approximate workflow scans hundreds of materials and screens outstanding new candidates. The high-accuracy workflow is then used on around 50 selected materials. Several novel high-conductivity 2D materials are found. The data provides valuable insights on electron-phonon scattering in 2D. I will discuss pathways to find or engineer high-conductivity 2D materials by identifying some influential aspects of phonon limited-transport such as intervalley scattering, screening, and band anisotropy.

**11:30**

**Nonlinear polaritons in monolayer semiconductor coupled to optical bound states in the continuum**

Ivan Iorsh<sup>1</sup>

<sup>1</sup>NRU ITMO, St. Petersburg

The talk is dedicated to the recent experimental results on the effects of strong light-matter coupling in the systems comprising a TMD monolayer covering periodic photonic nanostructures. The latter support sharp optical resonances called optical bound states in the continuum (BIC). These resonant states acquire large quality factors not due to the confinement by the cavity mirrors (as in conventional microcavities) and not due to the total internal reflection (as for the waveguide geometries) but rather due to the destructive interference of the outgoing far field radiation. These modes thus could be beneficial for the realization of strong light-matter coupling with TMD excitons, where the deposition of the upper mirror is usually a technologically challenging process and waveguide geometries suffer from the difficulties with the external excitation of these states. We have fabricated these structures and demonstrated enhanced nonlinear optical response.

**18:30****Anisotropy controls phonon thermalization in photoexcited black phosphorus**Timur Shegai<sup>1</sup>,<sup>1</sup>Physics, Chalmers University of Technology, Göteborg

In this talk, I will show that exciton-plasmon interactions between mono- and multi-layer TMDCs and individual plasmonic nanoantennas can reach the level of strong coupling, also known as vacuum Rabi splitting [1]. Specifically, I will discuss the formation of hybrid exciton-trion-plasmon polaritons in monolayer WS<sub>2</sub> – silver nano-prism system [2], spatially confined strong exciton-plasmon interaction between mono- and multilayer WSe<sub>2</sub> and gold bipyramids [3], as well as hierarchical micro-cavity-plasmon-exciton polaritons encompassing monolayer WS<sub>2</sub>, arrays of gold nanodisks and Fabry-Pérot microcavity [4]. I will also discuss our recent progress on self-hybridization in all-TMDC multilayer material platforms, which we believe will give birth to high-index TMDC nanophotonics [5, 6].

- [1] Baranov, D.G., et al. ACS Photonics, 2017, 5, 24.
- [2] Cuadra, J., et al. Nano Lett., 2018, 18, 1777.
- [3] Stührenberg, M., et al. Nano Letters, 2018, 18, 5938-5945.
- [4] Bisht, A., et al. Nano Letters, 2019, 19, 189-196.
- [5] Munkhbat, B., et al., ACS Photonics, 2019, 6, 139-147.
- [6] Verre, R., et al., Nature Nanotechnology, 2019, 14, 679.

**19:00****Studying Exciton Polaritons in van der Waals Materials**Patryk Kusch<sup>1</sup>, Sebastian Heeg<sup>1</sup>, Kirill Bolotin<sup>1</sup>, Stephanie Reich<sup>1</sup><sup>1</sup>Freie Universität Berlin - Institut für Experimentalphysik, Berlin, Germany

Polaritons in van der Waals materials promise new application in quantum technologies and nanophotonic circuits that operate in the terahertz to mid-infrared spectral region. Examples include plasmon polaritons in graphene and hyperbolic phonon polaritons in hBN. We will present near-field microscopy and spectroscopy of exciton polaritons (EPs) excited in transition metal dichalcogenides (TMDs). EPs in TMDs are formed due to the coupling between waveguide photons and excitons and exhibit a long propagation length together with a wavelength only of few hundred nanometers. By nanoimaging propagating EPs in MoS<sub>2</sub> and WSe<sub>2</sub>, we investigated their real space characteristics and get access to their dispersion relation allowing to determine the light-matter coupling strength. Finally, we will show waveguiding in a free-standing monolayer of WSe<sub>2</sub> and demonstrate interlayer excitons, excited in a TMD heterostructure build up of MoS<sub>2</sub> and WS<sub>2</sub>.

**19:30****Interaction-dominated transport in graphene: old mysteries and new regimes**Denis Bandurin<sup>1</sup><sup>1</sup>MIT, Cambridge

Electron–electron (e–e) collisions can impact transport in a variety of surprising and sometimes counterintuitive ways. Despite the long-time interest, experiments on the subject proved challenging because of the presence of momentum-relaxing scattering sources. Only recently, sufficiently clean electron systems in which transport dominated by momentum-conserving e–e collisions have become available, enabling the study of electron transport governed by interactions.

We will begin by discussing interaction-dominated transport in monolayer graphene. I will show that at elevated temperatures, the behavior of graphene's electron fluid resembles that of classical liquids with high viscosity. I will discuss approaches that can be used to probe the transport governed by e–e interactions and talk about the viscous Hall effect.

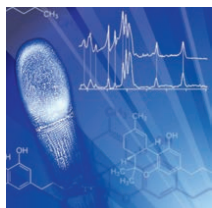
A very different behavior is found in twisted bilayer graphene (TBG). I will show that, unlike in monolayer, e–e collisions in TBG can lead to the relaxation of electrical current and result in the quadratic temperature dependence of its resistivity. This surprising behavior cannot be accounted for by existing scenarios and calls for alternative explanations.





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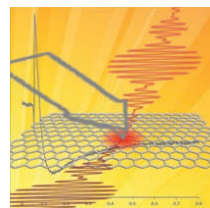
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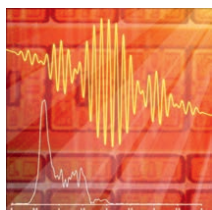
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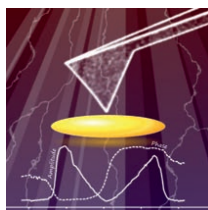
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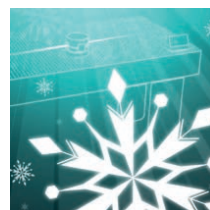
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- 08:30 – 09:00 K. Ensslin, Zurich  
*Gap Opening in Twisted Double Bilayer Graphene by Crystal fields*
- 09:00 – 09:30 R. Gorbachev, Manchester  
*Controlling optoelectronic properties of 2D semiconductors: band engineering and moiré superlattices*
- 09:30 – 10:00 L. C. Campos, Belo Horizonte  
*Topological valley transport in a folded bilayer graphene*
- 10:00 – 10:30 Coffee Break
- 10:30 – 11:00 F. Libisch, Vienna  
*The optical response of transition metal dichalcogenides*
- 11:00 – 11:30 R. Danneau, Karlsruhe  
*Conductance quantization, supercurrent and multiple Andreev reflection in bilayer graphene quantum point-contacts*
- 11:30 – 12:00 C. Schönenberger, Basel  
*Strain-engineered graphene and one-dimensional edge states in few-layer WTe<sub>2</sub>*
- 12:00 – 17:00 Mini Workshops
- 17:00 – 18:30 Dinner
- 18:30 – 19:00 D. Akinwande, Austin  
*Atomristor: 2D Memory and Applications*
- 19:00 – 19:30 G. S. Duesberg, Munich  
*Inorganic – organic monolayer stacks*
- 19:30 – 20:00 R. Boya, Manchester  
*Ångstrom-scale Capillaries: A Platform for investigating Confined flow*
- 20:00 Poster Session III





**08:30****Gap Opening in Twisted Double Bilayer Graphene by Crystal fields**Klaus Ensslin<sup>1</sup><sup>1</sup>Physics, ETH Zurich, Zurich

Crystal fields (CFs) occur due to a potential difference between chemically different atomic species. Here we show that the bandstructure of large-angle twisted double bilayer graphene (TDBG) is strongly modified by CFs. In particular, we experimentally demonstrate that TDBG, encapsulated between hBN layers, exhibits an intrinsic bandgap. By the application of an external field, the gaps in the individual bilayers can be closed, allowing to determine the CFs. We find that CFs point from the inner to the outer layers with strengths in the bottom/top bilayer  $E_b = 0.13\text{V/nm} \approx -E_t = 0.12\text{ V/nm}$ . We show both by means of first principles calculations and low energy models that CFs open a band gap in the groundstate.

This work was done in collaboration with Peter Rickhaus, Fokko de Fries, Giulia Zheng, Jose L. Lado, Yongjin Lee, Annika Kurzmann, Marius Eich, Riccardo Pisoni, Chuyao Tong, Rebekka Garreis, Carolin Gold, Michele Masseroni, Takashi Tamaguchi, Kenji Wantanabe, and Thomas Ihn.

**09:00****Controlling optoelectronic properties of 2D semiconductors: band engineering and moiré superlattices.**Roman Gorbachev<sup>1</sup><sup>1</sup>School of Physics and Astronomy, University of Manchester, Manchester

In this talk I will review our recent progress working with semiconducting 2D materials. I will start with discussing InSe, 2D material with high electronic quality and interesting optoelectronic properties. When placed on graphene, its valence band hybridize with graphene bands producing avoided crossing. This effect occurs in the second Brillouin zone of InSe, however ghost replicas of anti-crossing appear in the first zone through Umklapp reflection. Following this, I will discuss how direct optical transitions can be engineered by combining indirect materials, such as few-layer TMDs with InSe. Lastly, I will report our latest work on twisted TMDs, describing atomic reconstruction with TEM. For 3R stacking, a pattern of mirror reflected triangular 3R domains merges, featuring layer-polarized conduction band states caused by lack of both inversion and mirror symmetries. In contrast, for 2H stacking, stable 2H domains dominate, with nuclei of a second metastable phase. This appears as a kagome-like pattern at  $\theta \sim 1^\circ$ , transitioning at  $\rightarrow 0^\circ$  to a hexagonal array of large 2H domains. Tunnelling measurements show that such reconstruction creates strong piezoelectric textures.

**09:30****Topological valley transport in a folded bilayer graphene**E. Mania<sup>1</sup>, A. R. Cadore<sup>1</sup>, T. Taniguchi<sup>2</sup>, K. Watanabe<sup>2</sup>, L. C. Campos<sup>1</sup><sup>1</sup>Physics Department, Federal University of Minas Gerais, Belo Horizonte, Minas Gerais, Brazil<sup>2</sup>National Institute for Materials Science, Namiki 305-0044, Japan

The development of valleytronics demands long-range electronic transport with preserved valley index. A promising structure for this end is a topological 1D channel, called a domain wall, where valley-index defines the propagation direction of the charge carriers and the chiral edge states are robust over many kinds of disorder. Here, we present high-quality domain wall formed at the curved boundary of a folded bilayer graphene. Our experiments reveal long-range ballistic transport at such topological channels with the two-terminal resistance close to the ballistic resistance  $R = e^2/4h$  at zero-magnetic field and the four-terminal resistance near to zero. Investigating temperature dependence, we show that folded bilayer graphene regions (Bulk) preserve semi-conducting properties enabling quantum confinement of the one-dimensional edge states. On the other hand, the ballistic edge states show a monotonic increase of resistance with temperature. Such work presents robust ballistic transport at one-dimensional channels of bilayer graphene with strong potential for application on valleytronics.

Work supported by INCT in Carbon Nanomaterials, Fapemig, CAPES and CNPq

**10:30****The optical response of transition metal dichalcogenides**Florian Libisch<sup>1</sup><sup>1</sup>Institute for Theoretical Physics, Vienna University of Technology, Vienna

The optical response of monolayer transition metal dichalcogenides (TMDs) offers a wide range of intriguing properties, such as sharp lines in photoluminescence spectra that serve as single photon emitters, or highly sensitive second-order harmonic generation. I review our recent contributions to uncover the associated microscopic processes. To model single-photon emitters, we employ a multiscale tight-binding simulation for the optical spectra of WSe<sub>2</sub> under non-uniform strain and in the presence of point defects [1]. Strain locally shifts excitonic energy levels into the band gap where they hybridize with localized intragap defect states. We identify inter-valley defect excitonic states as the likely candidates for antibunched single-photon emission. We also calculate the second-order harmonic response of various TMDs and find excellent agreement to recent measurements [2]. We demonstrate and explain a surprisingly high sensitivity to small changes in the band structure, providing a way to sensitively probe strain in semiconducting TMDs.

[1] L. Linhart et al., PRL 123, 146401 (2019).

[2] L. Mennel et al., Nature Comm. 9, 516 (2018).

**11:00****Conductance quantization, supercurrent and multiple Andreev reflection in bilayer graphene quantum pointcontacts**Romain Danneau<sup>1</sup><sup>1</sup>Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany

By using local displacement fields in bilayer graphene (BLG), it is possible to electrostatically confine charge carriers. Connecting superconducting leads to a graphene nanostructure allows to induce high ballistic supercurrent. We demonstrate that it is possible to fully gate-control both amplitude and density profile of the supercurrent, making BLG a highly tunable superconducting weak link [1]. Adding an additional overall top gate, one better controls the 1D constriction and observes four fold degenerate quantized conductance down to full pinch-off [2]. We show that this ballistic effect is also reflected in the supercurrent and in the multiple Andreev reflection as the number of discrete channels is reduced [3].

[1] R. Kraft, J. Mohrmann, R. Du, P.B. Selvasundaram, M. Irfan, U.N. Kanilmaz, F. Wu, D. Beckmann, H.v. Löhneysen, R. Krupke, A. Akhmerov, I. Gornyi and R. Danneau. Nat. Commun. 9, 1722 (2018).

[2] R. Kraft, I.V. Krainov, V. Gall, A.P. Dimitriev, R. Krupke, I.V. Gornyi and R. Danneau. Phys. Rev. Lett. 121, 257703 (2018).

[3] R. Kraft, R. Mélin, R. Krupke, B. Douçot and R. Danneau. Unpublished.

**11:30****Strain-engineered graphene and one-dimensional edge states in few-layer WTe<sub>2</sub>**

Lujun Wang<sup>1,7</sup>, Artem Kononov<sup>1,5</sup>, Andreas Baumgartner<sup>1,7</sup>, Gulibusitan Abulizi<sup>1</sup>, David Indolese<sup>1</sup>, Peter Makk<sup>1,2</sup>, Kejin Qu<sup>3</sup>, Jiaqiang Yan<sup>3,6</sup>, David Mandrus<sup>3,6</sup>, Kenji Watanabe<sup>4,6</sup>, Takashi Taniguchi<sup>4</sup>, Simon Zihlmann<sup>1</sup>, Christian Schönenberger<sup>1,7</sup>

<sup>1</sup>Department of Physics, University of Basel, Basel Switzerland

<sup>2</sup>Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary

<sup>3</sup>Department of Materials Science and Engineering, University of Tennessee, Knoxville, USA

<sup>4</sup>National Institute for Material Science, Tsukuba, Japan

<sup>5</sup>Institute of Solid State Physics of the Russian Academy of Sciences - Chernogolovka, Russia

<sup>6</sup>Department of Material Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, USA

<sup>7</sup>Swiss Nanoscience Institute, University of Basel, Basel, Switzerland

We introduce a new technique and sample design to engineer strain in h-BN encapsulated graphene, avoiding valley mixing due to disorder. We show that strain and strain gradients can be deterministically generated. We then analyze the effect of strain on various transport phenomena, such as carrier mobility, conductance fluctuations, transverse magnetic focusing and Landau quantization, and critically discuss their origin based on both strain-induced scalar potential and pseudo-magnetic field. In the second part of the lecture, recent experiments on few-layer WTe<sub>2</sub> will be discussed. We show that Pd contacts induces superconductivity in few-layer WTe<sub>2</sub> crystals. We use this to engineer Josephson junctions and probe their critical current in magnetic field. We find 1D current carrying states on edges and steps in few-layer WTe<sub>2</sub>. The width of the states is deduced to be below 80 nm. The supercurrent in them is very robust and can be measured over distances up to 3  $\mu\text{m}$  and in perpendicular magnetic field up to 2 T.

We acknowledge support by the Georg H. Endress foundation, ERC project Top-Supra (787414), the Swiss Nanoscience Institute and the Swiss NSF.

**18:30**

**Atomristor: 2D Memory and Applications**

Deji Akinwande<sup>1</sup>

<sup>1</sup>Electrical and Computer Engineering, The University of Texas at Austin, US

This presentation focuses on the progress on 2D nanomaterials towards greater scientific understanding and advanced engineering applications. In particular the talk will highlight our pioneering work on monolayer memory (atomristors) that can enable various applications including zero-power devices, non-volatile RF switches, and memristors for neuromorphic computing. Non-volatile memory devices based on 2D materials are an application of defects and is a rapidly advancing field with rich physics that can be attributed to sulfur vacancies or metal diffusion. Areas with defects typically exhibit memory. It appears the memory effect is a 'universal' effect in monolayer non-conductors.



**19:00****Inorganic – organic monolayer stacks**

Georg S. Duesberg<sup>1,2</sup>, Rita Siris<sup>1</sup>, Laura Hoeltgen<sup>1</sup>, Kangho Lee<sup>1</sup>, John Mc Manus<sup>2</sup>,  
Conor Cullen<sup>2</sup>, Siwei Luo<sup>1</sup>, Kathrin Knirsch<sup>3</sup>, Andreas Hirsch<sup>3</sup>

<sup>1</sup>Institute of Physics, Universität der Bundeswehr München, Neubiberg, Germany

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Two-dimensional (2D) materials such as graphene and transition metal dichalcogenides (TMDs) are intensively studied because of their unique properties, such as thickness dependent band gaps and high carrier mobility. To harness those properties passivation and decoupling of the 2D layers have to be employed. For this, often very sophisticated techniques such as suspension or heterostack formation have to be realized. Furthermore, chemical functionalizations are highly sought to tune properties and to engineer defects of 2D materials. In this presentation, non-covalent, on-chip functionalization of chemical vapor deposition (CVD) grown monolayer 2D materials are presented. Perylene bisimide derivatives in organic or aqueous solution are used for self-assembly of monolayers (SAMs) on the 2D films. The formation of the stable, functional surfaces is selective to the monolayers, opening pathways for the creation of inorganic-organic heterostacks. Exemplarily we demonstrate the assembly of a MoS<sub>2</sub>-SAM-Graphene monolayer heterostructure. The presented films and heterostacks are comprehensively investigated by Raman spectroscopy, XPS, scanning probe techniques, and TOF-SIMS.

**19:30****Ångstrom-scale Capillaries: A Platform for investigating Confined flow**Radha Boya<sup>1</sup><sup>1</sup>Physics and Astronomy, The University of Manchester, Manchester

2D-materials are well known for their extraordinary properties and graphene is an archetypal example with most superlatives to its credit for the description of its properties, thinnest, strongest, most conducting, lightest etc. On the contrary, angstrom-scale capillary can be dubbed as “2D-nothing”; it is an antipode of graphene, created by focusing on what is left behind after extracting one-atomic layer out of a crystal. Angstrom-size capillaries are thus constructed out of 2D-materials, and we investigate properties of gas, liquids and ions confined in molecular scale. A core strand of the work that I will present is the development of Angstrom-capillaries as a platform to probe intriguing molecular-scale phenomena experimentally, including: water flow under extreme atomic-scale confinement, complete steric exclusion of ions, specular reflection and quantum effects in gas reflections off a surface. Previously such phenomena were only modelled by theoretical simulations and this is the first robust experimental platform with controlled angstrom-scale dimensions made from atomically smooth building blocks, alleviating the surface roughness which usually predominates at this scale.

**THU 1****Homogeneity of twisted bilayer graphene devices studied with STM**

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The homogeneity of the twist angle between the two layers of graphene is an important consideration for the validity of theoretic models describing MA-TBG. It is therefore essential to locally access and characterize how homogeneous this twist angle is. We employ STM to measure various twisted bilayer graphene devices with a range of nominal twist angles. The poster presents quantitative results of these measurements on different length scales.

**THU 2****Surface enhanced Raman spectroscopy of graphene on triangular silver nanoplates**

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Graphene covered metal nanoparticles is a novel type of hybrid material to study surface-enhanced Raman scattering (SERS) effects, and metal-graphene interactions. Such a hybrid nanostructure can be designed by transferring mechanically exfoliated graphene onto gold nanostructures on a silicon wafer [1]. An alternative method for such a system could be the deposition of mechanically exfoliated graphene on silver triangular nanoplates (Ag-TNPs) that show a strong localized surface plasmon resonance (LSPR) at their tips, tunable from the visible to the near-infrared spectrum depending mainly on their thickness, side and tip length [2]. Here we present a novel design of graphene deposited on Ag-TNPs on a transparent substrate. Our results show a dependence on the Raman response of graphene as a function of the location of the Ag-TNPs in the multilayer graphene lattice. We found a potential enhancement of the graphene Raman signal in the vicinity of the silver nanoparticles at the mono-layer site. Our findings open the possibility of using Ag-TNPs as a novel material to utilize its strong LSPR in graphene.

1. Nano Lett. 13(1), 301-308,(2012).

2. Nature Mat. 7, 442-453,(2008).

**THU 3****Two-dimensional  $\text{Ti}_3\text{C}_2\text{T}_x$  and DNA: a unique biointerface that can sense single mutations**C. Lorena Manzanares<sup>1</sup>, Martin Pumera<sup>1</sup><sup>1</sup>Center for Advanced Functional Nanorobots, Department of Inorganic Chemistry, University of Chemistry and Technology Prague

Discovered in 2011 as electrode materials for energy-related purposes, two-dimensional transition metal carbides (MXenes) have become attractive candidates for a wider spectrum of applications in recent years, including nanomedicine and sensors. The combination of their hydrophilic and active surface chemistry with their high surface area and broad absorption has attracted our interest in testing these materials as detection platforms for nucleic acids. We have evaluated the interaction between DNA oligonucleotides and MXene ( $\text{Ti}_3\text{C}_2\text{T}_x$ ) through monitoring the fluorescence of end-tethered 6-carboxyfluorescein (FAM) dye and by molecular dynamics simulations. Our findings reveal that MXenes possess selective response towards single-point mutations via a specific fluorescence kinetic behavior that differentiates a fully complementary strand from a single-point mutated strand. We hypothesize and elucidate the mechanisms behind such selective response by fluorescence spectroscopy and steady-state fluorescence anisotropy, as well as molecular dynamics simulations.

**THU 4****Optical properties of 2D metals and their influence on  $\text{WS}_2$** Katharina Nisi<sup>1</sup>, Margaux Lassaunière<sup>2</sup>, Shruti Subramanian<sup>3,4</sup>, Florian Sigger<sup>1</sup>, Hendrik Lambers<sup>2</sup>, David O. Tiede<sup>2</sup>, Joshua Robinson<sup>3,4</sup>, Ursula Wurstbauer<sup>2</sup><sup>1</sup>Physics Department, Walter Schottky Institute, Garching bei München, Germany<sup>2</sup>Institute of Physics, University of Münster, Münster, Germany<sup>3</sup>Department of Materials Science and Engineering, The Pennsylvania State University, USA<sup>4</sup>Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, USA

Two-dimensional metal films show distinctly different behavior compared to their three-dimensional cousins. Metals are no van der Waals materials, however 2D films can be prepared via confinement epitaxy by intercalating metals between epitaxial graphene and the hosting SiC crystal. Here, we explore the fascinating properties of 2D gallium, 2D indium and their alloys [1]. We are particularly interested in the dielectric properties and the light matter interaction of these novel 2D metals. We find resonances in the visible to near infrared regime that spectrally overlap with the excitonic interband transitions of semiconducting transition metal dichalcogenides (TMDCs). Hybrid structures of 2D metals and TMDCs are promising for enhancing and shaping their combined light matter interaction. We investigate the optical response of the 2D metal films as well as 2D metal-TMDC hybrid structure by a

combination of spectroscopic imaging ellipsometry, photoluminescence and Raman spectroscopy.

Work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – EXC 20891 – 390776260.

[1] B. Bersch et al. arXiv:1905.09938 (2019)

## THU 5

### **Property changes of atomically thin molybdenum disulphide by its environment**

Erik Pollmann<sup>1</sup>, Lukas Madau<sup>1</sup>, Tobias Foller<sup>1,2</sup>, Stephan Slezione<sup>1</sup>, Uttam Kumar<sup>1,2</sup>, Simon Schumacher<sup>1</sup>, Flemming Heuvel<sup>1</sup>, Christina vom Ende<sup>1</sup>, Marika Schleberger<sup>1</sup>

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Two-dimensional (2D) molybdenum disulphide (MoS<sub>2</sub>) is one of the novel materials, which is promising for next generation optoelectronic and spintronic devices. When measuring the properties of 2D materials, the properties of the 2D material are often determined under the influence of the environment to which the atomically thin materials are extremely sensitive. Therefore, there are two main challenges for industrial applications of 2D materials: (i) the large area homogeneous production of 2D materials, (ii) the control and maintenance of the physical properties.

In order to study optoelectronic and structural properties of the 2D material MoS<sub>2</sub> under typical environmental conditions (directly grown or exfoliated on dielectrics, on other van der Waals materials, or in contact to metals) we perform spectroscopy (e.g. Raman and photoluminescence spectroscopy) and scanning probe microscopy. We found i.a. that the difference between the exfoliated and chemical vapour deposited MoS<sub>2</sub> is much smaller than expected. Furthermore, MoS<sub>2</sub> undergoes an extremely strong change if in direct contact to a metal (here gold), apparent in an unusually strong change of its Raman spectrum.

## THU 6

### **Plasmons and thermoelectric properties of metal nanoparticles linked by conductive molecular bridges**

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It is analyzed plasmons and thermoelectric properties of systems consisting of small golden nanoparticles linked by narrow conductive molecular bridges, which are con-

sidered the conjugated polyacetylene molecule  $C_nH_n$ , terminated by sulfur atoms. Both properties are studied by an original hybrid model taking into account quantum effects. The model parameters are calculated using DFT and DFTB simulations. It is shown that in the dumbbell-like structures consisting of two metal nanoparticles connected by conductive polyacetylene molecule there are charge-transfer plasmons whose frequency lies in the IR region and strongly depends on the system geometry. During these plasmon vibrations, the charge flows through the conducting molecule, exhibiting quantum properties. It is argued this novel type of plasmons may be used in the area of chemical sensing.

Thermoelectric properties of periodic 1D systems consisting of nanoparticles connected by conducting bridges are also considered. The prospects of these properties of such systems depending on their geometry and composition are discussed.

This study was supported by the Russian Science Foundation, project no. 16-13-00060.

## THU 7

### **Superconductors and Correlated States in Magic Angle Twisted Bilayer Graphene**

Jaime Diez<sup>1</sup>

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Recently, it was discovered that a bilayer graphene with a twist angle of one sheet with respect to the other of around 1 degree leads to the emergence of ultra-flat moiré superlattice minibands. In such flat bands the group velocity tends to zero, leading to very high electron-electron interactions. Due to these interactions the material shows insulating states at certain band fillings and, more notably, when doping away from the insulating states superconductivity emerges. The fact that such an apparently “simple” system, as two graphene layers, allows to study the complex physics of highly correlated states such as Mott insulators, superconductivity, or even, magnetism and topology, makes it a very interesting system. Moreover, all these effects can be tuned by changing the carrier density of the material by using a gate electrode. In our group, fabrication techniques have been improved in order to get more homogeneous devices. The higher twist angle homogeneity leads to the appearance of superconducting domes at more band fillings than previously reported. On top of that, traces of possible orbital magnetism and some topological states are also seen.

## THU 8

### **Spin injection from BiTeBr with directional control over polarization**

Zoltán Kovács-Krausz<sup>1</sup>, Péter Makk<sup>1</sup>, Bálint Szentpéteri<sup>1</sup>, Anamul Md Hoque<sup>2</sup>, Bálint Fülöp<sup>1</sup>, Mátyás Kocsis<sup>1</sup>, Michael Yakushev<sup>3</sup>, Saroj Prasad Dash<sup>2</sup>, Szabolcs Csonka<sup>1</sup>

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The search for a reliable all-electric method of creating and manipulating spin polarization is one of the main goals of modern spintronics, leading to new practical applications where external magnetic fields are not needed. In the polar semiconductor BiTeBr, an electric field induced spin polarization can be achieved through the Rashba-Edelstein effect. By combining BiTeBr crystals with graphene that acts as a detector of spin current, we experimentally demonstrate the electrical generation of spins in BiTeBr. In addition, the ability to change the orientation of polarization is shown by using different contact geometries to alter the electric field orientation in BiTeBr. Detection of spins in graphene is achieved using ferromagnetic contacts, and the angle of spin polarization in BiTeBr is extracted using asymmetric Hanle spin precession, at room temperature. A tunneling model between BiTeBr and graphene is used to validate the consistency of observed polarization values with Rashba-Edelstein effect in BiTeBr.

#### THU 9

##### **Universal conductance and shot noise fluctuations in graphene**

Thomas Fabian<sup>1</sup>, Florian Libisch<sup>1</sup>

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The conductance in disordered quantum wires fluctuates with an universal value of the order of  $e^2/h$ , regardless of the size of the sample and the degree of disorder. Graphene samples show an unexpected increase of conductance fluctuations explained by the additional presence of valley symmetry.

We simulate conductance and shot noise fluctuations in graphene at energies away from the Dirac point. In a strongly disordered sample with broken valley symmetry we recover the universal value of a disordered wire. The conductance fluctuations increase when short-range scatterers are removed and only the long-range part of the potential is kept, highlighting their sensitivity to valley symmetry. Conductance fluctuations as a function of energy show a broad plateau at the predicted value. The level spacing statistics of both systems show the Gaussian-orthogonal universality class. In the presence of a magnetic field, the systems transitions into the Gaussian-unitary universality class and the conductance fluctuations decrease. We find a similar behavior for shot noise fluctuations, suggesting valley symmetry dependence of universal values also in this case.

#### THU 10

##### **Observation of 2D Noble Gas Crystals in Few Layer Graphene Encapsulation**

Manuel Längle<sup>1</sup>

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Graphene in its multi-layer forms has in the recent years been utilized as a 2D petri

dish to study the chemistry of materials in the transmission electron microscope (TEM). Here, we have used atomically resolved scanning TEM to study the effects of low energy ( $< 1$  keV) and high dose ( $> 10^{15}$  ions / cm<sup>2</sup>) ion irradiation in few-layer graphene.

Experiments have shown that implantation of noble gas atoms between a graphene layer and a metal is possible. Our observations show that ions with a suitable energy can pass through the first graphene sheets and become trapped in a sandwich-like configuration. In the presence of graphene encapsulation, these otherwise inert atoms form two-dimensional noble gas crystals with a remarkable stability under the 60 keV electron irradiation inside the microscope vacuum, and even individual atoms can thus be resolved.

## THU 11

### **The interplay of insulating and superconducting orders in magic-angle bilayer graphene**

Ipsita Das<sup>1</sup>

<sup>1</sup>ICFO-Institute of Photonic Sciences, Castelldefels

The behavior of strongly correlated states has been a puzzle for many years; especially unconventional superconductivity has become one of the main challenges in recent decades. Recently the discovery of an isolated low-energy flat band in moiré superlattice of twisted bilayer graphene has emerged as a platform to study these phenomena where superconductivity was found close to half filled band. In addition, we reported the correlated states at all integer fillings,  $\nu = 0, \pm 1, \pm 2, \pm 3$  and a set of previously unobserved superconducting domes close to  $\nu = 0, \pm 1$  filling states. However, coexistence of these two states raises an immediate question about the interplay of their orders. Recently we report on a new method to tune the electronic correlation by varying the distance of a metallic screening layer and MAG. We observed the correlated insulators disappear when the separation becomes smaller than the extent of Wannier orbitals, while superconductivity still exists sometimes taking the vacated position of insulator. Our new technique pioneers a pathway to probe directly microscopic origin of superconductivity and other correlated states in MAG.

## THU 12

### **Cascade of Phase Transitions and Dirac Revivals in Magic Angle Graphene**

Uri Zondiner<sup>1</sup>, Asaf Rozen<sup>1</sup>, Daniel Rodan Legrain<sup>2</sup>, Yuan Cao<sup>2</sup>, Raquel Queiroz<sup>1</sup>, Takashi Taniguchi<sup>3</sup>, Kenji Watanabe<sup>3</sup>, Yuval Oreg<sup>1</sup>, Felix von-Oppen<sup>4</sup>, Ady Stern<sup>1</sup>, Erez Berg<sup>1</sup>, Pablo Jarillo-Herrero<sup>2</sup>, Shahal Ilani<sup>1</sup>

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<sup>4</sup>Freie Universität Berlin, Germany



Twisted bilayer graphene near the magic angle (MATBG) exhibits remarkably rich electron correlation physics, displaying insulating, magnetic, and superconducting phases. In this work, we probe the local electronic compressibility of MATBG using a scanning single electron transistor. We find that when carriers are added into this system, they repeatedly refill the same bands, leading to a Dirac-like compressibility cascade near integer moiré fillings. Additionally, we present a clear compressibility asymmetry around the center of the conduction and valence bands, reflecting the evolution from low DOS at charge neutrality to high DOS at the band edges. A mean-field theory that includes this asymmetry reproduces the experimental results, and explains previous observations that were not yet fully understood. This cascade of Dirac revivals is visible already at relatively large temperatures ( $\sim 20\text{K}$ ) should thus serve as the starting point for understanding the unusual behavior in this system.

### THU 13

#### **Understanding the electronic interaction in the graphene-electrolyte interface**

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Electronic devices based on graphene are widely used in a number of applications; specially, in the field of biological and biochemical sensing. In these kind of sensing devices, graphene is in direct contact with an aqueous electrolyte. Thus, understanding the interaction of the material with the medium is crucial. The main objective of this work is to understand the graphene-electrolyte interface taking into account the influence of the adsorbed surface charge and the substrate. Spectroscopic techniques such as Raman and Impedance were used, complemented with theoretical simulations. The combination of the mentioned tools enables addressing charge carriers in graphene, as well as being an indirect measurement of the adsorbed charge and the coupling between the graphene and the substrate. Our results reveal the intriguing mechanisms of charge modulation in graphene via the electrolyte, and shed some light onto the intrinsic sensing capabilities of graphene (undoped and free of defects) and their modulation through the adsorbed surface charge and/or the substrate nature.

### THU 14

#### **Fabrication and Modification of free-standing 3D printed carbon nanofiber electrodes for energy conversion**

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Fused filament modeling is the most common and simplest type of 3D printing. Conductive composite filaments consisting of polylactic acid (PLA) and graphene have become widely used for 3D printing of electrochemical devices. To enhance the electrochemical performance of the 3D printed parts, post printing procedures like

the chemical activation were applied. For energy conversion via hydrogen evolution reaction (HER), the outstanding catalytic activity of transition metal dichalcogenides (TMD) like  $\text{MoS}_2$  have attracted immense interest as possible replacement of platinum. In this work, a simple post printing procedure by heating the printouts at  $350^\circ\text{C}$  for 3h in air is presented. The thermal removal of the PLA reveals a graphene based carbon fiber nanostructure which can be used as free-standing electrode. The applicability of such 3D printed carbon nanofiber electrodes for energy conversion application is demonstrated via its modification with TMD. The simple and easy scalable electrochemical modification of the electrodes resulted in an enhanced HER. Furthermore, scanning electrochemical microscopy provides valuable information about the heterogeneity of the catalyst activity.

## THU 15

### Resonant Raman Spectra of three-dimensional Weyl semimetal LaAlSi

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LaAlSi is a three-dimensional Weyl semimetal that has attracted a lot of interest for its topological properties. We measured polarized Raman spectra of LaAlSi for several laser energies. For analyzing the spectra, we have developed the computational programs of resonant Raman spectra by using the Quantum-espresso [1] and EPW [2] package. Here, we show the calculated results of polarized Raman spectra that depend on laser energy.

Another subject is the conservation of angular momentum of photon in the Raman process. Tatsumi et al. [3] predict several cases of Raman spectra that change the helicity of incident circularly polarized light, such as TMDs, graphene, black phosphorus. However, in his prediction, the material with four-fold symmetry does not exist even though he got the results from group theory. Since LaAlSi has the four-fold symmetry, we can predict the helicity-changing Raman spectra for LaAlSi by the present calculation and give the calculated results.

[1] P. Giannozzi, et al., J. Phys.: Condens. Matter 21, 395502 (2009)

[2] J. Noffsinger, et al., Compt. Phys. Commun. 181, 2140 (2010)

[3] Y. Tatsumi, et al., Phys. Rev. B 97, 195444 (2018)

## THU 16

### Condensation signatures of photogenerated interlayer excitons in a van der Waals heterostack

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Excitons are bound electron-hole pairs in semiconductors. At low temperature and high exciton density, the occupation numbers of the low-energy exciton states are predicted to increase leading eventually to quantum degeneracy and Bose-Einstein condensation. Atomistic van der Waals heterostacks are ideal systems for high-temperature exciton condensation because of large exciton binding energies and long lifetimes up to several tens of nanoseconds. We present signatures for exciton condensation at elevated temperatures in a  $\text{MoSe}_2\text{-WSe}_2$  heterostructure. We observe several criticalities in photogenerated exciton ensembles with respect to photoluminescence intensity, lifetime, linewidth, and temporal coherence on temperature and exciton density, accompanied by a relative occupation of the underlying exciton state of 100 %. The phenomena survive above 10 Kelvin consistent with the predicted critical condensation temperature. Our study provides a first phase-diagram of the many-body interlayer exciton states that paves ground for excitonic based integrated quantum optical circuits.

#### THU 17

##### Functionalization of Two-dimensional $\text{MoS}_2$

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Two-dimensional (2D) molybdenum disulfide ( $\text{MoS}_2$ ) has attracted increasing interests in both fundamental and industrial research owing to its unique structure and intriguing properties. The functionalization of this material allows for further tuning of the properties and improving its versatility. Herein, we demonstrate two approaches to functionalize chemically exfoliated  $\text{MoS}_2$  nanosheets (ce- $\text{MoS}_2$ ). In the first approach, controllably engineering the sulfur vacancies of ce- $\text{MoS}_2$  using a series of thiophenols in solution was achieved. The degree of functionalization can be tuned by varying the electron-withdrawing strength of substituents in thiophenols. We find that the intensity of 2LA(M) peak normalized to  $A_{1g}$  peak strongly correlates to the degree of functionalization. In the second approach, we develop a dual-functional  $\text{MoS}_2$  nanostructure through successively reacting of ce- $\text{MoS}_2$  with hexyl iodide and aryl diazonium salts. We anticipate the aforementioned approaches can provide deep insights into the fundamental reactivity of ce- $\text{MoS}_2$  and some practical guidance on the multi-angle tailoring of 2D  $\text{MoS}_2$  for various applications.

#### THU 18

##### The Raman response of confined linear carbon chains

Cla Duri Tschannen<sup>1</sup>, Georgy Gordeev<sup>2</sup>, Stephanie Reich<sup>2</sup>, Lei Shi<sup>3</sup>, Thomas Pichler<sup>4</sup>, Lukas Novotny<sup>1</sup>, Sebastian Heeg<sup>2</sup>

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Long linear carbon chains (LLCCs) encapsulated inside double-walled carbon nanotubes are the finite realization of carbyne, the truly one-dimensional allotrope of carbon. Due to a Peierls distortion, the confined carbon chains are polyynic with alternating single and triple bonds. This bond-length alternation (BLA) opens up a direct band gap and leads to the appearance of an optical phonon branch that can be probed by resonance Raman spectroscopy. The extent of the BLA and thus the electronic and vibrational properties of the carbon chains are determined by the chirality of the encapsulating host nanotube. Here, we present a combination of wavelength-dependent and tip-enhanced Raman measurements of single, isolated LLCCs. We particularly focus on the remarkable magnitude of the chains' Raman response and provide comparative measurements of 2D (graphene) and 3D (diamond) carbon-based materials of known Raman scattering efficiency.

## THU 19

### Field emission electron spectroscopy of carbon nanotube-based heterostructures

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Periodic oscillations of Fermi level in CNT are revealed via energy spectroscopy analysis of electrons emitted under action of DC voltage. The oscillations were observed for the micron-sized free standing thin SWCNT film mounted on a tungsten tip and for individual nanotubes grown on the apex of a diamond nanotip. The Fermi level position was determined from the kinetic energy spectra of electrons escaping from the CNT apex under applied voltage in UHV setup equipped with a hemispherical electron energy analyzer. Obtained experimental results and performed numerical simulations of electron transport through the field emitter indicate that the oscillations of Fermi level are caused by the Coulomb blockade effect in the hetero-

junctions at interfaces formed in the CNT-based emitters. The determined energies of single-electron transfer exceed 0.2 eV that permits observation of the Coulomb blockade at room temperature. In this work we will discuss structure of the CNT-based heterojunctions, the mechanisms and computer simulations of the observed single-electron effects and possibilities of their use in single-electron point cathodes.

The work was supported by RSF project 19-72-10067.

## THU 20

### Hexagonal boron nitride incorporation to achieve high performance $\text{Li}_4\text{Ti}_5\text{O}_{12}$ electrodes

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Today, Lithium titanium oxide (LTO) is considered one of the most attractive anode materials that can provide the desired ultra-fast charging ability (>10C) with high safety. However, it displays many serious drawbacks as compared to existing graphite anodes, including poor intrinsic conductivity, narrow electrochemical window, etc. Extensive research has been done to try to overcome these problems, especially developing new LTO composite materials with reduced graphene oxide (r-GO). However, even these methods have rapid capacity fading at high current densities, >5C, due to increased internal resistance and polarization losses. Here, we demonstrate an effective way to improve LTO composite materials with hexagonal boron nitride (h-BN) addition. Li-ion cells with h-BN incorporation exhibit excellent performance and operational stability especially at fast and ultra-fast charging rates, >10C.

## THU 21

### Optical properties of 2D metals and their influence on $\text{WS}_2$ and $\text{MoS}_2$

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Two-dimensional metal films show distinctly different behavior compared to their three-dimensional cousins. Metals are no van der Waals materials, however 2D films can be prepared via confinement epitaxy by intercalating metals between epitaxial graphene and the hosting SiC crystal. Here, we explore the fascinating properties of 2D gallium, 2D indium and their alloys [1]. We are particularly interested

in the dielectric properties and the light-matter interaction of these novel 2D metals. We find resonances in the visible to the near-infrared regime that spectrally overlap with the excitonic interband transitions of semiconducting transition metal dichalcogenides (TMDCs). Hybrid structures of 2D metals and TMDCs are promising for enhancing and shaping their combined light-matter interaction. We investigate the optical response of the 2D metal films as well as 2D metal-TMDC hybrid structure by a combination of spectroscopic imaging ellipsometry, photoluminescence and Raman spectroscopy.

Work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy – EXC 2089/1 – 390776260.

[1] B. Bersch et al. arXiv:1905.09938 (2019)

## THU 22

### Room-Temperature Single-Electron Behaviour in graphene-based GNR-FET

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In this work, I investigated the performance of graphene-based field-effect transistor when a molecularly-shaped graphene nanoribbon bridges the two leads. I measured the electrical properties in a dilution fridge from 25 mK to room temperature. Seven large Coulomb diamond structures are visible from cryogenic up to room temperature, thanks to the overcome of the additional energy ( $E_{add} = 156$  meV) over the thermal energy. The (almost) symmetric periodicity of the diamonds indicates the good quality of the graphene–nanoribbon junctions. I, therefore, suggest the use of graphene-based devices for performing magnetic measurements on graphene nanoribbons thanks to the small Schottky barriers and pinholes induced by the leads on the transport features. These measurements should help in elucidating long-standing topological predictions in graphene nanoribbons [1].

[1] Yazyev, Oleg V., and M. I. Katsnelson. "Magnetic correlations at graphene edges: basis for novel spintronics devices." *Physical Review Letters* 100.4 (2008): 047209.

## THU 23

### Optical properties of graphene quantum dots

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Graphene plays a key role as a central material for nanoelectronics. Nevertheless, its zero gap makes it unusable for applications needing semiconductors. Therefore, a lot of efforts are being made to develop materials with non-zero gap compatible with the hexagonal lattice of graphene. In this context, nano pieces of graphene such as 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, which is a prerequisite before you can imagine controlling their properties. Recently, we reported on single molecule spectroscopy experiments on graphene quantum dots (GQDs). We showed that GQDs are very bright and stable single-photon sources, demonstrating the high potential of GQDs as quantum emitters [1]. In this poster, we will show our latest results on the understanding of the photophysics of GQDs [2].

[1] S. Zhao, L. Rondin, . . . , and JS Lauret “Single photon emission from graphene quantum dots at room temperature”, Nature Communications, 9, 3470 (2018)

[2] T. Liu, S. Zhao, L. Rondin, . . . , and JS Lauret in preparation

## THU 24

### Cryogenic photoluminescence spectroscopy of interlayer excitons in TMD heterostructures

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The emerging field of van der Waals heterostructures provides the unique opportunity to rationally tailor the properties of solids. Within this innovative framework, heterostructures of atomically thin semiconductors with strong exciton transitions play a key role. The possibility to tune the excitonic response of heterobilayers by interlayer twist or doping effects provides novel opportunities for both basic and applied research in optics and optoelectronics. The design degrees of freedom are particularly rich in semiconductor heterobilayers, where the optical properties are intimately tied to layer-separated yet Coulomb-bound electrons and holes of interlayer excitons. Here, we report the results of cryogenic photoluminescence studies of MoSe<sub>2</sub>/WSe<sub>2</sub> and MoS<sub>2</sub>/WSe<sub>2</sub> heterobilayers for further progress towards developments of semiconductor van der Waals heterostructures with tailored optical and optoelectronic functionalities.

**THU 25****Synthesis of MoS<sub>2</sub> nanotubes based on boron nitride nanotubes**

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MoS<sub>2</sub> nanotubes have started to be produced in decent amounts and with promising potentials for large scale applications. The synthesis of single-walled MoS<sub>2</sub> nanotubes is still a challenge in the field, however, and a combined theoretical and experimental work indicated that large diameter multi-walled MoS<sub>2</sub> nanotubes are more stable than single-walled MoS<sub>2</sub>. In this work, we present a method of synthesizing core-shell hetero nanotubes of MoS<sub>2</sub> and boron nitride (BN) nanotubes. High-quality BNNTs are obtained by a template-assisted synthesis method via a CVD coating BN on pristine single-walled carbon nanotubes and subsequent removal of the template. The quality of BNNTs, a single crystalline, is examined by TEM and Raman spectra results. The optical bandgap of BNNTs is proven as 5.76 eV. In addition, the heterostructure of single-walled MoS<sub>2</sub> nanotubes encapsulated in BNNTs is demonstrated by a facile CVD process and characterized by the TEM measurement. Moreover, the Raman and photoluminescence spectra exhibit the optical features of single-walled MoS<sub>2</sub> nanotubes. This work paves a way for exploring the properties of other single-walled transition-metal dichalcogenides nanotubes.

**THU 26****Intrinsic and extrinsic defect-related excitons in TMDCs**

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We investigate an excitonic peak appearing in low-temperature photoluminescence of TMDCs, which is commonly associated with defects and disorder. First, to uncover the intrinsic origin of defect-related (D) excitons, we study their dependence on gate voltage, excitation power, and temperature in a prototypical TMDC monolayer, MoS<sub>2</sub>. We show that the behavior of D excitons can be understood in terms of a simple model, where neutral excitons are bound to ionized donor levels, likely related to sulphur vacancies, with a density of  $7 \times 10^{11} \text{ cm}^{-2}$ . Second, to study the extrinsic origin of D excitons, we controllably deposit oxygen molecules in-situ onto the surface of MoS<sub>2</sub> kept at cryogenic temperature. We find that in addition to trivial p-doping of  $3 \times 10^{12} \text{ cm}^{-2}$ , oxygen affects the formation of D excitons by functionalizing the vacancy. Combined, our results uncover the origin of D excitons, suggest a simple and conclusive approach to track the functionalization of TMDCs,



benchmark device quality, and pave the way towards exciton engineering in hybrid organic-inorganic TMDC devices.

## THU 27

### **Probing Enhanced Light-Matter Interaction In Graphene On Plasmonic-Photonic Crystals By Raman Spectroscopy**

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Graphene and carbon nanotubes have unique optical and electrical properties and are of great interest in nanoscale light emitting and light detection devices. Unfortunately, the intrinsic light-matter interaction of these graphene based nanomaterials is rather weak due to their low-dimensionality and measures to enhance it such as, eg., the integration into optical microcavities and photonic crystals have been considered in the past. In our present work, emphasis is laid on enhancements via so-called stacked complementary plasmonic-photonic crystal (SC PlasPhCs), which combine strongly localized plasmonic and high-Q photonic guided resonances to give rise to hybrid plasmonic-photonic resonances at visible and near infrared frequencies. SC PlasPhCs were previously employed as platforms to enhance fluorescence from molecules. Here, we study the enhancement of the light-matter interaction in graphene transferred onto SC PlasPhC substrates by Raman spectroscopy, complementary reflection measurements and simulations. By tuning the SC PlasPhC structural parameters (lattice distance and air-hole diameter), enhancement contributions of Raman excitation and emission can be tailored.

## THU 28

### **Topological defects in layered 2D crystals: Structure, properties and their applications**

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Point-like or extended defects in layered crystals, predominantly in graphene, have widely been studied and their impact on properties are manifold. Like in established semiconductor technologies, crystal defects yield novel functionalities, e.g., for optoelectronics and sensors.

For instance, dense dislocation networks, introducing extraordinary structural and electronic disorder, yield a perfectly linear magnetoresistance of bilayer graphene well suited for magnetic field sensing up to 100 T [1]. In layered semiconductors, similar defects may cause strong band-structure alterations with highly localized op-

tical response.

For advanced applications in optical communication, imaging, or light harvesting, multispectral devices with extended photosensitivity from the visible towards the IR range are desired. Defective few-layer  $\text{MoS}_2$  with broad IR-sensitivity has successfully been introduced into the established fabrication sequence of vertical photodetectors based on amorphous Si [2]. Bias-dependent charge utilization within the devices even allows for wavelength-selective sensing.

[1] Nature 505 2014 533 & Nat Phys 11 2015 650

[2] ACS Photonics 6 2019 1372

## THU 29

### Spin and valley lifetimes in monolayer TMDs

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Monolayer transition metal dichalcogenides (TMD) exhibit lifetimes in all-optical time-resolved Kerr rotation (TRKR) measurements which vary from several picoseconds up to the microseconds at low temperatures and can reach values of up to 100 ns at room temperature. We show that the latter can be linked to spin states not directly connected to a valley polarization. Furthermore, we report on nanosecond long, gate-dependent valley lifetimes of free charge carriers in monolayer  $\text{WSe}_2$  by combining gate-dependent photoluminescence and TRKR measurements with electrical transport measurements. This provides insight into the Fermi level position of the TMD and enables us to extract the respective valley lifetimes of free charge carriers and to disentangle it from the lifetimes of bound valley and spin states at elevated temperatures.

## THU 30

### Atomic reconstruction in twisted bilayers of transition metal dichalcogenides

Astrid Weston<sup>1,2</sup>, Yichao Zou<sup>2,3</sup>, Vladimir Enaldiev<sup>1,2,3</sup>, Alex Summerfield<sup>1,2</sup>, Nicholas Clark<sup>2,3</sup>, Viktor Zolyomi<sup>1,2</sup>, Abigail Graham<sup>4</sup>, Celal Yelgel<sup>1,2</sup>, Samuel Magorian<sup>1,2</sup>, Mingwei Zhou<sup>1,2</sup>, Johanna Zultak<sup>1,2</sup>, David Hopkinson<sup>2,3</sup>, Alexei Barinov<sup>5</sup>, Thomas Bointon<sup>2</sup>, Andrey Kretinin<sup>2,3</sup>, Neil Wilson<sup>4</sup>, Peter H. Beton<sup>6</sup>, Sarah J. Haigh<sup>2,3</sup>, Roman Gorbachev<sup>1,2,7</sup>

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Recent advances of Van der Waals heterostructures has permitted researchers to probe exciting new physics with the addition of relative rotation between adjacent atomic layers. We have used atomic resolution transmission electron microscopy and multiscale modelling to illustrate that the lattice of MoS<sub>2</sub> and WS<sub>2</sub> homo-bilayers with small relative twist reconstructs to form energetically favourable stacking domains separated by stacking faults. For angles close to 3R-like crystal alignment (0°) triangular domains are separated by a network of partial dislocations. In scanning tunnelling measurements we observe contrast in the tunnelling current between 3R-stacking domains due to layer-polarized conduction band states caused by a lack of both inversion and mirror symmetry (not seen in 2H domains). For twist angles close to 2H stacking (60°), 2H domains dominate where the nuclei of a previously unnoticed metastable stacking is limited to 5 nm in size. With relative twist of 1°, a kagome-like pattern appears which transitions to an hexagonal array of screw dislocations that separate large-area commensurate 2H domains at the smallest twist angles.

### THU 31

#### **Unexpected Photoluminescence Quenching in Ultrathin Molybdenum Disulphide Grown on Sapphire Substrates**

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Molybdenum disulphide (MoS<sub>2</sub>) is a transition metal dichalcogenide which is intensely studied due to its shift from an indirect semiconductor in its bulk form, to a direct semiconductor when thinned down. This results in the emergence of a photoluminescence signal in monolayer MoS<sub>2</sub>. A change of its optical properties could prove both as a problem for optoelectronic devices, and as an opportunity for creating new fields of application.

A common method to fabricate ultrathin MoS<sub>2</sub> chemical vapor deposition (CVD). Due to its defined and smooth surface, we chose sapphire as a substrate. Unexpectedly we observed a strong photoluminescence-quenching in CVD-grown monolayer MoS<sub>2</sub> on a specific batch of sapphire substrates. Our goal is to track down the cause of this phenomena in order to find a way to control the photoluminescence intentionally. Hence, we analysed the sapphire substrate itself, as well as the as-grown MoS<sub>2</sub> for its optical, chemical and structural properties. Furthermore, we

compared the growth process on different sapphire substrates. By combining different methods, we try to unravel the mystery of the lost photoluminescence signal.

## THU 32

### 2D Platforms for Majorana States and Phase Measurement of Topological Superconductivity

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A hallmark of topological superconductivity is the emergence of Majorana bound states (MBS). Their non-Abelian statistics allows for the implementation of quantum gates through braiding operations. To overcome the challenges of commonly studied 1D systems, we propose 2D platforms supporting scalable MBS and their braiding. Spin valves, known in spintronics, with their fringing fields [1,2] can proximitize 2D electron gas to implement MBS and their braiding [3,4]. Our measurements of topological superconductivity in epitaxial Al/InAs Josephson junctions demonstrate closing and reopening of the superconducting gap with increasing magnetic field, accompanied by the measurement of pi-jump in the superconducting phase [5]. Remarkably, this topological transition can be controlled by gate voltage. We propose X-shaped topological junctions[6] in which the observed topological transition can be used to realize scalable MBS and their braiding.

- [1] T. Zhou et al., PRB 99, 134505 (2019)
- [2] N. Mohanta et al., PR Applied 12,034048 (2019)
- [3] G. Fatin et al., PRL 117, 077002 (2016)
- [4] A. Matos-Abiague et al., SSC 262, 1 (2017)
- [5] W. Mayer et al., arXiv:1906.01179
- [6] T. Zhou et al., arXiv:1909.05386

## THU 33

### Neutral and charged excitons interplay in non-uniformly strain-engineered WS<sub>2</sub>

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We investigate the response of excitons in two-dimensional semiconductors to non-uniformity of mechanical strain. In our approach to non-uniform strain-engineering, a WS<sub>2</sub> monolayer is suspended over a triangular hole. Large ( $> 2\%$ ), strongly non-uniform ( $> 0.28\%/\mu\text{m}$ ), and in-situ tunable strain is induced in WS<sub>2</sub> by pressurizing it with inert gas. We observe a pronounced shift of the spectral weight from neutral to charged excitons at the center of the membrane, in addition to well-known strain-

dependent bandgap modification. We show that the former phenomenon is a signature of a new effect unique for non-uniform strain: funneling of free carriers towards the region of high strain followed by neutral to charged exciton conversion. Our result establishes non-uniform strain engineering as a novel and useful experimental 'knob' for tuning optoelectronic properties of 2D semiconductors. In addition, we present our recent results on engineering highly localized, non-uniform strain in  $\text{WS}_2$  by nano-indentation, which we realize with a custom-built, temperature-controlled AFM with full optical access.

#### THU 34

##### **Raman spectroscopy of carbon atomic wires interacting with metal nanoparticles and surfaces**

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Carbon-atom wires are the ultimate 1D systems comprising carbyne, the ideal infinite chain of  $sp$ -hybridized carbon atoms with two possible structures: semiconducting polyyne with alternated single-triple bond and metallic cumulene with all double bonds. In finite systems the length and the terminations significantly affect the wire structure opening the way to tune the electronic and optical properties [1]. We here discuss Raman and surface enhanced Raman scattering (SERS) to investigate the role of chain length and termination. By observing charge transfer effects between wires and metal nanoparticles pointing to a polyyne-to-cumulene transition (i.e. from semiconductor to metal-like), we show how the molecular design of the wire can tune the charge distribution and the charge transfer direction from a donor to an acceptor behaviour [2]. In addition, we discuss how Raman spectra of  $sp-sp^2$  polymeric wires on Au(111) unveil a peculiar interaction with the metallic surface [3].

[1] C.S. Casari et al. *Nanoscale* 8, 4414 (2016)

[2] A. Milani et al. *Scientific Reports* 9:1648 (2019)

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

#### THU 35

##### **Imaging the Collimation and Magnetic Focusing of Dirac Electrons**

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Van der Waals heterostructures have emerged as a new playground for exploring electron-optics - the solid-state analogues of optical devices, such as lenses, beam splitters and interferometers. A fundamental building block for constructing these

electron-optic devices is an electron source that can provide a narrow and collimated beam. In this work, we observe that the naturally occurring P-N junction formed at a metal-graphene interface leads to a strongly collimated beam of electrons, which can be turned on/off by simply changing the doping of the graphene. We non-invasively study this collimation by imaging magnetic focusing in real-space using a scanning single-electron transistor as an electrostatic potential probe. We observe a drastic transition of the potential landscape when the graphene doping changes sign, from featureless for electron-doped (no P-N junction) to oscillating for hole-doped. Additionally, we show that there is a universal relation between the measured contact resistance of the metal-graphene interface to the degree of collimation, which should be considered in future ballistic experiments.

### THU 36

#### **Magic-angle bilayer graphene nano-calorimeters – towards broadband, energy-resolving single photon detection**

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Because of the ultra-low photon energies in the mid-infrared and terahertz frequencies, in these bands photodetectors are notoriously underdeveloped, and broadband single photon detectors (SPDs) are non-existent. Advanced SPDs exploit thermal effects in nano-structured superconductors, and their performance is currently limited to the more energetic near-infrared photons due to their high electronic heat capacity. Here, we demonstrate a superconducting magic-angle twisted bilayer graphene (MAG) device that is capable of detecting single photons of ultra-low energies by utilizing its record-low heat capacity and sharp superconducting transition. We theoretically quantify its calorimetric photoresponse and estimate its detection limits. This device allows the detection of ultra-broad range single photons from the visible to sub-THz with response time around 4 ns and energy resolution better than 1 THz. These attributes position MAG as an exceptional material for long-wavelength single photon sensing, which could revolutionize such disparate fields as quantum information processing and radio astronomy.

**THU 37****Excellent electronic transport in heterostructures of graphene and monoisotopic boron-nitride grown at atmospheric pressure**Christoph Stampfer<sup>1</sup><sup>1</sup>II. Institute of Physics, RWTH Aachen, Aachen

Hexagonal boron nitride (BN), one of the very few layered insulators, plays a crucial role in 2D materials research. In particular, BN grown with a high pressure technique has proven to be an excellent substrate material for graphene and related 2D materials, but at the same time very hard to replace. Here we report on a method of growth at atmospheric pressure as a true alternative for producing BN for high quality graphene/BN heterostructures. The process is not only more scalable, but also allows to grow isotopically purified BN crystals. We employ Raman spectroscopy, cathodoluminescence, and electronic transport measurements to show the high-quality of such monoisotopic BN and its potential for graphene-based heterostructures. The excellent electronic performance of our heterostructures is demonstrated by well developed fractional quantum Hall states, ballistic transport over distances around 10 micrometer at low temperatures and electron-phonon scattering limited transport at room temperature.

**THU 38****High catalytic performance of tungsten and molybdenum disulphide rods in oxygen evolution reactions in alkaline solutions**Karolina Wenelska<sup>1</sup>, Klaudia Maslana<sup>1</sup>, Marcin Biegun<sup>1</sup>, Ewa Mijowska<sup>1</sup><sup>1</sup>West Pomeranian University of Technology, Szczecin, Faculty of Chemical Technology and Engineering, Szczecin, Poland

Transition-metal-based compounds such as carbides, nitrides, phosphides, sulfides, and selenides have been studied as alternative electrocatalysts for these reactions. Among all these compounds, transition metal dichalcogenides (TMDs) are of particular interest. Their layered structure with weak van der Waals forces between layers allowed to their exfoliation from bulk to monolayer, which shifted transition bandgap from indirect to direct. This makes them a promising candidate for optoelectronic devices, such as solar cells, photodetectors, light-emitting diodes.

Herein, we reveal two interesting findings with respect to the current state of the art: the design of WS<sub>2</sub>, MoS<sub>2</sub> in the form of rod-like structures, and the significant enhancement of the electrocatalytic activity of rod-like WS<sub>2</sub>, MoS<sub>2</sub> toward OER overpotential in respect to the exfoliated WS<sub>2</sub>, MoS<sub>2</sub>. To prepare rods of WS<sub>2</sub> and MoS<sub>2</sub> first bulk WS<sub>2</sub> or MoS<sub>2</sub> was exfoliated and functionalized by nickel oxides nanoparticles. Next, exfoliated WS<sub>2</sub> and MoS<sub>2</sub> were reshaped to the rods in the high-temperature process in a hydrogen atmosphere and then treated with ethylene. As-prepared rods have been tested as electrocatalyst in OER.

**THU 39****Ultrafast dynamics in transition metal dichalcogenides probed by terahertz spectroscopy**

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We investigate sub-picosecond dynamics in high-quality multi- and bi-layers (ML and BL) of prototypical TMDC MoSe<sub>2</sub>, using THz time-domain spectroscopy.

We observed strong THz emission from both BL and ML samples in response to ultrashort optical excitation. In ML samples, the pattern of emitter THz suggests that the excited currents are in-plane of the sample, while for BL—out-of-plane. Moreover, in BL sample we observed time-resolved beating at 25 THz in the signal.

The model we developed suggests the domination of the photoexcited surge current in ML signal and shift current in BL signal. The beating is attributed to coherent oscillations between two excitonic states with separation of 100 meV.

Combined, our results provide a consistent explanation of THz emission from TMDCs.

**THU 40****“Real-world” waste plastics versus biomass derived porous carbons in Supercapacitors**

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<sup>1</sup>Nanomaterials Physicochemistry Department, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology, Szczecin, Szczecin, Poland

Nowadays, porous carbons derived from waste plastics and biomass have been widely studied for supercapacitors. It is of great significance to convert waste plastics into high value-added carbons because of terrible environmental problems caused by the growing amount of waste plastics. On the other hand, biomass, an easily available and cheap natural resource, is the common precursor to synthesize carbon materials with low cost and naturally heteroatoms doping. Herein, porous carbons from “real-world” waste plastic bottles and biomass are used in supercapacitors. The capacitance is 158, 190, 359, 452 F/g at 0.5 A/g in 6M KOH for waste PET[1], waste mixed plastics[2], eucalyptus, and egg-white, respectively. The performance of biomass-derived carbons is greater, however, the facile way of transforming waste plastics into carbons is a promising route to recycle waste plastics and hopefully mitigate the waste plastics-related environmental issues.

This work was financially supported by the NAWA PROM 2 (No. PPI/PRO/2019/1/00008/DEC/01).



- [1] Y. Wen, et al., E. Mijowska, J. Appl. Polym. Sci. 137 (2020), 48338.  
[2] Y. Wen, et al., E. Mijowska, Waste Manage. (Oxford) 87 (2019), 691-700.

#### THU 41

##### **Preparation of Ultrahigh–Aspect–Ratio Two–Dimensional Bismuth Microsheets: Toward Selective Vapor Sensing**

Seyyed Mohsen Beladi Mousavi<sup>1</sup>, Martin Pumera<sup>1</sup>

<sup>1</sup>Inorganic chemistry, University of chemistry and technology, Prague

Discovery of atomically thin pnictogens, especially black phosphorus, has revealed their great potential as novel two-dimensional (2D) semiconductors for a wide range of electronic and optoelectronic applications. Here, a novel thermal approach allowing the preparation of ultrahigh aspect-ratio bismuthene microsheets as a stable aqueous dispersion is demonstrated. This method is based on controlled recrystallization of bismuth particles to form homogeneously shaped 2D microsheets. Spectroscopic and microscopic analyses confirmed the formation of ultrathin bismuthene with large lateral dimensions (area:  $4\ \mu\text{m}^2$ , thickness:  $2.5\ \text{nm}$ ). Notably, although the preparation is performed in an oxygenated solution, the sheets are not oxidized, and they are stable in the air or water for at least three months. The bismuthene nanosheets are used to construct a vapor sensor based on an electrochemical impedance spectroscopy method. The device is highly selective toward methanol vapors, it has a fast response, and it shows long-term stability.

#### THU 42

##### **Atomically precise graphene nanoribbon heterojunctions: spectroscopic characterization and charge transport measurements**

Boris V. Senkovskiy<sup>1</sup>, Seyed K. Alavi<sup>2</sup>, Yannic Falke<sup>1</sup>, Martin Hell<sup>1</sup>, Dmitry Y. Usachov<sup>3</sup>, Alexander V. Fedorov<sup>4</sup>, Alexander Chernov<sup>1</sup>, Dmitry Rybkovskiy<sup>5</sup>, Kenya Shimada<sup>6</sup>, Taichi Okuda<sup>6</sup>, Thomas Szkopek<sup>7</sup>, Felix R. Fischer<sup>8</sup>, Klas Lindfors<sup>2</sup>, Alexander Grüneis<sup>1</sup>

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<sup>7</sup>McGill University, Department of Electrical and Computer Engineering, Canada

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We synthesize aligned armchair graphene nanoribbons of 7 carbon atoms width (7-AGNRs) having a wide band gap, and perform their controlled partial conversion into narrow-band-gap 14-AGNRs. This allows us to create a unique system – an aligned array consisting of heterojunctions of narrow- and wide-band-gap GNRs. We identify characteristic Raman modes and visualize 1D electronic band disper-

sion of 14-AGNRs by angle-resolved photoemission spectroscopy. We integrate the GNR heterojunctions array into the field-effect-transistor (FET) geometry with variable source-drain channel length. Weak temperature dependence of the charge transport indicates that the thermal activation is not a dominant factor. Strong dependence of the FET characteristics on the electric field and the gate potential points towards the importance of the modulation of 14-AGNRs/7-AGNR barrier and the carrier tunneling under the barrier. We discuss the mechanisms responsible for the charge transport in GNR heterojunctions. Our results suggest that GNR heterojunctions, which can be engineered with atomic precision, are a promising platform for novel nanoscale devices, such as energy-efficient tunnel FETs.

### THU 43

#### **The Epoxide Route as a tuneable synthetic approach to the obtaining of 2D layered hydroxides and their hybrid phases**

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<sup>2</sup>Departamento de Física de la Materia Condensada, GlyA, CAC-CNEA. Instituto de Nanociencia y Nanotecnología, CNEA-CONICET, Argentina

<sup>3</sup>INQUIMAE-DQIAQF, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Argentina

Layered hydroxides (LH) are a special sort of anionic layered two-dimensional materials. Recently they received increasing attention for their applications in energy storage - especially oxygen evolution reaction -, pollution removal, catalysis -as precursors of carbon nanoforms- or magnetism, to name a few. They can be classified in three groups depending on their structure: single LH, layered double hydroxides (LDH) and simonkolleite-like LH (alpha-LH).

In this work we present the Epoxide Route, a one-pot room temperature synthetic approach based on the nucleophilic attack over an epoxide ring which drives the alkanilization for the obtaining of different LH phases and their hybrid forms. LDH and alpha-LH were successfully synthesized where their anionic interlayer chemistry (covalent or electrostatic) and the nature of the cation in the layers (oxidation state and crystallographic environment) were tuned on demand. The nature of the growth mechanism, electronic, electrochemical and magnetic properties and the DFT+U description of some of the most representative phases are discussed.

- 08:30 – 09:00 T. Susi, Vienna  
*Electron-beam manipulation of lattice impurities*
- 09:00 – 09:30 J. Sloan, Warwick  
*Atomically Thin Confined Nanowires - the Final Orderable Structural Domain?*
- 09:30 – 10:00 A. N. Khlobystov, Nottingham  
*Molecules in Carbon Nanotubes: Structure, Property and Reactivity*
- 10:00 – 10:30 Coffee Break
- 10:30 – 11:00 R. Deblock, Orsay  
*Dynamically induced 0- $\pi$  transition in a carbon nanotube-based Josephson junction*
- 11:00 – 11:30 A. K. Hüttel, Regensburg  
*Nanotube quantum dots: from microwave optomechanics to novel materials*
- 11:30 – 12:00 S. Reich, Berlin  
*Plasmonic nanoparticle crystals for deep strong light-matter coupling*
- 12:00 – 17:00 Mini Workshops
- 17:00 – 17:30 P. Bøggild, Lyngby  
*Lithographic bandgap engineering of graphene: the crucial role of edges*
- 17:30 – 18:00 S. Hofmann, Cambridge  
*On the Fundamental Mechanisms that underpin CVD Technology for Atomically Thin 2D Films*
- 18:00 – 18:30 SUMMARY: A. Jorio, Belo Horizonte  
*Kirchberg 2020 - Conference Summary*
- 18:30 – 20:00 Break
- 20:00 – 22:00 Bauernbuffet – Farewell Dinner

Friday, March 13th

Topological properties, applications

**08:30****Electron-beam manipulation of lattice impurities**Alexander Markevich<sup>1</sup>, Kimmo Mustonen<sup>1</sup>, Mukesh Tripathi<sup>1</sup>, Jani Kotakoski<sup>1</sup>, Toma Susi<sup>1</sup><sup>1</sup>University of Vienna, Faculty of Physics, Vienna, Austria

Covalently bound impurity atoms in crystal lattices can be manipulated via the elastic backscattering of probe electrons from moving C nuclei [1] using the atomically focused electron irradiation of a scanning transmission electron microscope.

This capability was first realized for incidental silicon impurities in single-layer graphene, with our recently reported manipulation rate already nearly on par with any atomically precise technique [2]. Such manipulation is also possible in large-diameter single-walled carbon nanotubes [3].

Although more challenging, P dopants in graphene can also be manipulated [4], but significantly heavier Ge impurities cannot [5]. Even more excitingly, electron-beam manipulation of Bi dopants in bulk silicon was recently reported [6], with a novel indirect exchange mechanism uncovered by our latest modeling.

- [1] T. Susi et al., Nat. Rev. Phys. 1, 397–405 (2019)
- [2] M. Tripathi et al., Nano Lett. 18, 5319 (2018)
- [3] K. Mustonen et al., Adv. Func. Mat. 29, 1901327 (2019)
- [4] C. Su et al., Sci. Adv. 5:eaav2252 (2019)
- [5] M. Tripathi et al., ACS Nano 12, 4641 (2018)
- [6] B. Hudak et al., ACS Nano 12, 5873 (2018)

**09:00****Atomically Thin Confined Nanowires - the Final Orderable Structural Domain?**Jeremy Sloan<sup>1</sup><sup>1</sup>Department of Physics, University of Warwick, Coventry CV4 7AL

Atomically regulated (1D) nanowires can be as small as a single atom in width and are the smallest ordered materials. They allow the study of the fundamental properties of matter, such as nanoscale phase transformations and the energetics of confined crystal structure formation. Carbon nanotubes are ideal templates for forming and observing such transitions in 1D nanowires. These materials test the state of the art in electron microscopy and associated spectroscopies but their extremely small size also lends them to ab initio theoretical investigations whereby their stability, electronic properties can be studied. This work is leading to ground-breaking new studies including the physical realisation of Peierls distortions, novel phonon optics and spectacular modification of thermal properties. A further recent innovation is the study of phase transformations at the smallest volume scale ever attempted (i.e.  $\sim 1 \text{ nm}^3$ ). In this presentation, the interrelationships between nanoscale structural synthesis and characterisation, theoretical investigations will be discussed and new methodologies for investigating their structural evolution with time will also be presented.

**09:30****Molecules in Carbon Nanotubes: Structure, Property and Reactivity**Andrei N. Khlobystov<sup>1</sup><sup>1</sup>School of Chemistry, University of Nottingham, Nottingham, UK

How do we know that molecules react in one way rather than another? Even in an ideal case, a reaction observed in a laboratory experiment by ensemble-averaging analytical techniques, such as spectroscopy or diffraction, can only support rather than confirm a proposed mechanism. In practice, definitive information about the reactions can be provided only by a direct observation of dynamics at the single-molecule level. We entrap and study chemical reactions of individual molecules in nanotubes triggered and controlled by heat [1], electric potential [2] or electron beam [3]. Reactions in nanotubes often deliver unusual materials, such as nanoribbons of graphene [4], or enable improvements of important physical and chemical processes. Loaded with metal nanoparticles the nanotubes exhibit remarkable catalytic properties that can be exploited in many applications, including electrocatalysis in fuel cells, outperforming traditional materials [5]. All this becomes possible due to the nanoscale confinement of molecules in carbon nanotubes.

[1] Adv.Funct.Mater. 2019,29,1808092

[2] Adv.Mater. 2019,31,1904182

[3] Nature Comm. 2018,9,3382

[4] ACS Nano 2017,11,2509

[5] Adv.Mater. 2016,28,9103

**10:30****Dynamically induced 0- $\pi$  transition in a carbon nanotube-based Josephson junction**Diana Watfa<sup>1</sup>, Raphaëlle Delagrangé<sup>1</sup>, Alik Kasumov<sup>1</sup>, Raphaël Weil<sup>1</sup>, Meydi Ferrier<sup>1</sup>, Hélène Bouchiat<sup>1</sup>, Richard Deblock<sup>1</sup><sup>1</sup>Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, Orsay, France.

A carbon nanotube (CNT) between two superconducting is an ideal model system for studying electronic transport and investigating the competition between two important effects in condensed matter: the Kondo effect and superconducting proximity effect. The Kondo effect is a many-body interaction between a localized impurity spin and free conduction electrons leading to the screening of the impurity spin and the appearance of a Kondo resonant state at the Fermi energy of the contacts. We have measured the DC Josephson current and AC Josephson emission of a CNT Josephson junction. The AC emission is probed by coupling the CNT to an on-chip detector (a Superconductor-Insulator-Superconductor (SIS) junction), via a coplanar waveguide resonator. The measurement of the photo-assisted current of the SIS junction gives direct access to the signal emitted by the CNT. We focus on the gate regions that exhibits Kondo features in the normal state. We demonstrate that, strikingly, when the DC supercurrent is enhanced by the Kondo effect, the AC Josephson effect is strongly reduced. This could be explained by a dynamically induced quantum transition between a singlet and a doublet doublet.



**11:30****Nanotube quantum dots: from microwave optomechanics to novel materials**Andreas K. Hüttel<sup>1</sup><sup>1</sup>Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg

Placing a vibrating carbon nanotube next to a coplanar microwave resonator at cryogenic temperatures results in a microwave optomechanical system. This system, however, has a fundamentally new property: the nanotube is also a quantum dot, and strong interaction of motion and single electron tunnelling dominates its behaviour. We have characterized such a system at millikelvin temperatures via optomechanically induced transparency (OMIT) [1]. The interaction of charge transport and vibration leads to a strongly enhanced, gate-dependent optomechanical coupling. The typical figure of merit for optomechanical systems, the single-photon coupling, reaches up to  $g_0 = 2\pi \times 95$  Hz. With this, the manipulation of a carbon nanotube at the quantum limit of motion enters technological reach.

In the end I will briefly report on our recent work introducing transport spectroscopy of straight, low-defect multiwall MoS<sub>2</sub> nanotubes. We demonstrate clear quantum dot behaviour, with tentative indications of excited states and quantum state transitions [2].

[1] S. Blien et al., arXiv:1904.12188 (2019)

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

**11:30****Plasmonic nanoparticle crystals for deep strong light-matter coupling**Niclas Mueller<sup>1</sup>, Yu Okamura<sup>1</sup>, Bruno Vieira<sup>1,2</sup>, Sabrina Juergensen<sup>1</sup>, Holger Lange<sup>3</sup>, Eduardo B. Barros<sup>2</sup>, Florian Schulz<sup>3</sup>, Stephanie Reich<sup>1</sup>,<sup>1</sup>Freie Universitaet Berlin, Berlin, Germany<sup>2</sup>Universidade Federal do Ceara, Fortaleza, Brazil<sup>3</sup>University of Hamburg, Hamburg, Germany

Metal nanoparticles absorb and scatter light through the collective excitations of their free electrons. These plasmons give rise to the bright red color of nanoparticle-stained glass. They also enhance optical processes close to the metal, which is used for sensing and analytics. We consider crystals of metal nanoparticles, where the interparticle distance is much smaller than the particle size. The interaction of light with the crystal plasmons is so strong that the interaction strength exceeds the plasmon frequency. The light-matter Hamiltonian becomes dominated by counter-rotating terms and the photon self interaction. We synthesized face centered cubic crystals of gold nanoparticles. Their optical properties reveal Rabi frequencies up to 3eV, almost a factor of two higher than the plasmon frequency. We discuss the dispersion of the plasmon-polaritons and how the properties of the material are defined by its interaction with light. Metallic and semiconducting nanoparticles may work as building blocks for a class of materials with extreme light-matter interaction. They will have application in nonlinear optics, the search for novel ground states, polariton chemistry, and quantum technology.

**17:00****Lithographic bandgap engineering of graphene: the crucial role of edges**Peter Bøggild<sup>1</sup><sup>1</sup>DTU Physics, Technical University of Denmark, Kgs. Lyngby

In the light of graphene's rich electronic properties one of the most obnoxious road-blocks have been to pattern graphene on a small scale. Early theoretical work predicted that the bandstructure of graphene can be engineered by nanopatterning. Unfortunately, edge disorder and contamination associated with lithographic processes effectively ruins the transport properties. This has held back development of graphene nanoelectronics for more than a decade. The key is to control the chemistry and roughness of the edges, which has a striking impact on charge distribution and scattering, leading to QHE breakdown and ferroelectric behavior in graphene devices. We fabricated graphene devices with lithographic patterning on the 10 nm scale, which exhibited distinct magnetotransport features in quantitative agreement with numerical and analytical calculations, and with a ca. 150 meV bandgap. Also, the subtle moiré-superlattice signatures associated with a small finite twist angle between the graphene and hexagonal boron nitride survives the aggressive lithographic patterning, suggesting that nanoscale circuits and components that exploit the novel properties of twisted 2D layers are feasible.

**17:30****On the Fundamental Mechanisms that underpin CVD Technology for Atomically Thin 2D Films**Stephan Hofmann<sup>1</sup><sup>1</sup>Engineering, University of Cambridge, Cambridge

Driven by the industrial demand for “electronic-grade” 2D material films, we focus on developing scalable process technology, and in this talk I will review our recent progress in scalable (MO)CVD and device integration approaches for highly crystalline graphene, h-BN and TMD ( $\text{WS}_2$ ) films [1]. We employ a “deconstructed” MOCVD process for  $\text{WS}_2$ , based on a simple sequential exposure pattern, as model system to systematically explore each growth aspect. Using Au support, we find not only allows a significant reduction of the carbon contamination but also a self-limiting behaviour to mono-layer  $\text{WS}_2$  with reasonable crystallinity, and full coverage within 10 min exposure time. We also report that  $\text{WS}_2$  post-growth treatment with oleic acid can greatly enhance the PL yield and mobility [2]. I will also report on our efforts to find new methods for high-throughput quality monitoring of 2D layers, incl. the use of ellipsometric contrast micrography [3] and super-resolution imaging [4].

[1] ACS Nano 13, 2114 (2019); 2D Mat. 7, 024005 (2020).

[2] Nano Lett. 19, 6299 (2019).

[3] ACS Nano 12, 8555 (2018).

[4] ACS Nano 13, 4538 (2019).

Topological properties, applications

Friday, March 13th

**18:00**

**Kirchberg 2020 - Summary**

Ado Jorio<sup>1</sup>

<sup>1</sup>Physics, UFMG, Belo Horizonte



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