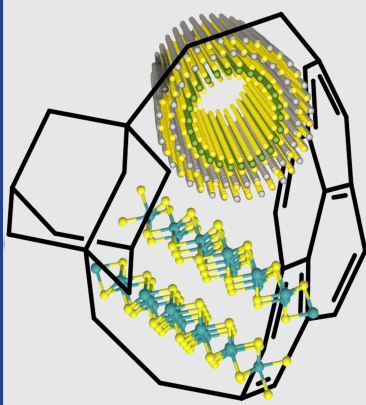
Name

XXXIII[nd] International Winterschool on Electronic Properties of Novel Materials

Molecular Nanostructures

Program

IWEPNM 2018



Hotel Sonnalp
Kirchberg/Tirol
Austria

17 - 24 March, 2018

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
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LAYOUT

María Machón, Felix Herziger

Logo designed by Christoph Tyborski.
The logo shows an 'easter basket' of graphene and a diamondoid ([2](1,3)Adamantano[2](2,7)pyrenophane) filled with layers of transition metal dichalcogenides and inorganic nanotubes.

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Financial assistance from the sponsors and supporters is greatly acknowledged.

Dear Friend:

Welcome to the 32nd International Winterschool on:

Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of thirty-one 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
Christoph Tyborski	accommodation
Dirk Heinrich	accommodation, technical assistance
Hans Tornatzky	finances, communications
Harald Scheel	website
Roland Gillen	technical assistance, video transfer, sponsoring, abstract booklet
Felix Kampmann	announcements, website assistance
Emanuele Poliani	technical assistance
Narine Ghazaryan	technical assistance
Anja Sandersfeld	visa applications, general assistance

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

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

Sincerely yours,
Janina, Christian, Andreas and Stephanie

Chairpersons

J. Maultzsch (Erlangen)
C. Thomsen (Berlin)
A. Hirsch (Erlangen)
S. Reich (Berlin)

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Scope

This winterschool will provide a platform for reviewing and discussing new developments in the field of electronic properties of molecular nanostructures and their applications. Subjects included are:

- Materials science of graphene and nanographene
- Novel two-dimensional materials
- Carbon nanotube / graphene optics and electronics
- Carbon nanotube / graphene growth and selection
- Theory of novel materials
- Applications of novel materials
- Nanostructure spintronics
- Topological materials
- Single-molecule experiments

INFORMATION FOR PARTICIPANTS

Time and location
The IWEPNM 2018 starts on Saturday, 17 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, 24 March, breakfast. There will be a reception party on Saturday, 17 March, after dinner, and a farewell party including dinner on Friday, 23 March.

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

Addresses
The address of the Winterschool is:
IWEPNM 2018 Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria
e-mail: info@hotelsonnalp.info, web: www.hotelsonnalp.info

All questions concerning the IWEPNM 2018 should be directed to:
Prof. Dr. Janina Maultzsch,
Department für Physik, FAU Erlangen, Staudtstr. 7, 91058 Erlangen, Germany
or
Prof. Dr. Christian Thomsen,
Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany
Tel: 0049-(0)30-31423187, Fax: 0049-(0)30-31427705
email: iwepnm-info@physik.tu-berlin.de, web: www.iwepnm.org

Participation
Participation at the IWEPNM 2018 is possible for students and scientists working in the field covered by the scope of the meeting. Because of the limited space the participation requires prearranged acceptance by the organizers.

Contributions
All oral contributions will be presented in the big seminar room of the Hotel Sonnalp. All participants are invited to contribute comments to research and tutorial lectures, where 10 minutes for discussion are reserved within each lecture. Video projection will be available for presentations. Invited speakers please test the video projection with the technical staff at the latest a few minutes before your session begins. Posters will be presented in the hall of the seminar room.
We kindly ask you NOT to take any pictures or videos of the presentations.

Childcare
Childcare is provided by Michaela Kisch and her team (michaela@kitzkids.com). If you need childcare during the winterschool, please contact us at the registration desk.

Ski pass and internet connection
If you wish to buy a ticket for the ski lifts, please ask at the hotel reception.
Internet connection through WLAN is available for all participants, even if they are not accommodated at the Hotel Sonnalp. Please check at the front desk. There will be a room in the basement with fixed LAN connections, and limited number of laptops for free internet use.

Poster awards
There will be a poster award for the best poster presentation in each poster session on Monday, Tuesday, and Thursday. All participants are welcome to cast their vote and choose the best poster presentation. Poster awards are kindly provided by Wiley VCH.

Conference Publication
Invited and contributed presentations from IWEPNM 2018 are scheduled for publication as a special issue in physica status solidi (pss) (b). **Manuscript submission is due on April 27th.** In selected cases articles are highlighted in pss (RRL) (Reviews@RRL, Rapid Research Letters) or Advanced Electronic Materials. A hardcover 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**. Manuscripts of contributed presentations are limited to 6 pages (no page limit for invited presentations). We strongly recommend using the Word or Latex templates to get an accurate estimate of the article length.
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 option "IWEPNM 2018: Electronic Properties of Novel Materials". If you intend to submit a "Rapid Research Letter", a "Feature Article" or a manuscript to Advanced Electronic Materials, please consult with the editors at iwepnm-publication@physik.fu-berlin.de.

IWEPNM 2018
CHAIRPERSONS FOR THE ORAL SESSIONS

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

Sunday, 18.03.	morning	Janina Maultzsch
	morning, after coffee break	Hans Kuzmany
	evening	Siegmar Roth
Monday, 19.03.	morning	Andreas Hirsch
	morning, after coffee break	Christophe Voisin
	evening	Anke Krüger
Tuesday, 20.03.	morning	Sebastian Heeg
	morning, after coffee break	Xi Ling
	evening	Agnieszka Kuc
Wednesday, 21.03.	morning	Stephanie Reich
	morning, after coffee break	Shigeo Maruyama
	evening	Toby Hallam
Thursday, 22.03.	morning	Andreas Knorr
	morning, after coffee break	Ralph Krupke
	evening	Elena Obraztsova
Friday, 23.03.	morning	M. Eugenia Pérez-Ojeda
	morning, after coffee break	Aravind Vijayaraghavan
	evening	Claudia Backes

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

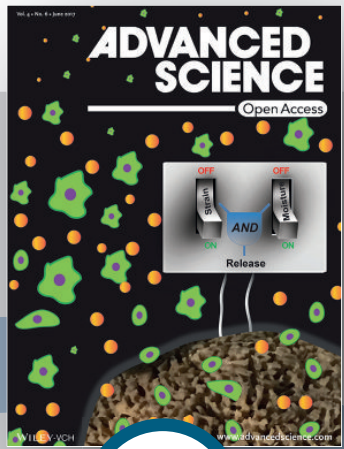
ABSTRACTS

Final program

	Sunday, March 18	Monday, March 19	Tuesday, March 20	Wednesday, March 21	Thursday, March 22	Friday, March 23
Topics	**Graphene QD, topological materials, electron microscopy**	**Carbon nanostructures: synthesis and applications**	**2D materials: optics; graphene**	**CNT optics and applications**	**2D, 1D, 0D materials: optoelectronics and magnetism**	**Chemistry of 2D materials; CNT and graphene synthesis**
08:30	Tuning pseudospin polarization and valley splitting of graphene by a STM MORGENSTERN	Bottom-up synthesis of functional molecule-based nanosheets SAKAMOTO	Exciton propagation in atomically thin semiconductors CHERNIKOV	TUTORIAL Optical and Charge Transport Properties of Dense Films of Semiconducting Carbon Nanotubes ZAUMSEIL	TUTORIAL Interaction and Topological Effects in Atomically Thin Two-dimensional Materials LOUIE	2D Nanomaterials, Nanomachines and Sensing PUMERA
09:00	Conductance quantization and Coulomb blockade in bilayer graphene IHN	The synthesis and properties of diamond nanomaterials KRÜGER	Excitons in monolayer-thin transition metal dichalcogenides GLAZOV			Liquid exfoliation as versatile technique to study fundamental properties of 2D materials BACKES
09:30	Topological Materials with liquid electrons FELSER	Graphene Nanoribbon Heterostructures RUFFIEUX	Exciton Based Description of Atomically Thin Semiconductors: Optical Lineshape, Intervalley Coupling, Luminescence Dynamics KNORR	Bright and tunable single-photon source with carbon nanotubes. VOISIN	Realization of an Electrically Tunable Narrow-Bandwidth Atomically Thin Mirror Using Monolayer $MoSe_2$ KRONER	Tuning Electronic Structure of 2D Chalcogenide Materials KUC
10:00	**Coffee break**					
10:30	Topology and Correlations in Monolayer WTe_2 WU	Electronic band structure characterization and *in-situ* Raman Spectroscopy of Chemically Functionalized Graphene Nanoribbons GRÜNEIS	Charge Versus Energy Transfer in Atomically Thin Graphene-Transition Metal Dichalcogenide van der Waals Heterostructures BERCIAUD	Direct measurement of a locally modulated gap transition at defects in carbon nanotubes SENGA	Light-Matter coupling in two dimensional materials SCHNEIDER	Structure Characterization of Catalysts and Single-Walled Carbon Nanotubes in Chirality-Specified Synthesis LI
11:00	The many faces of the 2D topological semimetal WTe_2 COBDEN	Optical properties of graphene nanopieces LAURET	Resonance Raman Spectroscopy of 2-dimensional materials CHEONG	Diameter-controlled stacking of functional molecules in single wall carbon nanotubes WENSELEERS	Tuning a Circular p-n Junction in Graphene from Quantum Confinement to Optical Guiding JIANG	Separation of Double Walled Carbon Nanotubes FLAVEL
11:30	Robust spin-polarized midgap states at step edges of topological crystalline insulators DI SANTE	Light-field-driven electron dynamics in graphene HIGUCHI	Theory of Resonant Raman Spectroscopy and Valley-Depolarization in Transition Metal Dichalcogenides WIRTZ	Monopole nanoantennas for near-field scanning optical microscopy CANCADO	Graphene as a 'tunneling barrier' in vertical magnetoresistive junctions GRIGORIEVA	Size-Controlled Growth of Single-Crystal Graphene Domains by CVD CHENG

	Sunday, March 18	Monday, March 19	Tuesday, March 20	Wednesday, March 21	Thursday, March 22	Friday, March 23
12:00 - 17:00	Mini workshops	Mini workshops	Mini workshops	Mini workshops	Mini workshops	Mini workshops
17:00 - 18:30	Dinner					17:00 Phonon spectroscopy of nanomaterials using angstrom-size electron beams LAGOS
18:30	TUTORIAL Transmission Electron Microscope Imaging of 2D Heterostructures Stacks HAIGH	Toxicity of Nanomaterials HADRUP	Controlling optical absorption of graphene by gate voltage in dielectric multilayer SAITO	Coiling and twisting nanotubes JOSELEVICH	Endohedral metallofullerenes as robust single molecule magnets POPOV	17:30 Probing interlayer interaction in van der Waals materials VAN DER MOLEN
19:00		Carbon nanotube based electronic and optoelectronic devices PENG	Flat bands, magnetism, half-metallic behavior and spin current polarization in multilayer rhombohedral graphene MAURI	Excitons in two-dimensional semiconductors 'talking' to their environment BOLOTIN	Molecular quantum spintronics GANZHORN	18:00 Conference Summary STAMPFER
19:30	Towards atomically precise manipulation of 2D nanostructures in the electron microscope SUSI	Aligning liquid crystals and rotating light polarization with carbon nanotube sheets SCALIA	Material challenges and opportunities in next generation electronics KIM	Van-der-Waals heterostructures based on dry transferred high-mobility CVD graphene BANSZERUS	Photovoltaic perovskite nanowires: from fundamental aspects to applications FORRO	18:30 - 20:00 Break
20:00	Electron Microscopy and Spectroscopy of Low-dimensional Nano-Materials at the Single Atom Level SUENAGA	Poster I Monday	Poster II Tuesday	Polaritons in layered two-dimensional materials KOPPENS	Poster III Thursday	Bauernbuffet Farewell
20:30						
Topics	**Graphene QD, topological materials, electron microscopy**	**Carbon nanostructures: synthesis and applications**	**2D materials: optics; graphene**	**CNT optics and applications**	**2D, 1D, 0D materials: optoelectronics and magnetism**	**Chemistry of 2D materials; CNT and graphene synthesis**

Materials Science Matters



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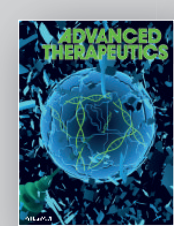

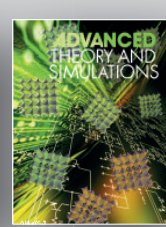

* 2017 Release of Journal Citation Reports® Source: 2016 Web of Science Data

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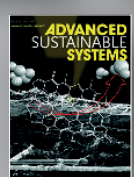

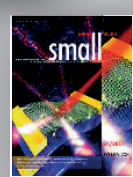

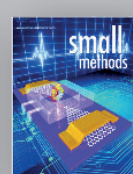

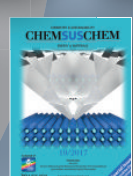

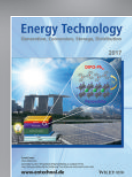

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ADVANCED SCIENCE NEWS

WILEY

08:30 – 09:00 M. Morgenstern, Aachen
Tuning pseudospin polarization and valley splitting of graphene by a scanning tunneling microscope

09:00 – 09:30 T. Ihn, Zurich
Conductance quantization and Coulomb blockade in bilayer graphene

09:30 – 10:00 C. Felser, Dresden
Topological Materials with liquid electrons

10:00 – 10:30 coffee break

10:30 – 11:00 S. Wu, Boston
Topology and Correlations in Monolayer WTe_2

11:00 – 11:30 D. Cobden, Washington
The many faces of the 2D topological semimetal WTe_2

11:30 – 12:00 D. Di Sante, Würzburg
Robust spin-polarized midgap states at step edges of topological crystalline insulators

12:00 – 17:00 mini workshops

17:00 – 18:30 Dinner

18:30 – 19:30 TUTORIAL: S. Haigh, Manchester
Transmission Electron Microscope Imaging of 2D Heterostructures Stacks

19:30 – 20:00 T. Susi, Vienna
Towards atomically precise manipulation of 2D nanostructures in the electron microscope

20:00 – 20:30 K. Suenaga, Tsukuba
Electron Microscopy and Spectroscopy of Low-dimensional Nano-Materials at the Single Atom Level

08:30

Tuning pseudospin polarization and valley splitting of graphene by a scanning tunneling microscope

Markus Morgenstern[1]
[1]II. Institute of Physics B, RWTH Aachen, Aachen

Graphene provides two extra binary degrees of freedom, -sublattice and valley-, which are adequately described as a pseudospin. The sublattice pseudospin is chiral mimicking the relativistic real spin completely. Here, I firstly show that application of large pseudomagnetic fields B_{ps} ($\sim$1000 T) can be used to polarize the sublattice pseudospin up to 40 %. Therefore, the van-der Waals force of an STM tip lifts graphene from the SiO_2 substrate and, thus, induces huge strain gradients, i.e. $|B_{ps}|$. The resulting sublattice imbalance, directly read from STM images, is in excellent agreement with analytic calculations based on the strain field from molecular dynamics.
Secondly, the valley degree of freedom is tuned using a quantum dot which is induced by the tip potential in combination with a B field. The laterally changing orientation of graphene's C atoms with respect to the B and N atoms on an aligned BN substrate changes the valley splitting of the confined state by up to 15 meV including an inversion. The mapped valley addition energies as a function of position of the quantum dot are reproduced by tight-binding calculations based on parameters from DFT.

9:00
Conductance quantization and Coulomb blockade in bilayer graphene
Thomas Ihn[1]
[1]Physics Department, ETH Zurich, Zürich

It is possible to open a band-gap in bilayer graphene by applying a so-called displacement field normal to the layer plane. We exploit this property for confining charge carriers laterally by electrostatic means. One-dimensional quantum point contact geometries show indications of conductance quantization. The quantized energy levels exhibit interesting degeneracies at zero magnetic field and peculiar magnetic field dispersions. In quantum dot geometries, we are able to analyze the single-particle energy spectrum of states for few-electron and hole dots. In addition to the four-fold level degeneracies and level-bunching effects well-known from carbon nanotubes, we measure a strong orbital Zeeman effect, which completely dominates over the spin-related Zeeman effect in a perpendicular magnetic field. The latter can, however, be quantitatively measured in parallel field configuration, giving the expected g-factor of 2. The behavior of the lowest energy states for the first few electrons or holes in a magnetic field are in good agreement with existing theories for quantum dots in bilayer graphene.

09:30
Topological Materials with liquid electrons
Claudia Felser[1]
[1]Max Planck Inst. for Chemical Physics of Solids, Dresden

Topology a mathematical concept became recently a hot topic in condensed matter physics and materials science. One important criteria for the identification of topological material is the band inversion and the crystal symmetry. In my talk, I focus on new topological semimetals: Weyl semimetals. Binary phosphides are the ideal material class for a systematic study of Weyl physics. Weyl points, a new class of topological phases was also predicted in NbP, NbAs, TaP, MoP and WP_2. In NbP micro-wires we have observed the chiral anomaly but NbP has served also as a model system for astrophysics: realizing the gravitational anomaly in NbP and the hydrodynamic flow of electrons in WP_2. MoP and WP_2 show exceptional properties such as high conductivity higher than copper, high mobilties and a high magneto-resistance effect. In magnetic materials, the Berry curvature measured via the classical anomalous Hall effect helps to identify interesting candidates for magnetic topological materials and devices.

10:30
Topology and Correlations in Monolayer WTe_2
Sanfeng Wu[1]
[1]Physics, Massachusetts Institute of Technology, Cambridge

Topology and correlations are two fundamental aspects that determine the electronic states of condensed matter systems. Both aspects individually have led to striking observations such as the quantum spin Hall insulating state and superconductivity, respectively. The combination of them can result in exotic phenomena including topological superconductivity and non-abelian anyons. In this talk I will discuss our recent study on monolayer tungsten ditelluride (WTe_2), where we find that topology and correlations are simultaneously important in understanding its ground state properties. I will first talk about our quantum transport measurements for identifying the undoped monolayer WTe_2 as a two-dimensional topological insulator. The observation of the quantum spin Hall effect surviving up to 100 K will be discussed. I will then report the observation of superconductivity below 1 K when the same monolayer is electrostatically doped through dielectric gating. Our results establish monolayer WTe_2 as a novel material platform for studying rich electronic phenomena driven by topology and correlations, allowing for the creation and detection of non-abelian quantum particles.

11:00

The many faces of the 2D topological semimetal WTe_2

David Henry Cobden[1]
[1]Department of Physics, University of Washington, Seattle

Semimetals, with their small and often complicated Fermi surfaces, have received renewed attention recently as hosts of topological features such as Dirac and Weyl points. Many have van der Waals layered structures, allowing exploration of their physics down to the monolayer limit. In the case of WTe_2, we have found a diverse range of interconnected phenomena in this limit. The monolayer exhibits edge conduction consistent with the helical boundary modes of a 2D topological insulator persisting up to room temperature, albeit with substantial backscattering at low temperatures of unknown origin. Meanwhile, the bulk of a monolayer varies between insulating, metallic and superconducting states as a function of temperature and gate voltage. Quantum oscillations indicate that a weak Fermi surface is present down to the level of a bilayer, but in the non-superconducting monolayer state the magnetic field dependence is very weak, raising questions as to how the extreme magnetoresistance of the 3D bulk arises. The material is also polar, and behaves as a highly controlled ferroelectric up to room temperature. We speculate that electron-hole correlations play a role in all these phenomena.

11:30

Robust spin-polarized midgap states at step edges of topological crystalline insulators

Domenico Di Sante[1], Paolo Sessi[2], Martin Greiter[1], Titus Neupert[3], Giorgio Sangiovanni[1,3], Tomasz Story[4], Ronny Thomale[1], Matthias Bode[2]
[1]Institut fuer Theoretische Physik und Astrophysik, Universitaet Wuerzburg, Wuerzburg
[2]Experimentelle Physik II, Universitaet Wuerzburg
[3]Physik Institut, Universitaet Zuerich, Switzerland
[4]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Topological crystalline insulators are materials in which the crystalline symmetry leads to topologically protected surface states with a chiral spin texture, rendering them potential candidates for spintronics applications. In this talk, I report on the discovery of one dimensional midgap states at odd atomic surface step edges of the three dimensional topological crystalline insulator (Pb,Sn)Se. A minimal toy model and realistic tight-binding calculations identify them as spin polarized flat bands connecting two Dirac points. The midgap states inherit stability through the two dimensional Dirac metal from the three dimensional bulk insulator. This makes (Pb,Sn)Se the first example for a crystal symmetry protected hierarchy of one and two dimensional topological modes, which we experimentally prove to result in a striking robustness to defects, strong magnetic fields, and elevated temperature.

P.Sessi, D. Di Sante *et. al*, Science 354 1269 (2016)

18:30
TUTORIAL: Transmission Electron Microscope Imaging of 2D Heterostructures Stacks

Sarah Haigh[1,2], Aidan Rooney[1,2], Lan Nguyen[1], Daniel Kelly[1,2], Nick Clark[2], Irina Grigorieva[2], Andre Geim[2], Roman Gorbachev[2]
[1]Materials, University of Manchester, Manchester
[2]National Graphene Institute, UK

2D crystals can be layered together to create new van der Waals (vdW) crystals with bespoke properties. The performance of such materials is strongly dependent on the quality of the crystals and the interfaces at the atomic scale. Transmission electron microscopy (TEM) is the only technique able to characterize the structure of encapsulated crystals and reveal the nature of buried interfaces in these engineered vdW crystals. In this talk I will introduce some of the latest capabilities of (scanning) TEM imaging for heterostructure characterisation. I will report the use of TEM imaging and analysis techniques to provide insights to aid the development of 2D heterostructures for a range of applications including electronics and ion membranes.[1-5] I will further report on the use of the 2D heterostructure platform to enable new capabilities for STEM and TEM imaging of samples in liquids [6].

[1] Boya *et al.*, Nature, 538, 222–225 (2016)
[2] Vasu *et al.*, Nature Comms, 7, 12168 (2016)
[3] Cao *et al.*, Nano Letters, 15, 4914-4921 (2015)
[4] Nguyen *et al.*, ACS Nano, 11, 2894-2904 (2017)
[5] Rooney *et al.*, Nano Letters, 17, 5222–5228 (2017)
[6] Kelly *et al.*, Nano Letters, article asap 2017

19:30

Towards atomically precise manipulation of 2D nanostructures in the electron microscope

Toma Susi[1], Mukesh Tripathi[1], Jannik C. Meyer[1], Jani Kotakoski[1]
[1]University of Vienna, Faculty of Physics, Vienna

Single-atom manipulation using the Ångström-sized electron probe of a scanning transmission electron microscope is emerging as a fundamentally new tool for the direct assembly of nanostructures. While momentum transfer from highly energetic electrons often leads to atom ejection [1], interesting dynamics can be induced when the transferred kinetic energies are comparable to bond strengths in the material [2]. Operating in this regime, targeted 60-keV irradiation allows us to manipulate Si impurities in graphene. In our latest experiments, we have achieved 34 controlled single-site jumps with a rate already comparable to state-of-the-art in fully automated scanning tunneling microscopy [3]. Sample quality thus appears to be the principal challenge in creating 2D nanostructures from multiple Si atoms in the near future [4]. I will also discuss the beam-driven dynamics and manipulation potential of other heteroatoms [5].

[1] T. Susi et al., Nat. Commun. 7:13040 (2016)
[2] T. Susi et al., Phys. Rev. Lett. 113, 115501 (2014)
[3] T. Susi et al., arXiv:1712.08755
[4] D. Nosraty Alamdary et al., Phys. Status Solidi B, 1700188 (2017)
[5] T. Susi et al., 2D Materials 4, 042004 (2017)

20:00
Electron Microscopy and Spectroscopy of Low-dimensional Nano-Materials at the Single Atom Level
Kazu Suenaga[1]
[1]AIST, Tsukuba

Properties of nano-materials are largely influenced by its structural imperfections, such as defects, impurities, edges or boundaries. Hence, analytical technique at single atom level is becoming crucial to fully understand the physical/chemical performance of nano-devices. In my presentation, single atom spectroscopy by means of electron energy-loss spectroscopy (EELS) will be shown to discriminate individual atoms in low-dimensional materials at their interrupted periodicities. It is emphasized here that information of the bonding/electronic states has become accessible for single atoms through the EELS fine-structure analysis as well as the spin state [1]. Large variations of local electronic properties of low-dimensional materials with different atomic coordinates will be investigated. Further, a high-energy resolution EELS offers us possibilities to obtain local optical/vibrational properties. Some of the recent examples for such experiments on low-dimensional nanomaterials will be also presented [2, 3].

[1] Y.-C. Lin *et al.*, Phys. Rev. Lett., 115, 206803 (2015)
[2] J. Lin *et al.*, NanoLett., 16, 7198 (2016)
[3] L. Tizei *et al.*, Phys. Rev. Lett., 114, 107601 (2015)

08:30 – 09:00	R. Sakamoto, Tokyo *Bottom-up synthesis of functional molecule-based nanosheets*
09:00 – 09:30	A. Krüger, Würzburg *The synthesis and properties of diamond nanomaterials*
09:30 – 10:00	P. Ruffieux, Dübendorf *Graphene Nanoribbon Heterostructures*
10:00 – 10:30	coffee break
10:30 – 11:00	A. Grüneis, Cologne *Electronic band structure characterization and in-situ Raman Spectroscopy of Chemically Functionalized Graphene Nanoribbons*
11:00 – 11:30	J. Lauret, Orsay *Optical properties of graphene nanopieces*
11:30 – 12:00	T. Higuchi, Erlangen *Light-field-driven electron dynamics in graphene*
12:00 – 17:00	mini workshops
17:00 – 18:30	Dinner
18:30 – 19:00	N. Hadrup, Copenhagen *Toxicity of Nanomaterials*
19:00 – 19:30	L. Peng, Beijing *Carbon nanotube based electronic and optoelectronic devices*
19:30 – 20:00	G. Scalia, Luxembourg *Aligning liquid crystals and rotating light polarization with carbon nanotube sheets*
20:00	Poster Session I

08:30

Bottom-up synthesis of functional molecule-based nanosheets

Ryota Sakamoto[1,2]

[1]Department of Chemistry, School of Science, The University of Tokyo, Tokyo

[2]JST-PRESTO

Molecule-based two-dimensional polymers are ultrathin polymeric frameworks with in-plane periodicity. They can be synthesized in a direct, bottom-up fashion using atomic, ionic, or molecular components. However, few are based on carbon–carbon bond formation, which means that there is a potential new field of investigation into these fundamentally important chemical bonds. Here we describe the bottom-up synthesis of all-carbon, pi-conjugated graphdiyne nanosheets. A liquid/liquid interfacial protocol involves layering a dichloromethane solution of hexaethynylbenzene on an aqueous layer containing a copper catalyst at room temperature. A multilayer graphdiyne (thickness: 24 nm; domain size: >25 microns) emerges through a successive alkyne–alkyne homocoupling reaction at the interface. A gas/liquid interfacial synthesis is more successful. Sprinkling a very small amount of hexaethynylbenzene in a mixture of dichloromethane and toluene onto the surface of the aqueous phase at room temperature generated single-crystalline graphdiyne nanosheets, which feature regular hexagonal domains, a lower degree of oxygenation, and uniform thickness (3.0 nm) and lateral size (1.5 microns).

09:00

The synthesis and properties of diamond nanomaterials

Anke Krüger[1]
[1]Institute for Organic Chemistry, Wuerzburg University, Wuerzburg

The properties of carbon materials strongly depend not only on the type of hybridization (sp^2 vs. sp^3) but also on the size of the carbon nanoobject and the actual orientation and morphology of its surface. Additionally, the surface termination plays a major role in the surface chemistry that is subsequently accessible for the respective carbon nanomaterial.
Here we discuss the production of differently terminated nanodiamond materials and their physicochemical properties. Furthermore, the functionalization of different types of nanodiamond and its influence on the materials properties will be presented. Such efforts aim at the synthesis of tailored functional diamond materials for applications such as (photo)catalysis, energy transformation and storage as well as biomedical applications.
This project has received funding from the European Union´s Horizon 2020 Program under Grant Agreement no. 665085 (DIACAT).

09:30
Graphene Nanoribbon Heterostructures
Pascal Ruffieux[1]
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The bottom-up fabrication strategy [1] has introduced the possibility to grow carbon nanostructures with atomic precision and hence allows to controllably tune their electronic properties. The approach building on the predefined covalent assembly of specifically designed precursor monomers has been successfully applied for the synthesis of various types of graphene nanoribbons (GNRs), including armchair GNRs with width-controlled electronic band gaps [2] as well as zigzag GNRs with their characteristic edge states [3]. Here, I will review recent advances in the bottom-up fabrication of GNRs and describe the fabrication of prototypical devices with GNRs as active material [4]. An even wider range of properties is accessed by creating GNR heterostructures where different types of GNRs are seamlessly stacked along the GNR axis [5]. An overview of properties achieved in these systems will be presented.

[1] J. Cai *et al.*, Nature 466, 470 (2010).
[2] L. Talirz, *et al.*, Adv Mater Weinheim 28, 6222 (2016).
[3] P. Ruffieux, *et al.*, Nature 531, 489 (2016).
[4] J. P. Llinas, *et al.*, Nature Communications 8, 633 (2017).
[5] S. Wang, *et al.*, Nano Lett 17, 4277 (2017).

10:30

Electronic band structure characterization and *in-situ* Raman Spectroscopy of Chemically Functionalized Graphene Nanoribbons

Alexander Grüneis[1], Boris Senkovskiy[1], Martin Hell[1], Markus Pfeiffer[2], Klas Lindfors[2], Danny Haberer[3], Felix Fischer[3]
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[2]Department für Chemie, Universität zu Köln, Germany
[3]Department of Chemistry, University of California at Berkeley, USA

Graphene nanoribbons (GNRs) combine the advantages inherent to graphene (flatness and uniformity) and nanotubes (one-dimensionality and large structural variety). GNRs can be grown by bottom-up polymerization from organic precursors. The choice of the precursor molecule alone dictates all resulting GNR properties. In the present work we investigate functionalized GNRs on Au(788) by a combination of angle-resolved photoemission and Raman spectroscopy carried out in a unique ultra-high vacuum (UHV) Raman system. UHV Raman spectroscopy [1] is especially important for *in-situ* synthesis and characterization of air-sensitive GNRs. In particular we show that 1) alkali metal doping can turn semiconducting GNRs into 1D metallic wires [1], 2) hydrogen sp3 defects can render GNRs luminescent [2] and 3) substitutional boron atoms alter the GNR-substrate interactions. The Raman spectra of functionalized GNRs are rationalized by calculations and comparison to the corresponding graphene system. Finally, we perform alignment-preserving bubbling-transfer and spectroscopy [2] of GNRs transferred onto plasmonic substrates.

[1]Adv.El.Mat. 3,1600490,(2017).
[2]Nano Lett. 17,4029(2017).

11:00

Optical properties of graphene nanopieces

Shen Zhao[1], Loïc Rondin[1], Julien Lavie[2], Lucile Orcin-Chaix[1,2], Klaus Müllen[4], Akimitsu Narita[4], Christophe Voisin[3], Stéphane Campidelli[2], Jean-Sébastien Lauret[1]
[1]Laboratoire Aimé Cotton, CNRS, Univ Psud, ENS Cachan, Orsay, France
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[3]LPA, ENS Paris, France
[4]MPG, Mainz, Germany

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 [1], which is a prerequisite before you can imagine controlling their properties. In this presentation, we will show our recent results on the optical properties of both graphene quantum dots and nanoribbons synthesized by bottom-up chemistry.

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

11:30
Light-field-driven electron dynamics in graphene
Takuya Higuchi[1]
[1]Department of Physics, University of Erlangen (FAU), Erlangen

When solids are exposed to intense optical fields, the intraband electron motion may influence interband transitions, potentially causing a transition of light-matter interaction from a quantum (photon-driven) regime to a semi-classical (field-driven) regime. We demonstrate this transition in monolayer graphene [1]. We observe a carrier-envelope-phase-dependent current in graphene irradiated with phase-stable two-cycle laser pulses, showing a striking reversal of the current direction as a function of the driving field amplitude at 2 V/nm. This reversal indicates the transition into the field-driven (or strong-field) regime. We show furthermore that in this regime electron dynamics are governed by sub-optical-cycle Landau-Zener-Stückelberg interference, comprised of coherent repeated Landau-Zener transitions. We expect these results to have direct ramifications for light-wave driven electronics in graphene.

[1] T. Higuchi, C. Heide, K. Ullmann, H. B. Weber, and P. Hommelhoff, Nature 550, 224 (2017).

18:30
Toxicity of Nanomaterials
Niels Hadrup[1]
[1]National Research Centre for the Working Environme, Copenhagen

Toxicity deals with the unwanted effects of materials on the human body. In theory everything is toxic if the dose is high enough. The drinking of pure water has e.g. caused deaths. Thus, the question is not whether nanomaterials are toxic – but at which doses?
For determining this, a range of data can be used, including human, animal, cell culture, and computational data. Also the route of exposure is important. Do we foresee that humans will be exposed e.g. by food (oral) by skin or by inhalation? And can we foresee how high the exposure will be?
When developing a novel nanomaterial we can already at the scoping stage look into the toxicity literature. This can help predict at which levels the material is likely to become toxic and whether these levels are sufficiently low compared to the expected exposure. This is what we call "safe by design".
Also upon manufacture we can determine safe nanomaterial dose levels in animals. These levels are then used to assess levels that are safe for humans by the application of so called assessment factors. By division with these we take into account that animals are not humans and that all humans are not equally healthy.

19:00

Carbon nanotube based electronic and optoelectronic devices

Lian-Mao Peng[1]
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CNT-based electronics has been considered one of the most promising candidates to replace Si CMOS technology. Prototype device studies on individual CNTs revealed that CNT based devices have the potential to outperform Si CMOS technology in both performance and power consumption, especially at sub-10 nm technology nodes, which are close to the theoretical limits; and various optoelectronic device such as light-emitting diodes, photodetectors and photovoltaic cells have been demonstrated. Very recently, both p-type devices and integrated systems were fabricated using CNT films. However, the key performance metrics demonstrated by these devices are still substantially lower than those of conventional semiconductor based devices. In this talk, I will discuss the use of randomly oriented CNT film to build CNT CMOS and optoelectronic devices, and show that the performance of CNT film devices and systems can be dramatically improved by optimizing the material purity, device structure and fabrication processes, thus yielding CNT devices with outstanding performance comparable to that of Si CMOS and ICs working in the GHz regime, and integrated electronic and optoelectronic systems for communications between nanoelectronic circuits using CNT devices.

19:30

Aligning liquid crystals and rotating light polarization with carbon nanotube sheets

Kieu-Thuy Truong[1], Ji Hyun Park[2], MD Asiqur Rahman[3], Hakam Agha[3], Dongseok Suh[1], Giusy Scalia[3]

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[3]Physics and Material Science Unit, University of Luxembourg, 162a, avenue de la Faïencerie, L-1511, Luxembourg

Multifunctional layers for liquid crystals (LCs) can be realized using sheets of carbon nanotubes (CNTs). In typical configurations for LC displays key functions are implemented with passive layers as transparent electrodes, usually made by indium tin oxide, and aligning layers by rubbed polymer films. The former are needed for applying electric fields to reorient LC molecules while the latter to promote LC alignment. Interestingly, also CNT sheets can be used for creating monodomains of unidirectionally aligned LCs. This means that sheets of CNTs can act as aligning layers as well as transparent electrodes combining functions traditionally supplied by different layers in LCDs. We show that LCs can be indeed aligned and reoriented in structures containing sheets of CNTs. The type and strength of anchoring of LC on surfaces determines the electro-optic behavior of LCs however, the aligning effect of CNT sheets is also due to geometrical constrain of LC molecules between the oriented CNT ridges. As we will describe the optical anisotropy of CNT sheets has also importance when they are combined with LCs due to its effects on polarized light.

MON 1
Formation and Characterization of Black Phosphorus Intercalation Compounds with Alkali Metals

Vicent Lloret[1], Gonzalo Abellán[1], Stefan Wild[1], Christian Neiss[2], Katharina Werbach[3], Julio C. Chacón-Torres[4], Filippo Fedi[3], Andreas Görling[2], Herwig Peterlik[3], Thomas Pichler[3], Frank Hauke[1], Andreas Hirsch[1]
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[2]Lehrstuhl für Theoretische Chemie, Friedrich-Alexander-Universität-Erlangen-Nürnberg (FAU)
[3]Faculty of Physics, University of Vienna
[4]Yachay Tech University, School of Physical Sciences and Nanotechnology

The formation of Black Phosphorus Intercalation Compounds (BPICs) has been pursued for many years yet its synthesis and characterization remain rather unexplored.[1,2] Herein, we report the bulk synthesis of BPIC with alkali metals by vapor phase as well as in solid state reaction.[3] The characterization of BPICs in vapor phase has been studied in detail by in-situ Raman spectroscopy, energy-dispersive X-ray spectroscopy (EDX) and X-ray diffraction (XRD) complementing the obtained results with DFT calculations. Furthermore, through a vapor transport intercalation under ultra-high vacuum monitored by in situ Raman spectroscopy, a series of novel Raman modes ascribed to the BPICs have been determined. Our results provide a glimpse into the very first steps of a new family of intercalation compounds, with a distinct behavior as compared to its graphite analogues (GICs), showing a remarkable structural complexity and a dynamic behavior.

[1] Synth. Met. 18, 559–564 (1987)
[2] Nat. Commun. 8, 15036 (2017)
[3] Angew. Chem. Int. Ed. 56, 15267 (2017)

MON 2
Chemical Vapor Deposition of MoS2 Monolayer and heterostructures

Xi Ling[1]
[1]Department of Chemistry, Boston University, Boston

Atomically thin two-dimensional (2D) materials, due to its ultra-flexible nature and diverse properties covering from metal (e.g. graphene), to semiconductor (e.g. MoS_2) to insulator (e.g. hexagonal boron nitride), have been considered as promising candidates not only to advance the forefront of semiconductor industry, but also as the key elements for future ubiquitous electronics. For their practical application, some challenges should be solved, such as the large-area synthesis and assembly, properties study, and applications exploration. In this talk, I will introduce the synthesis of 2D materials (e.g. MoS_2) using chemical vapor deposition (CVD) method, and our research progress in direct assembly of diverse 2D materials into both vertically stacked and horizontally stitched heterostructures during growth process. The

methodology enables the large-scale fabrication of diverse heterostructures with arbitrary patterns, and clean and precisely aligned interfaces, regardless of lattice matching between the components, which offers tremendous potential for its application in integrated circuits.

MON 3
Optomechanical measurement of thermal properties of $MoSe_2$

Nicolas Morell Bennasser[1], Antoine Reserbat-Plantey[1], Slaven Tepsic[1], Xavier Marie[2], Adrian Bachtold[1]
[1]Quantum NanoMechanics, ICFO-Institute of Photonic Sciences, Castelldefels (Barcelona)
[2]INSA, Toulouse, France

Thermal properties of 2D solids is a key parameter for both 2D based applications and fundamental studies (role of dimensionality in thermal transport, hybrid devices). While Raman and electrical measurements have established the record thermal conductivity of graphene, thermal properties of monolayer transition metal dichalcogenides (TMD) remains challenging to measure.

I will show our latest results on thermal conductance (K) of $MoSe_2$ suspended monolayers. We report a variation from K=2·10^{-6} W/K at room temperature, in agreement with previous calculations, given the sample geometry. By reducing the temperature, the thermal conductance first slightly increases before drastically going down at lower temperatures. It separates a regime where thermal conduction is governed by phonon-phonon interactions (high temperatures) from a regime where the phonon mean free path becomes larger than the grain size (diffusive) or the sample dimensions (ballistic). At low temperatures, such optomechanical measurement remains efficient at low laser power (0.1-1 μW), thus avoiding lattice heating by more than 1 K.

MON 4
In-situ modification of two-dimensional materials

Kyrylo Greben[1], Kirill Bolotin[1]
[1]Department of Physics, Freie Universität Berlin, Berlin

An attractive strategy to create new types of 2D matter is to functionalize defect sites in original 2D materials. However, freshly generated defects are extremely reactive to the environment, which immediately influences the quality and homogeneity of a functional layer.

Here we explore the controlled chemical functionalization of freshly generated defects inside 2D materials in a vacuum environment.

We developed the set-up that combines *in-situ:* 1) generation of functional and structural defects by means of controllable RF-plasma, 2) doping and surface functional-

ization using gasses and organic molecules and 3) measurement of the Raman and photoluminescence spectra of various 2D materials.
We generated more than 10^{13} cm^{-2} defects in graphene and TMDCs. These defects are stable in vacuum and do not cause doping. During the controllable exposure to ambient conditions, we observe the gradual reduction of the defect density to less than 10^{12} cm^{-2}, accompanied by a simultaneous increase in doping reaching densities more than 10^{13} cm^{-2}.

MON 5
Coupling a terahertz-cavity to a carbon nanotube quantum dot

Federico Valmorra[1,2], K. Yoshida[3], L. Contamin[1], T. Cubaynes[1], M. Dartiailh[1], M. Desjardins[1], S. Massabeau[1], K. Hirakawa[3], J. Mangeney[1], A. Cottet[1], T. Kontos[1]
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One of the most interesting aspects of physics is the fundamental, coherent interaction of light and matter, down to the quantum level of countable photons and single electronic transitions. Studying the coupling of quantum dots to cavities lies at the basis of mesoscopic Quantum ElectroDynamics, the condensed-matter counterpart of cavity- and circuit-QED. Up to now these investigations have focussed on the microwave range, but it comes natural to extend them to the THz, where the energies of the quantum dots realised in a carbon nanotube lie. In this study we demonstrate the coupling of a THz-cavity, namely a split-ring resonator, to such quantum dots: the transport characterisation of the devices shows a region of suppressed conductance, close to zero bias, as large as the photon energy. This gap is reminiscent of the Franck-Condon blockade effect transposed to photons. Some transport features also hint at the presence of strong coupling between the cavity mode and the electronic transition, paving the way towards more complex condensed matter studies and pushing forward quantum optics in the THz frequency range.

MON 6
B-Doped Single Walled Carbon Nanotubes with record substitutional atoms

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[2]Department of Physics, Tokyo Metropolitan University, 1-1 Minami-Osawa, Hachioji-shi, Tokyo 192-0397 Japan

Introducing substitutional heteroatoms like boron on the C sites of single-walled carbon nanotubes (SWCNTs) imposes several dificulties. Among those, the use of a

setup able to withstand the aggressive B chemistry, the low yields of nanotubes, the low incorporation of dopants and the final presence of impurities that cannot be removed by standard purification make the production of these materials a considerable challenge. In this poster we report on various methods we have used towards the production of B-doped SWCNTs that grow in enough amounts that allow purification and keep a record substitutional doping. For instance, we have developed a method to use solid precursors in high vacuum CVD, which contain both carbon and the boron in its stoichiometry, which do not only effectively circumvent the experimental problems reported so far in the synthesis of these materials, but they are able to incorporate up to 19 at.% of B atoms in the samples as-grown. A purification process was developed in this work achieving a 8 % of sp^2 like substitution. The morphology of the tubes has been throughly examined and the B content has been estimated from XPS at bulk level.

MON 7
Impact of Many-Body Effects on Landau Levels in Graphene

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[2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany
[3]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg
[4]Radboud University, Institute for Molecules and Materials, 6525AJ Nijmegen, Netherlands
[5]Institute for Theoretical Physics, Vienna University of Technology, 1040 Vienna, Austria

We present magneto-Raman spectroscopy measurements on suspended graphene to investigate the charge carrier density-dependent electron-electron interaction in the presence of Landau levels. Utilizing gate-tunable magneto-phonon resonances, we extract the charge carrier density dependence of the Landau level transition energies and the associated effective Fermi velocity v_F. In contrast to the logarithmically divergence of v_F at zero magnetic field [1], we find a linear scaling of v_F as a function of charge carrier density, due to magnetic field-induced suppression of the long-range Coulomb interaction. We quantitatively confirm our experimental findings by performing tight-binding calculations on the level of the Hartree-Fock approximation [2]. We further estimate that the involved transition energies are reduced by an exciton binding energy of 6 meV [3].
[1] G. Yu *et al.*, Proc. Natl. Acad. Sci. U.S.A. 110, 3282 (2013)
[2] L. Chizhova *et al.*, Phys. Rev. B 92, 125411 (2015)
[3] J. Sonntag *et al.*, arXiv 1712.05648 (2017).

MON 8
Synthesis of Large-Area 2-Dimensional Molybdenum Disulfide Nanomaterials for Application in Solar Cells

Yang Qian[1], Taiki Inoue[1], Anton Anisimov[2], Shohei Chiashi[1], Esko I. Kauppinen[3], Jing Kong[4], Shigeo Maruyama[1,5]
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[5]Energy NanoEngineering Laboratory, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba 305-8564, Japan

2-dimensional transition metal dichalcogenide (TMD) nanomaterials have been focused on in recent years because of their intriguing properties that are different from bulk materials [1]. Unlike graphene, there is an intrinsic band gap in TMD nanomaterials, which further becomes direct gap in their monolayer forms. As a representative of TMD nanomaterials, monolayer molybdenum disulfide (MoS2) has a direct band gap of $\sim$1.9 eV, and thus opens its exciting prospects for a variety of optoelectronic applications, especially for solar cells [2, 3]. In this research, monolayer/multilayer MoS_2 films have been synthesized by low-pressure chemical vapor deposition. The as-synthesized large-area MoS2 films (cm level) show high quality through the characterizations of Raman and photoluminescence spectroscopy. The MoS_2 films have been further applied to heterojunction solar cells by fabricating MoS_2-carbon nanotube (CNT) hybrids. The properties and mechanisms of MoS_2-CNT hybrid solar cells will also be discussed.

[1] A. Geim et al., Nature 499, 419 (2014)
[2] Q. Wang et al., Nat. Nanotech. 7, 699 (2012)
[3] A. Polman et al., Science 352, 6283 (2016).

MON 9
Effect of SWCNT Composition on Polyfluorene-Based SWCNT Dispersion Selectivity

Han Li[1], Shuai Liang[2], Alex Adronov[2], Benjamin Flavel[1,3]
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[2]Department of Chemistry and Chemical Biology, McMaster University, Canada
[3]Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

Applications of single-walled carbon nanotubes (SWCNTs) are hampered by the mixtures of metallic and semiconducting SWCNTs that are present in commercial samples. Polyfluorene-based conjugated polymers are the most promising

candidates for the separation of SWCNTs according to electronic type. However, the mechanism responsible for this selectivity is poorly understood. To determine whether this polymer is only selective for semiconducting SWCNTs, we exposed it to mixtures of metallic and semiconducting SWCNTs in different ratios. We found that the polymer is indeed selective for semiconducting SWCNTs in toluene, but only when the starting ratio is below 75:25 metallic:semiconducting. When the starting ratio is increased to 75:25 or higher, the amount of metallic SWCNTs dispersed dramatically increases. If the solvent is changed to THF, the threshold ratio at which metallic SWCNTs begin to be dispersed is much lower. This indicates that the interaction selectivity is under kinetic control, where the polymer exhibits a preference for interaction with semiconducting SWCNTs, but is not precluded from interaction with metallic SWCNTs if exposed to a high enough concentration

MON 10

The Frst Molecular Dumbbell Consisting of an Endohedral Sc3n@C80 and an Empty C60-Fullerene Building Block

Tao Wei[1], M. Eugenia Pérez-Ojeda[1], Andreas Hirsch[1]
[1]Organische Chemie II, Friedrich-Alexander-Universität, Erlangen

An unprecedented hybrid dumbbell consisting of a metallofullerene and an empty fullerene was afforded via simple click reaction of suitable precursor derivatives of Sc3N@C80 and a C60 hexakisadduct. The structure of synthetic endohedral clusterfullerene-based dumbbell was unambiguously characterized by MALDI-TOF mass spectrometry and 1H NMR spectroscopy. The electronic structure was carefully studied by UV-vis-NIR spectroscopy revealing its exceptional electronic behaviour compared to parental building blocks. In combine with the electronic property study of congener dimer on basis of solo C60, the peculiar electronic property of dumbbell is unveiled. Our success on the first construction of endohedral clusterfullerene dumbbell opens up a new perspective in fullerene chemistry.

MON 11

Catalytically active single oxygen sites in the basal plane of 2D MoS_2 crystals by ambient oxidation

Levente Tapasztó[1], Janos Pető[1], Tamas Ollar[1], Peter Vancso[1], Zakhar Popov[2], Pavel B. Sorokin[2]
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[2]National University of Science and Technology MISiS, 119049 Moscow, Russia

A major objective in catalysis is the atomic level identification and control of catalytically active sites for a specific reaction. Here we propose that this can be realized in molybdenum disulfide (MoS_2) through a simple oxidation process. In contrast to the generally accepted view of environmentally inert basal plane, we found that during ambient exposure oxygen gradually incorporates into the basal plane of two-

dimensional (2D) MoS_2 crystals by replacing individual sulfur atoms. We were able to image this slow substitutional oxidation process at single-atom level by scanning tunneling microscopy. The O substitutional sites were identified as single-atomic active reaction centers for H2 evolution, extending the catalytic activity of MoS_2 crystals from edges over the entire basal plane. The substitutional oxidation of 2D MoS_2 crystals provides a novel chemical engineering method of unprecedented control to design highly efficient 2D electrocatalysts with a high density of single-atomic active basal plane sites.

MON 12
Towards Bottom-Up Synthesis of Carbon Nanostructures on Insulating Surfaces

Konstantin Amsharov[1]
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The sp2-carbon based nanostructures such as fullerenes, nanographenes, nanoribbons and single-walled carbon nanotubes display outstanding electronic properties and are considered to be leading materials for future electronics. The possibility to fabricate complex carbon nanostructures on metal surfaces has generate enormous expectations. However in order to construct truly working nano devices these structures should be transferred to an insulator. The next challenge in this field is a controlled synthesis of these unique materials directly on insulating surfaces. We have found that synthesis of such architectures can be realized rather effectively on various metal oxides via selective cyclodehydrofluorination of specially programmed precursor molecules. Our finding opens up a venue towards rational synthesis of carbon based nanomaterial by bottom-up strategy directly on insulating metal oxide surfaces.

MON 13
Microscopic theory of plasmon-enhanced light absorption and Raman scattering in graphene

Niclas Sven Mueller[1], Stephanie Reich[1]
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Plasmonic excitations in metallic nanostructures generate intense electromagnetic near fields that enhance optical processes in nearby materials. As a two-dimensional material, graphene interacts only weakly with light. The combination of graphene with plasmonic nanostructures is promising for enhancing its Raman response and its quantum efficiency in photo detectors.
We present a microscopic description of plasmon-enhanced optical absorption and Raman scattering in graphene, which is based on perturbation theory. We consider the interaction of graphene with a lattice of plasmonic nanoparticles, as was previously realized experimentally. By using tight-binding wave functions for the electronic states of graphene and the dipole approximation for the plasmon, we obtain

analytic expressions for the coupling matrix elements. The plasmonic nanostructure induces non-vertical optical transitions in the band structure of graphene with selection rules for the momentum transfer that depend on the periodicity of the plasmonic lattice. Our study leads to a better understanding of plasmon-induced optical transitions in graphene and can be used to improve graphene-based photonic devices.

MON 14
Perylene-based functionalization of carbon nanotubes

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Functionalization grants compounds with additional features, typically by attaching novel groups to the original systems. The characteristics of the yielded complexes often result in more than just the mere sum of the initial products. The specific character of the functionalized structure, moreover, depends upon the way the functionalization strategy has been pursued.
We focus here on carbon nanotubes (CNTs) functionalization through perylene, an aromatic molecule emitting in the excitation window of most single-walled CNTs. We showed that the perylene core of custom surfactants attached though $\pi - \pi$ stacking interactions onto the sidewall of CNTs while ensuring efficient excitation transfer to the tubes. Here we will show how starting from the same elements (perylene and CNTs) and pursuing different functionalization routines, we achieve systems with different features and functions. In particular, we will compare the characteristics of perylene-comprising polymers wrapped around the tubes with the peculiarities of perylene covalently attached to to the nanotubes following a novel conjugation-preserving routine we recently developed (Nat. Comm. 8, 14281 (2017)).

MON 15
Spin detection using a nanotube mechanical resonator

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Micro-scale mechanical resonators are highly sensitive force sensors, enabling the detection of very small ensembles of nuclear spins. Recently, we showed that mechanical resonators made of suspended carbon nanotubes display outstanding properties, such as quality factors up to 5 million, and force noise as low as 10^{-21} N/Hz$^{1/2}$. We propose to use this excellent sensitivity capability to detect and manipulate the nuclear spins of the ^{13}C atoms naturally present in the carbon nanotube. For this, we use a metallic nanowire patterned very close to the nanotube to

generate both the oscillating magnetic field and the magnetic field gradient, which are needed to manipulate the nuclear spins of the nanotube, and to detect them.

MON 16
CVD Growth and Heterostructures of Transition Metal Dichalcogenides

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Atomically-thin, -layered, two-dimensional (2D) materials such as graphene, transition-metal dichalcogenides (TMDs) and hexagonal boron nitride (h-BN) have gained ever increasing interest since the first isolation of monolayer graphene. TMDs are an interesting class of materials as they can be either (semi-)metallic or semi-conducting and their properties depend on the number of layers.
For the large- area synthesis of TMDs different methods such as thermally assisted conversion (TAC), atomic layer deposition (ALD) and chemical vapour deposition (CVD) are possible. To create large, highly- crystalline surfaces CVD is the most suited growth method. In this research the focus has been on microreactor CVD growth of WSe_2, MoS_2 and $MoSe_2$ and the production of TMD heterostructures. TMD heterostructures can facilitate efficient electron-hole separation due to the type-II band alignment and can be used for optoelectronic applications and pn-junctions.
The grown materials were characterised by optical microscopy, Raman spectroscopy, photoluminescence, atomic force microscopy (AFM) and electrical measurements.

MON 17
Observation of large strain-induced band gap modifications in MoS_2 nanobubbles formed at the 2D MoS_2/Au (111) interface

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Unlike graphene, most materials from the 2D transition metal dichalcogenide family exhibit semiconductor behavior possessing a direct band gap. This makes these crystals especially useful in electronic and optoelectronic applications. To fully realize their potential we have to be able to fine-tune their properties according to specific requirements. One way to accomplish this feat is using mechanical strain to engineer the band gap. DFT calculations predict a significant band gap decrease of

0.2 eV for 1 % strain introduced to the system. However, the experimental observation of this phenomenon has so far been limited to measuring the modified optical (direct) gap. Here we report the direct observation of nanobubbles with diameters in the range of 10–300 nm emerging in the MoS_2 monolayer deposited on Au (111) surface by Scanning Tunneling Microscopy. Raman spectroscopy measurements revealed that such nanobubbles locally induce large strains of up to 6 % in the MoS_2 lattice. Using tunneling spectroscopy measurements we were able to directly measure the band gap modification of up to 1 eV due to such large mechanical strains.

MON 18

Effect of pore size of gel on the structure sorting of single-wall carbon nanotubes

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Gel column chromatography method has shown a substantial potential for scalable metal/semiconductor (M/S) separation and further single-chirality separation of single-wall carbon nanotubes (SWCNTs). Commercial Sephacryl S-200 gel has been widely used for the separation of SWCNTs. In order to obtain gels of higher separation efficiency or special functions, we have been working on the synthesis of novel gels. In this study, we prepared novel separation gels synthesized by crosslinking the dextran chains with epichlorohydrin. In this system, only dextran chains in the gel provide adsorption sites. We investigated the influence of dextran concentration on the M/S separation performances. Interestingly, a gel of lower dextran concentration shows higher separation performance. Because higher dextran concentration gel possesses smaller pores, the pore size of the gel should play a critical role for the SWCNT separation. For the low concentration gel, large pores allow the fast access of SWCNTs to adsorption sites inside the gel, while the small pores of high concentration gel inhibit the access of SWCNTs into the gel. We claim that the pore size of a gel is one of the most important parameters of the gel performance for the separation of SWCNTs, which was not discussed previously.

MON 19

Carbon nano-onions (CNOs): insights into reductive covalent functionalisation

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Despite carbon nano-onions (CNOs) are well known since 1992, they have not received as much attention as other synthetic carbon allotropes. However, they exhibit outstanding properties for many applications such as large surface area to volume ratio.[1]
Herein we report the synthesis of covalently functionalised CNO via reductive route using intercalation compounds, in particular KC8.[2] For the first time, an in situ Raman study of the controlled intercalation process with potassium has been carried out, revealing a Fano resonance formation. We have compared the K doped-CNO functionalisation using phenyl iodide and n-hexyl iodide as electrophiles in model nucleophilic substitution reactions. We have performed an exhaustive characterization of the functionalised CNOs by employing statistical Raman spectroscopy (SRS), thermogravimetric analysis coupled with gas chromatography and mass spectrometry (TGA/GC/MS), DLS, UV-vis and FTIR-ATR spectroscopy and STEM. This work provides important insights into the reductive CNO functionalisation and paves the way for the development of complex hybrid architectures.
[1] Chem. Commun. 49, 2406 (2013)
[2] J. Am. Chem. Soc. 139, 5175 (2017)

MON 20
Resonances of valley depolarization in TMDCs and phonon dispersion measurements by IXS

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We present the resonance behaviour of the conservation of circular polarization in single-layer MoS_2 and $MoSe_2$ by photoluminescence measurements with varying excitation energies [1]. We find that the circular polarization of the emitted light is conserved to 100 % in MoS_2 and 84 %/79 % (A/A^- peaks) in $MoSe_2$ close to resonance. The values for $MoSe_2$ surpass any previously reported value. However, in contrast to previous predictions, the degree of circular polarization decreases clearly at energies less than the 2 LA phonon energy above the resonance. Our findings indicate that at least two competing processes underly the depolarization of the emission in single-layer transition metal dichalcogenides.
Further, we present the first complete measurement of the phonon dispersion of MoS_2 along the high symmetry directions Γ-K, Γ-M, K-M and Γ-A. Thereby, we resolve the previous contradiction of inelastic neutron scattering (INS) and electron

energy loss spectroscopy (EELS) data. Along with our experimental data we present the dispersion as calculated from ab initio.

[1] H. Tornatzky et al., Resonance profiles of valley polarization in single-layer MoS_2 and $MoSe_2$, submitted to Phys. Rev. Lett. (2018); arXiv:1801.09497

MON 21

Resonant anti-Stokes Raman scattering in single walled carbon nanotubes

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In this work, we present a resonant Raman study of anti-Stokes and Stokes scattering of the G mode in carbon nanotubes [1]. The Raman scattering cross section of chirality enriched nanotube (6,5) (7,5) (8,3) (6,4) species is investigated. The excitation range covered incoming and outgoing resonances of the second excitonic transition. Both anti-Stokes and Stokes scattering profiles exhibit an asymmetric shape. The outgoing (incoming) resonance is dominant in the anti-Stokes (Stokes) scattering. The fifth-order Raman process incorporating the scattering interferences between bright and dark excitionic states explains the asymmetry of the Raman profiles. The chirality dependent degree of asymmetry is due to the varying exciton-phonon matrix elements, as we confirmed by tight-binding calculations. We have developed excitation energy dependent Stokes/anti-Stokes resonant ratios for future evaluation of the effective temperature via Raman spectroscopy.

[1] G. Gordeev *et al.*, Phys. Rev. B 96, 245415 (2017)

MON 22

Atomically precise graphene nanoribbons through on-surface synthesis

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There has been tremendous progress in the bottom-up synthesis of graphene nanostructures. In particular, atomically well-defined graphene nanoribbons (GNRs) have been shown to provide precise control over the width and edge geometry of the ribbon [1]. By changing the monomer design, the fabrication of a wide range of GNRs including different widths and doping can be achieved with engineered chemical and electronic properties. Embedding heterojunctions into single nanoribbons gives access to a wider range of functionalities. We demonstrate the GNR equivalent of a

metal-semiconductor junction by joining armchair GNRs belonging to the metallic (5-atom wide) and semiconducting (7-atom wide) families through on-surface synthesis [2,3]. In addition to a single junction, we have realized more complicated structures combining several interfaces. These structures constitute the first steps towards encoding more functionality into a single GNR for electronic applications.

[1] L. Talirz *et al*, Adv. Mater. 28, 6222 (2016)
[2] A. Kimouche *et al*, Nat. Commun. 6, 10177 (2015)
[3] P.H. Jacobse, A. Kimouche *et al*, Nat. Commun. 8, 119 (2017)

MON 23
Triplet excitons in single walled carbon nanotubes

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Photophysics of single-wall carbon nanotubes (SWCNTs) is intensively studied due to their potential application in light harvesting and optoelectronics. The excited states of SWCNTs form strongly bound electron-hole pairs, excitons, of which only those with a singlet spin symmetry participate in application relevant optical transitions. The presence of long-living spin-triplet states affects the application relevant optical properties and are also candidates for quantum information storage. Therefore knowledge of the triplet exciton energy structure, in particular in a SWCNT chirality dependent manner, is greatly desired. The development of a unique optically detected magnetic resonance (ODMR) spectrometer, which is tailored to match the requirements of energy selective excitation and energy resolved detection in the near-infrared range, was the key to this study. We report the direct observation of light emission from the triplet state recombination, *i.e.* phosphorescence, for several SWCNT chiralities. This yields the singlet-triplet gap as a function of SWCNT diameter and it closely follows the theoretical predictions based on quantum confinement effects.

MON 24
Spin-orbit coupling and large spin relaxation lengths in high-quality encapsulated bilayer MoS_2

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In transition metal dichalcogenides (TMDCs) the spin degree of freedom is pre-

served as a result of their strong intrinsic spin-orbit coupling (SOC) in combination with the weak Bychkov-Rashba SOC. Here, we present results from weak localization in high quality bilayer MoS_2 that is encapsulated with hexagonal boron nitride (h-BN). Using the recently developed theory for weak localization and antilocalization in TMDCs by H. Ochoa et al., we obtain information about the spin relaxation of the electrons and the spin-orbit induced Zeeman splitting. We find a spin relaxation length that is the largest reported so far for TMDCs, which we attribute to the high mobility of the electrons. We also extract a gate-dependent Zeeman splitting that is larger than theoretical predictions, indicating a possible spin dependent shift of the band edge due to the external electric field in combination with a larger value for the mass of the electrons.

MON 25
Atomic-resolution STEM imaging of monolayer $CuPcCl_{16}$ films on graphene

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High-resolution studies on monolayer organic crystals have only been carried out with scanning probe methods so far. On the one hand, they are usually prepared on surfaces of bulk materials, which are not accessible by (S)TEM. On the other hand, the critical electron dose of a monolayer organic crystal is orders of magnitudes lower than the one for bulk crystals, making (S)TEM characterization very challenging. In this work we present an atomically resolved study on the dynamics of a monolayer $CuPcCl_{16}$ crystal under the electron beam as well as an image of the undamaged molecules obtained by low-dose electron microscopy. The results show the dynamics and the radiation damage mechanisms in the 2D layer of this material, complementing what has been found for bulk crystals in earlier studies. Furthermore, being able to image the undamaged molecular crystal allows the characterization of new composites consisting of 2D materials and organic molecules.

MON 26
Reductive Covalent Functionalization of Black Phosphorous

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The bulk covalent functionalization of Black Phosphorous (BP) is a matter of utmost importance because it allows the modification of its electronic and optical properties as well as to improve the solubility and the processing for further applications. Currently, a few works on the neutral covalent functionalization of BP have been reported, however the reductive route –well known from graphene chemistry– re-

mains unexplored. Herein, we report a detailed study on the synthesis and characterization of bulk functionalized BP starting from black phosphorous intercalation compounds (BPICs). The activated BP-sheets are dispersed in an inert solvent and further reacted with electrophiles. The reactions were followed using in-situ Raman spectroscopy and the covalently functionalized BP were studied by temperature dependent Raman spectroscopy, IR spectroscopy, TG-MS and X-Ray photoelectron spectroscopy (XPS). Furthermore, these studies were supported by DFT calculations, providing hints on the reaction mechanism. These preliminary results will pave the way for improving the solubility, processability and stability of BP.

MON 27

Graphene-like Carbon Nanostructures from Combustion Synthesis: qualitative and quantitative Description

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Exfoliated nanocarbon materials could be classified by their different degree of graphitization. Among many known methods used to determine the La and Lc parameters, one may point out the XRD data modelling as one of the most efficient. Although there is the variety of approaches how to address the experimental data to obtain the trustable results about nanocrystallities size, there are still some issues to be considered. Within this study the new model is proposed and discussed. Finally, those XRD modelling considerations were verified on the carbonaceous nanomaterial resulting from the fast magnesium reduction of calcium carbonate (Ar, starting pressure 1 MPa) characterized by the following equation: 2 Mg + $CaCO_3 \rightarrow$ 2 MgO + CaO + C, using combustion synthesis approach. The progressive onset of an incandescence signal from the combustion zone was recorded. The solid products were purified (leaching of Mg-related compounds). The final residue contained almost pure C (elemental analysis) and was characterized using XRD, SEM/EDS, TGA, and Raman spectroscopy. Mostly layered petal-like carbon nanostructures and some C-encapsulated MgO nanocrystallites dominated the product.

MON 28

Room temperature valley polarization and coherence in transition metal dichalcogenide-graphene van der Waals heterostructures

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Van der Waals heterostructures made of graphene (Gr) and transition metal dichalcogenides (TMD) are an emerging platform for opto-electronic as well as opto-valleytronic

devices that could benefit from (i) strong light-matter interactions and spin-valley locking in TMDs and (ii) exceptional electron and spin transport in graphene. However, the valley contrasts in TMD/Gr heterostructures have not been investigated so far. Here, using a comprehensive polarimetry analysis, we directly measure the Mueller matrix of monolayer TMD/monolayer Gr heterostructures. Room temperature valley contrasts up to 40 % and valley coherences up to 20 % are unveiled in tungsten diselenide (WS_2)/Gr heterostructures. Remarkably, valley contrasts have been particularly elusive in molybdenum diselenide ($MoSe_2$), even at cryogenic temperatures. Upon interfacing MoSe2 with graphene, we, observe sizeable room temperature valley polarization and valley coherence in excess of 10 % at room temperature. Our results are discussed in light of recent reports of highly efficient interlayer coupling and energy transfer in TMD/Gr heterostructures and hold promise for room temperature opto-valleytronics.

MON 29
Two-dimensional tungsten suboxides

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Semiconductor metal oxides are the basis of smart, multifunctional materials and applicable as sensors and in nanoelectronics. Their common feature is a deficit of oxygen atoms, which determines transport properties, and mixed oxidation numbers of metal atoms. Therefore, it is possible to control physical (electrical, optical, magnetic) and chemical properties by stoichiometry of these materials.
Nonstoichiometric phases of the WO_3 compound, *i.e.* in the form of WO_{3-x}, attracted a lot of interest due to their well-defined phases and distinctive morphological structure. At the nanoscale, these suboxides can be found as nanoplates, nanowires and nanoparticles.
We will present tungsten suboxide compounds that are found in form of platelets and nanotiles a few micrometers wide and around 100 nm thick. Results of structural characterization performed by electron microscopy (SEM, TEM) and X-ray diffraction will be shown. Surface topography and electronic properties will be revealed based on AFM, STM and XPS studies, while optical properties will be investigated with UV-Vis spectroscopy and Raman spectroscopy.

MON 30
Strain and excitonic effects in TMDs - a tight-binding approach

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Strain engineering offers a wide playground in the field of two-dimensional materi-

als with possible applications in future electronic devices. Depending on strength, orientation and local variation strain alters the materials properties and leads to interesting phenomena such as pseudo-magnetic fields [1] or single-photon emitters [2].
We develop a general simulation approach to model non-uniform strain in two-dimensional materials. Using a multi-scale approach including DFT, Wannier functions and tight-binding calculations we are able to calculate - with reasonable accuracy - various physical properties including excitonic binding-energies for system sizes up to 10^5 atoms. This multi-scale approach allows to include local defects accurately and efficiently [3]. We present calculations performed on strained WSe_2 and discuss preliminary results.

[1] N. Levi, S. Burke and K. Meaker et. al., Science, 329 (5), 544 (2010)

[2] M. Koperski, K. Nogajewski, et. al., Nature Nanotechnology 10, 503-506 (2009)

[3] L. Linhart, F. Libisch and J. Burgdörfer, PRB, in press, (2017)

MON 31
Structure and Dynamics of Alkali-Metal Intercalated Black Phosphorus

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Phosphorene, i.e. single or few-layer sheets of black phosphorus (BP), raised the interest of the scientific community due to its many unusual properties, such as a high p-type charge carrier mobility and a tunable direct band gap. Superconducting properties of a metallic BP phase at low temperatures and under high pressures have been observed since 1968. More recently, surface doping of few-layer single crystal BP with K atoms was found to result in a metallic state. Intercalating BP with alkali metals therefore is considered a promising strategy to electronically dope BP at atmospheric pressure. For this work, the structural change of BP after intercalating with alkali metals in various concentrations was investigated via X-Ray diffraction. By determining the structure directly after synthesis as well as over longer time intervals the stability of the different systems was evaluated. A careful analysis of the diffraction patterns also allows to grasp the dynamic of the intercalated systems, which was found to be dependent on the type and concentration of the alkali metal. Through this, an insight into the dynamics and possible long-term stability of the system is gained.

MON 32
WS_2-graphene composites, a route to enhance the mobility of printed transistor

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Printed electronics made of 2D materials is a promising field to provide low-cost electronic devices. Since the first demonstration of printed transistors made of 2D nanosheets networks[1] researchers's interest focused on improving their performance (mobility, I_{on}/I_{off}, threshold voltage...).

Embedding a more conductive material in a network of semiconducting flakes is one of the most straightforward paths. In this work, we will show how it is possible to tune printed WS_2 transistor's properties by controlling the graphene loading level in a WS_2/graphene composite

[1] A.G. Kelly et al., Science, 356, 69 (2017)

MON 33
Dexter-like intervalley coupling in TMDs: valley polarization and excitonic effects

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Controlled access to spin- and valley-polarized states in TMDs is achievable through their large spin-orbit coupling in combination with circular dichroism. Technological applications, such as spin-valleytronics devices, require a thorough understanding of the underlying mechanisms of intervalley coupling. In this work, we present a joint theory-experiment study on the effect that Dexter-like intervalley coupling has on the valley polarization decay and the excitonic broadening and renormalization in TMDs. Such a coupling is similar to the one between spatially separated systems, however now between different valleys in momentum space. We show that this coupling occurs between A and B excitonic states in different valleys and gives rise to an efficient intervalley transfer of coherent exciton populations, which affects the valley polarization. Also, it enables the hibridization of B and A states that are quasi-resonant, leading to an additional broadening of the B peak linewidth and to significant renormalization in the system. The gained insights allow to understand the intrinsic limit for spin and valley polarization and the properties of lowest lying excitonic states.

MON 34
2D Pnictogens (P and Sb) catalyze the alkylation of soft nucleophiles with esters

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Group 15 elements in zero oxidation state (P, As, Sb and Bi), also called pnictogens, are rarely used in catalysis due to the difficulties associated in preparing well–structured and stable materials. Here, we report the synthesis of highly exfoliated, layered 2D-BP and 2D-Sb in zero oxidation state, suspended in an ionic liquid, with the native atoms ready to interact with external reagents while avoiding aerobic or aqueous decomposition pathways, and their use as efficient catalysts for the alkylation of nucleophiles with esters. The 2D pnictogen material circumvents the extremely harsh reaction conditions associated to previous superacid–catalyzed alkylations, by enabling an alternative acid–base mechanism on surface, protected from the water and air by the ionic liquid. Thus, the Calkyl–O bond of the ester is selectively activated on the catalytic 2D pnictogen surface with respect to the much reactive neighboring C–C and C=O bonds, allowing the alkylation of a variety of acid–sensitive organic molecules and giving synthetic relevancy to the use of simple esters as alkylating agents.

MON 35
Unraveling the structure of 2D polymers by low-dose TEM imaging and diffraction

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Two-dimensional (2D) covalent crystals, which are laterally infinite, one to a few atom- or monomer-unit thin and freestanding, are promising candidates for next-generation electronics, optoelectronics, sensors, and membranes. Organic synthesis opens up an emerging route to the realization of novel 2D covalent crystals, i.e., crystalline 2D polymers (2DPs). Through self-assembly of well-defined building blocks, the crystal structure of the 2DPs can be engineered at the molecular- or even atomic-level. However, the elucidation of the molecular structures of the synthetic

2DPs remains challenging due to the interaction of the imaging electrons with the specimen.
In this work, we have successfully applied low-dose selected-area electron diffraction (SAED) and aberration-corrected high-resolution transmission electron microscopy (AC-HRTEM) to the characterization of synthetic 2D polyimide and polyamide, and unambiguously determined their molecular structures. Atomic-resolution imaging of beam-sensitive 2DPs, on the other hand, remains a formidable task and warrants further investigation.

MON 36
Excitonic transitions in heterostructured Mo and W transition metal dichalcogenides from first principles

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Novel two-dimensional materials from the group of layered transition metal dichalcogenides (TMDC) have recently attracted scientific interest for their unusual physical properties, such as their strong optical response. Recent experiments have suggested the occurrence of long-lived interlayer excitons in stacked heterostructures, with spatial separation of electrons and holes across the layers, possibly allowing for exploitation in solar cells.
Based on recent simulations [1], we have computed the theoretical absorption spectra of bilayer $MoSe_2$-WSe_2 heterostructures by solution of the excitonic Bethe-Salpeter equation with GW quasiparticle corrections and inclusion of spin-orbit-coupling. Our calculations suggest two possible contributions to the experimentally observed interlayer exciton: (i) A spatially indirect, momentum indirect recombination at the indirect fundamental band gap of the heterostructure with an exciton binding energy of order 0.1-0.2 eV and (ii) spatially indirect, momentum direct recombinations of electron-hole pairs with relatively high binding energy on the order of 0.2 eV at the K point. We predict that the second contribution should dominate in MoS_2-WSe_2 heterostructures [2].
[1] Gillen *et al.*, IEEE JSTQE 23, 1 (2017); arXiv:1605.01972 (2016)
[2] Gillen *et al.*, under review; arXiv:1801.06310 (2018)

MON 37
Manipulation of Transition Metal Dichalcogenides: Nanomachining 2D $PtSe_2$ with AFM

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In recent years, two-dimensional (2D) layered materials such as graphene and tran-

sition metal dichalcogenides (TMDs), have been heavily studied due to their high potential for use in a wide range of future nanoelectronic devices. While it is known that some semiconducting TMDs such as MoS_2 change their bandgap with decreasing layer thickness, other TMDs, such as $PtSe_2$, have been shown to develop a band gap, ie. go from semi-metallic to semiconducting.
By using novel manipulative techniques such as nanomachining with an atomic force microscopy (AFM), TMDs can be incrementally machined down and their electrical properties monitored. The change in surface potential can be characterised by Kelvin probe force microscopy (KPFM). Further nanomachining of contacted TMD channels can be performed while monitoring the device performance with each layer removal down to the monolayer. This would enable the design of 'self-contacted' devices based on TMDs through the creation of a semiconducting channel via nanomachining with high performance expectations.

MON 38
Second Harmonic Generation in strained MoS_2

Valerie Smejkal[1], Lukas Mennel[2], Marco M. Furchi[2], Lukas Linhart[1], Stefan Wachter[2], Matthias Paur[2], Dmitry K. Polyushkin[2], Thomas Müller[2], Florian Libisch[1], Joachim Burgdörfer[1]
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Second harmonic generation (SHG) has proven to be a versatile probe for surfaces and interfaces as well as for imaging of complex molecules. With the advent of two-dimensional materials, this technique has now been extended to optically probe local strain variations in those materials which strongly effects their optoelectronic properties.
We have set up first experiments measuring strain in monolayer MoS_2 using SHG [1]. The experimental calibration and data acquisition are based on the optoelastic properties of the crystal in the linear regime. We compare the measured data with a first-principles study of SHG in MoS_2 using DFT and second-order perturbation theory as implemented in the exciting-code [2]. The joint experimental and theoretical study allows to delineate the regime of applicability of the linear description and provides information on the importance of effects beyond lowest-order perturbation theory.
[1] L. Mennel, T. Müller, *et al.*, accepted in Nat. Comm. (2018).
[2] A. Gulans, C. Draxl, *et al.*, J. Phys. Condens. Matter 26, 363202 (2014).

MON 39
Nanomechanical characterization of the charge evolution in a Kondo quantum dot

K. J. G. Götz[1], D. R. Schmid[1], F. J. Schupp[1], P. L. Stiller[1], Ch. Strunk[1], A. K. Hüttel[1]
[1]Institute for Experimental and Applied Physics, University of Regensburg, Regensburg, Germany

Suspended single wall carbon nanotubes are at cryogenic temperatures both extraordinary nano-electromechanical systems and prototypical clean and defect-free single electron devices. The interaction of the corresponding two fields of physics allows for many interesting studies. In particular, by measuring the gate voltage dependence of the transversal vibration frequency, the evolution of the charge on a quantum dot embedded in the nanotube can be evaluated.
We apply this technique to the limit of strong Kondo correlations between a nanotube quantum dot and its contacts. The current through the nanotube displays a clear odd-even pattern (i.e., a "Kondo ridge" at odd electron number) as a function of gate voltage. The time-averaged charge on the quantum dot, however, shows no such odd-even pattern, and can be well modelled via sequential tunnelling only. We conclude that the Kondo current is carried via virtual occupation of the quantum dot alone. This is in excellent agreement with recently published results coupling a nanotube to a coplanar waveguide resonator, where the transmitted radio-frequency phase depends on the compressibility of the electronic system.

MON 40
The optical features of 7-armchair graphene nanoribbons

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The graphene nanoribbons (GNRs) are attracting much interest globally due to strong quantum confinement effects. An electron and phonon dispersion, an electrical conductivity type, an energy bandgap of GNRs are defined by a width and an edge type of a nanoribbon. An armchair GNR (AGNR) with H atoms on the edges can have an optical bandgap. For such nanoribbon type the width of an energy bandgap increase with the decrease of the AGNR width. To form semiconducting ultra-narrow graphene nanoribbons with a controlled morphology is a challenging goal. One of the most promising methods to produce GNRs with an atomically smooth structure is based on a bottom-up approach. In this work we report the modified bottom-up approach to facilitate synthesis of 7-AGNRs (7 carbon atoms in width, armchair edge type, H-passivation) on a large scale. The obtained GNR thin films have characteristic Raman features that are typical for a 7-AGNR and bright photoluminescence especially in a red spectrum range. We also demonstrate the characteristic spectral features in the optical absorption and in the photoluminescence spectral map of 7-AGNRs.
We acknowledge funding from project RSF- 17-72-10154.

MON 41
Thermal Expansion of Colloidal CdSe/CdS Core/Shell Quantum Dots

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[2]Physics and Chemistry of Nanostructures, Ghent University, Ghent, Belgium

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[4]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

This work uncovers the thermal properties of colloidal CdSe/CdS quantum dots (QDs) associated with additional epitaxial strain at the core/shell interface. We investigate the temperature-dependent behavior of the longitudinal optical (LO) phonon frequencies of these QDs by Raman spectroscopy over a temperature range of 7 K to 300 K. For Wurtzite and zincblende structured QDs, a characteristic red shift of the CdSe and CdS LO frequencies with increasing temperature is found. The extent of this red shift, however, depends on the interplay between the two materials in the heterostructure as well as on the temperature. We propose a simple method to decouple the pure thermal properties of each material from characteristics determined by the interaction of core and shell.

MON 42
Atomic structure and electrical properties of graphene oxide synhesized by different routes

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[2]Danubia Nanotech, Bratislava, Slovakia

Graphene oxide (GO) is considered as a precursor for the large-scale production of graphene for industrial applications. Chemical routes to GO are based on using strongly oxidizing agents. As a consequence of covalent functionalization, charge localization eliminates electrical conductance in GO. By removing the oxid groups the conductance would, to some extent, restore. The processes of oxidation and reduction, however, often cause a sever structural disorder which strongly degrades graphene properties. Here we compare properties of GO materials prepared by two different chemical processes. In contrast to the well-established Hummer´s method, a newly-developed synthesis of GO introduces only minor defects in the atomic structure of graphene. Our STEM investigations on atomic scale show not only the well-preserved structural order but also very large graphene flakes up to 100 μm. This leads to a significant improvement in macroscopic physical properties like electrical conductivity (2000 S/cm)and mechanical modulus (6.8 GPa) in a paper made of reduced GO. It offers a very promising alternative to a waste majority of graphene on the market.

MON 43
Molecular Fingerprints and Electronic Structure of DNA/RNA Nucleobases on Graphene

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Academy of Sciences, Prague

Fast, cheap and reliable identification of the exact order of nucleobases within a DNA/RNA molecule is an important goal of next-generation genome sequencing. Graphene has recently attracted enormous attention for next-generation DNA/RNA sequencing and sensing thanks to its unique electronic and structural properties. Here we present a systematic study of the electronic structure of a graphene-nucleobase system for various molecular orientations and concentrations using density functional theory [1]. We identify that the in-plain dipole moments of the nucleobases play the dominant role in the modification of the electronic structure of graphene, demonstrating both p- and n-type of doping depending on the direction of the dipole moments. We demonstrate that intermolecular interactions have a strong influence on the adsorption geometry, resulting in a tilt of the molecules on graphene. The predicted tilt of nucleobases causes significant changes to the electronic structure and molecular fingerprints of nucleobases in graphene.
[1] Y. Yin, J. Cervenka and N. V. Medhekar, J. Phys. Chem. Lett. 8, 3087 (2017).

MON 44
Covalent modification of black phosphorus via neutral route

Aleksandra Mitrovic[1,2], Gonzalo Abellán[1,2], Frank Hauke[1,2], Andreas Hirsch[1,2]
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[2]Zentralinstitut für Neue Materialien und Prozesstechnik (ZMP), Fürth

From material aspects, black phosphorus (BP) is unique. Resembles graphite/graphene, but to date its potentials are far less discovered. Our research aims to systematically investigate the inherent reactivity principles of BP as well as to synthesize, isolate, and characterize a variety of families of covalent BP derivatives. The appealing aspects of covalently functionalizing BP are: a) an increased solubility and processability, b) the possibility of its stabilization against oxidation, c) the modification of its electronic and optical properties (band gap engineering), d) the combination of the properties of BP with those of other compound classes, and e) the development of real world applications such as electronic devices. Here, we describe the covalent modification of neutral, solvent exfoliated BP while addressing two reaction modes, namely, a) the reaction of BP with carbenes and nitrenes as well as b) with Lewis acids.

MON 45
Tuning the electronic properties of materials by molecular self-assembly

Juan Carlos Moreno-Lopez[1], Paola Ayala[1], Thomas Pichler[1]
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The self-assembly of organic molecules on well-defined surfaces is generally accepted as one of the most promising methods to develop advanced materials. Usually, the molecular precursors are sublimated onto a well-defined substrate where the competition between molecule-molecule and molecule-substrate interactions

defined the final arrangement of the molecules. By choosing molecular precursors wisely it is possible to create molecular patterns with a regular array of pores. This periodical arrangement of pores commonly acts as an electrostatic barrier for the surface electrons of the substrate, creating quantum confinement effects [1]. This approach allows us to tune the electronic properties of multiple surfaces, including 2D materials. Here, by means of Angle-Resolved Photoemission Spectroscopy (ARPES) and X-ray Photoelectron Spectroscopy (XPS), as main experimental techniques, we studied the influence of molecular networks on the electronic structure of several materials.
[1] J. Lobo-Checa *et al.*, Science, 325, 300 (2009)

MON 46
Electronic Band Structure of Pristine and Boron-doped N=7 Armchair Graphene Nanoribbons

Boris Senkovskiy[1], Dmitry Usachov[2], Alexander Fedorov[2,3], Danny Haberer[4], Felix Fischer[4], Alexander Grüneis[1]
[1] Institute of Physics II, University of Cologne, Köln, Germany
[2]St. Petersburg State University, St. Petersburg, Russia
[3]IFW-Dresden, Dresden, Germany
[4]Department of Chemistry, University of California at Berkeley,USA

Using angle-resolved photoemission spectroscopy (ARPES), we obtain the first true experimental band structure of pristine and boron-doped armchair GNRs of N=7 carbon atoms width, assembled from the molecular precursors on a stepped Au(788) crystal. We demonstrate that the photoemission intensity of each sub-band of quasi-1D GNRs is a peaked function of the 2D momentum in the ribbon plane. ARPES mapping in the full 2D momentum space allows us to extract effective masses, charge carrier velocities and band offsets. Periodic incorporation of B atoms in GNRs strongly modifies the interaction with the Au substrate. Particularly, hybridization of the B-derived frontier flat valence sub-band with Au states results in energy spreading of the band. From another hand, the second parabolic sub-band with C contribution remains particularly non-changed. Complementary to the ARPES, we investigate the vibrational properties of GNRs by in situ Raman spectroscopy. We find that boron doping strongly affects the Raman active phonon freqencies. In particular, we observe a frequency shift and a doubling of the so-called radial breathing-like mode for boron doped GNRs.

MON 47
Synthesis and Properties of Monolayer 1T'-Phase $MoTe_2$, WTe_2, and Their Lateral Heterostructures

Meng-Qiang Zhao[1], Carl H. Naylor[1], Qicheng Zhang[1], Zhaoli Gao[1], William M. Parkin[1], Jinglei Ping[1], A. T. Charlie Johnson[1]
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Two-dimensional (2D) transition metal dichalcogenides (TMDs) in 1T' phase are predicted to be large-gap quantum spin Hall topological insulators, with great promise in future electronic applications. However, the metastable nature of 1T' TMDs makes their direct growth by chemical vapor deposition (CVD) a great challenge.
Recently, our group achieved the successful CVD growth of monolayer, single-crystal flakes of 1T'-$MoTe_2$ and WTe_2, through a fast operation process. The 1T' structure was well demonstrated by the high-resolution microscopy images and Raman spectrum. To achieve on-demand tuning of electronic properties, the growth of 1H-WSe_2/1T'-WTe_2 monolayer lateral heterostructure was achieved by a two-step CVD method. The 1H-WSe_2 was synthesized first, followed by an epitaxial growth of 1T'-WTe_2 on the edge. Transmission electron microscopy revealed a single crystalline structure and a clear transition between the two different phases. Electrical transport studies demonstrated the formation of lateral p-type semiconductor and semi-metal heterojunctions. Monolayer 1H-MoS_2/1T'-$MoTe_2$ lateral heterostructure was obtained by a similar method.

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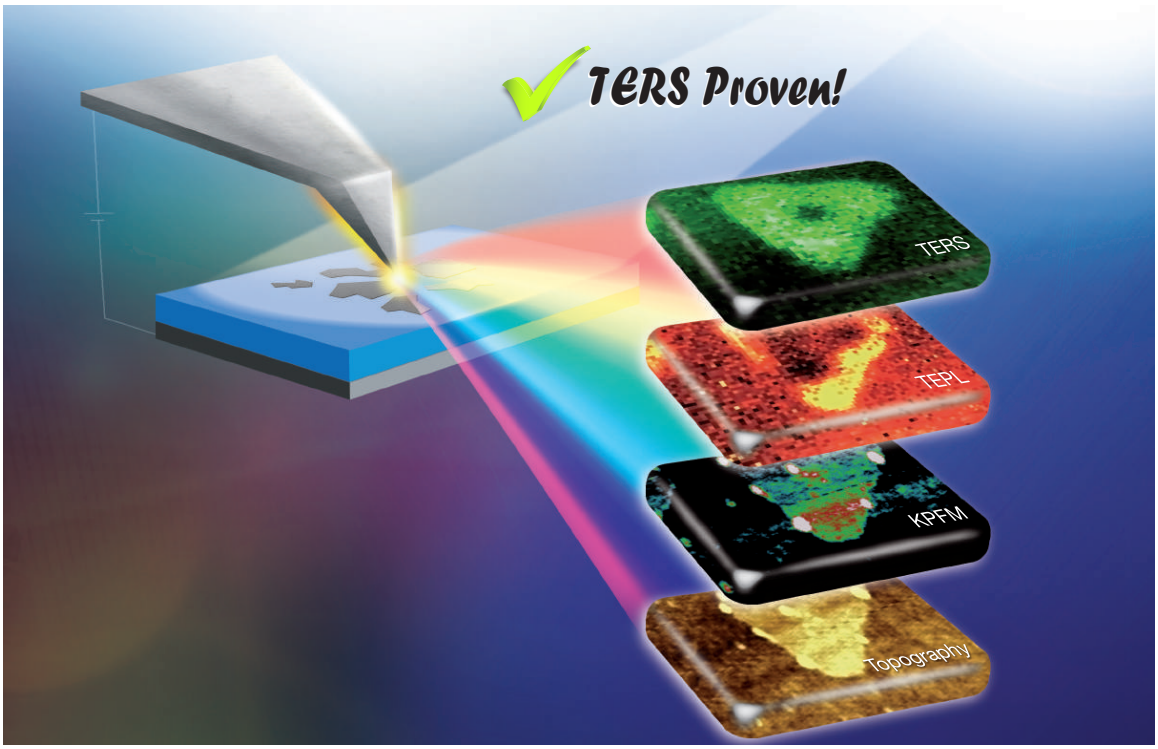

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08:30 – 09:00 A. Chernikov, Regensburg
Exciton propagation in atomically thin semiconductors

09:00 – 09:30 M. Glazov, St. Petersburg
Excitons in monolayer-thin transition metal dichalcogenides

09:30 – 10:00 A. Knorr, Berlin
Exciton Based Description of Atomically Thin Semiconductors: Optical Lineshape, Intervalley Coupling and Luminescence Dynamics

10:00 – 10:30 coffee break

10:30 – 11:00 S. Berciaud, Strasbourg
Charge Versus Energy Transfer in Atomically Thin Graphene-Transition Metal Dichalcogenide van der Waals Heterostructures

11:00 – 11:30 H. Cheong, Seoul
Resonance Raman Spectroscopy of 2D materials

11:30 – 12:00 L. Wirtz, Luxembourg
Theory of Resonant Raman Spectroscopy and Valley-Depolarization in Transition Metal Dichalcogenides

12:00 – 17:00 mini workshops

17:00 – 18:30 Dinner

18:30 – 19:00 R. Saito, Tohoku
Controlling optical absorption of graphene by gate voltage in dielectric multilayer

19:00 – 19:30 F. Mauri, Rome
Flat bands, magnetism, half-metallic behavior and spin current polarization in multilayer rhombohedral graphene

19:30 – 20:00 J. Kim, Boston
Material challenges and opportunities in next generation electronics

20:00 Poster Session II

08:30
Exciton propagation in atomically thin semiconductors
Alexey Chernikov[1]
[1]Department of Physics, University of Regensburg, Regensburg

Coulomb-bound electron-hole pairs, or excitons, have been in the focus of the solid-state research for many decades. They are of paramount importance for the fundamental understanding of interacting charge carriers in semiconductors. Recently, excitons in single layers of semiconducting transition-metal dichalcogenides (TMDCs) were found to combine a number of intriguing properties, including binding energies on the order of 0.5 eV, strong light-matter interaction and spin-valley coupling.
Here, we address the topic of exciton transport in TMDCs by directly monitoring spatial behavior of excitons in single layers of WS_2 through spatially- and time-resolved photoluminescence. We find highly nonlinear behavior with characteristic, qualitative changes in the spatial profiles of the exciton emission and an effective diffusion coefficient increasing by two orders of magnitude, depending on the injected exciton density. Including Auger recombination into the diffusion equation allows us to identify the main origin of the nonlinearity. At elevated densities, the exciton distribution evolves into long-lived halo shapes with micrometer-scale diameter, indicating memory effects.

09:00
Excitons in monolayer-thin transition metal dichalcogenides
Mikhail Glazov[1]
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Atomically thin materials such as graphene and monolayer transition metal dichalcogenides exhibit fascinating physical properties resulting from their reduced dimensionality and crystal symmetry. The family of semiconducting transition metal dichalcogenides is a very promising platform for fundamental studies of two-dimensional systems. A lack of inversion symmetry combined with strong spin-orbit interactions leads to a unique combination of the spin and valley degrees of freedom, while weak dielectric screening yield a significant enhancement of the Coulomb interaction. The resulting formation of bound electron-hole pairs, or excitons, dominates the optical and spin properties of the material. I review recent progress in understanding of the excitonic properties in monolayer TMDs and lay out future challenges. The emphasis is made on the exciton fine structure and manifestation of excitons in polarization-dependent linear and nonlinear optical effects.

09:30

Exciton Based Description of Atomically Thin Semiconductors: Optical Lineshape, Intervalley Coupling and Luminescence Dynamics

Andreas Knorr[1], Malte Selig[1], Dominik Christiansen[1], Florian Katsch[1], Gunnar Berghäuser[2], Ermin Malic[2]
[1]Institut für Theoretische Physik, Technische Universität Berlin, Berlin
[2]Chalmers University of Technology, Department of Physics, Gothenburg

Monolayers of Transition Metal Dichalcogenides (TMDs) are atomically thin two dimensional structures which, due to a reduced dielectric screening of the Coulomb interaction, exhibit a remarkable exciton physics. This involves optically accessible (bright) as well as spin- and momentum-forbidden (dark) excitonic states including intervalley excitons. Here, we develop a theory for (a) the linear optical properties, dominated by exciton-phonon interaction, (b) the intrinsic exciton-exciton interaction resulting from different Coulomb-scattering phenomena in nonlinear optics, and (c) the luminescence dynamics of TMDs. A comparison of the theory with experimental results is given (R. Bratschitsch *et al.*, (Münster): asymmetric absorption line shapes, pump-probe; T. Heinz *et al.*, A.Chernikov *et al.*, (Stanford, Regensburg): contribution of dark excitons to the homogeneous linewidth and luminescence dynamics).

G. Moody *et al.*, Nat. Commun. 6, 8315 (2015)

E. Malic *et al.*, Phys. Rev. Mat. 2, 014002 (2018)

M. Selig *et al.*, Nat. Commun. 7, 13279 (2016)

D. Christiansen *et al.*, Phys. Rev. Lett. 119, 187402 (2017)

R. Schmidt *et al.*, Nano Letters 16 (2016)

10:30

Charge Versus Energy Transfer in Atomically Thin Graphene-Transition Metal Dichalcogenide van der Waals Heterostructures

Guillaume Froehlicher[1], Etienne Lorchat[1], Stéphane Berciaud[1]
[1]Université de Strasbourg, CNRS, IPCMS (France)

Made from stacks of 2D materials, van der Waals heterostructures (vdWH) exhibit unique light-matter interactions and are promising for novel optoelectronic devices. The performance of such devices is governed by near-field coupling phenomena (e.g., through interlayer charge and/or energy transfer) that remain poorly understood. Here, using a combination of photoluminescence (PL) and Raman scattering spectroscopies, we disentangle contributions from interlayer charge and energy transfer processes in an atomically-thin graphene (Gr) -transition metal dichalcogenide (TMD, here molybdenum diselenide, $MoSe_2$) vdWH.
The PL intensity in Gr/TMD is massively quenched and increases linearly with the incident photon flux, demonstrating a room temperature TMD exciton lifetime of about 1 ps. Complementary insights are provided from a comprehensive analysis of the Gr and TMD Raman modes, which reveals a net photoinduced electron transfer from TMD to graphene. Remarkably, exciton dynamics in Gr/TMD vdWH is independent of the existence of a net charge transfer. This key result strongly suggests that picosecond interlayer energy transfer from TMD to Gr dominates the photoresponse of Gr/TMD vdWH.

11:00
Resonance Raman Spectroscopy of 2-dimensional materials
Hyeonsik Cheong[1]
[1]Dept. of Physics, Sogang University, Seoul, Korea

Raman spectroscopy is broadly used in the studies of 2-dimensional materials to determine the number of layers or other physical properties. In the case of graphene, the line shape and the position of the 2D band depend on the excitation energy and can be used to determine the number of layers and the stacking order. In the case of transition metal dichalcogenides, the Raman spectrum varies greatly depending on the excitation energy, and many unusual effects have been reported. The Raman intensities of high-frequency intra-layer vibration modes are enhanced near resonance with exciton states. Some Raman peaks that are either forbidden or weak in non-resonant cases show strong enhancement near resonances. In the low-frequency Raman spectra, some unusual features, in addition to shear and breathing modes, appear near resonance with exciton states. Some intra-layer vibration modes exhibit Davydov splitting due to inter-layer interactions when the excitation energy is close to resonances. In this presentation, some of the latest results in resonance Raman spectroscopy of MoS2, MoSe2, WS2, and WSe2 will be reviewed.[1]

[1] J. Raman Spectroscopy, in press (DOI 10.1002/jrs.5200).

11:30

Theory of Resonant Raman Spectroscopy and Valley-Depolarization in Transition Metal Dichalcogenides

Ludger Wirtz[1], Henrique Miranda[1,2], Sven Reichardt[1,5], Alejandro Molina-Sánchez[1,3], Davide Sangalli[4], Andrea Marini[4]

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[2]Institute of Materials Science (ICMUV), University of Valencia, Spain

[3]Institute of Condensed Matter and Nanosciences (IMCN/NAPS), Université catholique de Louvain, Belgium

[4]CNR-ISM, Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy

[5]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany

We present recent results on theoretical spectroscopy involving electron-phonon scattering.
In the first part of the talk, we will present calculations of resonant Raman spectra of few-layer transition metal dichalcogenides (TMDs). We have implemented both an approach using finite displacements and a diagrammatic approach using many-body perturbation theory. With increasing number of layers, N, the A1' mode splits into several peaks which can be used to determine N. We show that the non-intuitive intensity distribution of the various sub-peaks can be explained through quantum interference.
In the second part, we will show examples how time-dependent many-body perturbation theory can help to understand ultra-fast spectroscopy of 2D materials. In particular, we show that electron-phonon coupling is the driving mechanism for the temperature-dependent valley depolarizion in time-resolved Kerr rotation spectroscopy of TMDs.

18:30

Controlling optical absorption of graphene by gate voltage in dielectric multilayer

Riichiro Saito[1], Muhammad Shoufie Ukhtary[1], Sylvain Alexandre Nulli[1], Haihao Liu[1]
[1]Department of Physics, Tohoku University, Sendai

The optical absorption probability of *monolayer* graphene can be changed from 0 % to 100% by changing the Fermi energy and/or by using dielectric multilayer. In the doped graphene, retarded surface plasmon can absorb the light significantly at the interface of two dielectric materials with the incident angle more than the critical angle in which the total reflection occurs. By changing the Fermi energy, we can change the absorption probability for such a geometry from 0 % to 100 %[1], which is experimentally observed by the THz measurement[2]. Further, using the dielectric multilayer which consists of two dielectric materials A and B, such as ABABGBABA (G is graphene), the electric field of the light at the G is enhanced exponentially by interference effect[3]. For such geometry we can get up to 50 % absorption for the incident light propagating in the direction perpendicular to the surface[4].

[1] M. S. Ukhtary, *et al.*, Appl. Phys. Exp. 8, 055102 (2015).
[2] Y. Harada *et al.*, ACS photonics 4, 121 (2017).
[3] H. Liu, *et al.*, J. Phys. Cond. Matt. 29, 455303 (2017).
[4] S. A. Nulli, M. S. Ukhtary, R.Saito, *unpublished.*

19:00

Flat bands, magnetism, half-metallic behavior and spin current polarization in multilayer rhombohedral graphene

Francesco Mauri[1,2]
[1]Physics, Universita' di Roma - La Sapienza, Roma
[2]Graphene Labs, Fondazione Istituto Italiano di Tecnologia

Attempts to induce in graphene a clean and stabilized or a robust magnetism have not been successful yet. An alternative procedure is to explore correlated states in flat electronic bands hosted by multilayer graphene with rhombohedral (ABC) stacking [1]. I will show how to use Raman spectroscopy to identify long-sequence of ABC stacking [2,3,4] and to isolate large graphitic flake containing up to 14 layers. On such samples we reveal the flat electronic bands and identify a gapped magnetic state by comparing ARPES with DFT calculations [4]. The gap is robust and stable at liquid nitrogen temperature. Finally using first-principles calculations, I demonstrate that field-effect doping of these graphene multilayers induces a perfect half-metallic behavior with 100 % spin current polarization that can be reversed simply by changing the gate potential [5].
We acknowledge support of the European Union under Grant agreement No. 696656-GrapheneCore1.

[1] Pamuk *et al.*, PRB 95, 075422 (2017)
[2] Henni *et al.*, Nano Lett. 16, 3710 (2016)
[3] Torche *et al.*, PRMat 1, 041001 (2017)
[4] Henck *et al.*, arXiv:1708.03220
[5] Baima Mauri Calandra, submitted

19:30
Material challenges and opportunities in next generation electronics
Jeehwan Kim[1]
[1]MIT, Cambridge

The current electronics industry has been completely dominated by Si-based devices due to its exceptionally low materials cost. However, demand for non-Si electronics is becoming substantially high because current/next generation electronics requires novel functionalities that can never be achieved by Si-based materials. Unfortunately, the extremely high cost of non-Si semiconductor materials prohibits the progress in this field. I will discuss about my group's efforts to address these issues. Our team has recently conceived a new crystalline growth concept, termed as "'remote epitaxy"', which can copy/paste crystalline information from the wafer remotely through graphene, thus generating single-crystalline films on graphene. These single-crystalline films can be easily released from the slippery graphene surface, and the graphene-coated substrates can be reused infinitely to generate single-crystalline films. Therefore, the remote epitaxy technique can produce expensive non-Si semiconductor films with unprecedented cost efficiency while allowing additional flexible device functionality required for current ubiquitous electronics.

TUE 1
Spin splitting in quasi-one dimensional systems

Marko Milivojević[1], Nataša Lazić[1], Saša Dmitrović[1], Tatjana Vuković[1], Milan Damnjanović[1]
[1]Department of Physics, University of Belgrade, Serbia

Spin-orbit induced phenomena in quasi-one dimensional systems are analyzed using the derived double line groups symmetry and their irreducible representations. Orbital band splitting and consequent removal of the spin degeneracy are found to be incompatible with vertical mirror symmetry, as well as with simultaneous invariance under the time reversal and horizontal (roto) reflections. This singles out only the systems with the first and the fifth family line group symmetry as candidates for obtaining spin polarized currents. Interesting insight into the band topology arises even when spin-orbit term is not added to the Hamiltonian. The results, illustrated on carbon nanotubes, show why the spin polarization is possible only in the direction of the tube's axis, while the absence of overall spin polarization of the band is a consequence of the non-crossing rule.

TUE 2
Optical absorption and resonance Raman scattering for ribbon molecules

Lei Shi[1], Claudia Berkmann[1], Thomas Pichler[1], János Koltai[2], Jenő Kürti[2], Hans Kuzmany[1]
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Chemical reactions inside single-walled carbon nanotubes are presently of high scientific and technological interest. In a recent report[1] we showed molecules related to oligorylenes to be responsible for extra resonance enhanced Raman lines in ferrocene-filled carbon nanotubes after high temperature transformation. In order to learn more about the new compounds we performed optical absorption and resonance Raman experiments for the ribbon molecules, e.g. terrylene and quaterrylene, inside and outside the nanotubes. The experiments allowed determining electronic transition energies, their modulation by the filling process, ground state as well as excited state vibrational frequencies, and electron-vibron coupling constants. Experimental findings are supplemented by quantum-chemical calculations on a DFT level for electronic transition energies, frequencies, and coupling constants. Results are compared to the Raman lines after filling the tubes with ferrocene and subsequent heat treatment.

[1] H. Kuzmany, L. Shi, J. Kürti, J. Koltai, A. Chuvilin, T. Saito, and T. Pichler. Phys. Status Solidi RRL 11, 1700158 (2017)

TUE 3
Extraction of Linear Carbon Chains from Carbon Nanotube Host

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Recently we demonstrated synthesis of linear carbon chains inside double-walled carbon nanotubes (LCCs@DWCNTs) with a record length of more than 6000 carbon atoms [1]. The experimentally determined electronic energy gaps ranging from 2.253 to 1.848 eV follow a linear relation with Raman frequency [2]. Furthermore, the interaction and charge transfer [3] between the LCCs and their host DWCNTs lead to an increase of the photoluminescence signal of the inner tubes of DWCNTs [4]. In order to unravel the role of the host nanotubes, the LCCs were extracted and separated by ultrasonication and density gradient centrifugation methods. Resonance Raman spectral results suggest that the inner tubes play much greater roles than the outer tubes in modifying the property of the LCCs [5].
This work was supported by the FWF (P27769-N20) and EU projects (2D-Ink FA726006).
[1] Nat. Mater. 15, 634 (2016)
[2] Phys. Rev. Materials 1, 075601 (2017)
[3] Phys. Rev. B 94, 195422 (2016)
[4] Adv. Funct. Mater. 26, 4874 (2016)
[5] Submitted.

TUE 4
Liquid-Phase Exfoliation as Versatile Technique for 2D-Nanomaterial Preparation

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Liquid-phase exfoliation (LPE) techniques coupled with centrifugation methods have become popular to prepare dispersions of a versatile class of materials in bulk quantities of variable nanosheet sizes and thicknesses. The properties of these materials are drastically changing from bulk to few- and monolayer sheets and even vary for different sizes of the same thickness. This makes the control over sheet size and thickness by post-exfoliation treatments extremely important. In this regard, liquid phase cascade centrifugation has been suggested as promising methodology to obtain narrower sheet size and thickness distributions. [1]
In this contribution, we show progress in producing nanosheet dispersions of materials beyond graphene and TMDs, such as LaSeTe2, NiPS3 or RuCl3 with well-defined size and thickness extracted from statistical AFM and correlated with UV-Vis

and Raman measurements. This allows to establish valuable metrics for size and thickness for new classes of layered materials.

[1] C. Backes, B. Szydłlowska, A. Harvey, *et al.*, ACS Nano 10, 1589 (2016)

TUE 5

Superconducting quantum point contact with split gates in the two-dimensional $LaAlO_3/SrTiO_3$ superfluid

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One of the hallmark experiments of quantum transport is the observation of the quantized resistance in a point contact formed with split gates in GaAs/AlGaAs heterostructures. It has been a long standing goal to achieve similar experimental conditions also in superconductors. In principle, this has come within reach with the discovery of gate tunable superconductivity at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface. Here we demonstrate the formation of a superconducting quantum point contact (SQPC) with split gate technology in a superconductor, utilizing the unique gate tunability of the two dimensional LAO/STO superfluid. When the constriction is tuned through the action of metallic split gates we identify three regimes of transport: (1) SQPC for which the supercurrent is carried only by a few quantum transport channels. (2) Superconducting island strongly coupled to the equilibrium reservoirs. (3) Charge island with a discrete spectrum weakly coupled to the reservoirs. Our experiments demonstrate the feasibility of a new generation of mesoscopic all-superconductor quantum transport devices in LAO/STO.

TUE 6

Tunable quantum interference in bilayer graphene in double-resonant Raman scattering

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The line shape of the double-resonant 2D Raman mode in bilayer graphene is often considered to be characteristic for a certain laser excitation energy. Here, in a joint experimental and theoretical study, we analyze the dependence of the

double-resonant Raman scattering processes in bilayer graphene on the electronic broadening parameter. We demonstrate that the ratio between symmetric and antisymmetric scattering processes sensitively depends on the lifetime of the electronic states, explaining the experimentally observed variations of the complex 2Dmode line shape.

TUE 7

Biosensing with Graphene Tunnel Junctions - intrinsic and environmental limitations

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Biosensing with tunnelling electrodes has become an active research field, promising fast and accurate characterization of DNA strands and proteins. Graphene was identified as a candidate for electrode material in such biosensing tunnel junctions.
We developed a method of a feedback controlled electroburning which allows us to fabricate nanometre-sized Graphene Tunnel Junctions (GTJs), with a tunnelling distance which can be adjusted to the analyte of interest. Two important features of devices for biosensing are temporal resolution, related to the pace of translocation of an analyte through the GTJ and the minimum detectable signal. Both of these properties can be limited by the electric noise due to the noise sources intrinsic to the device itslef, and environmental noise sources due to the liquid environment necessary for the biosensing and sequencing measurements.
Here we analyse the intrinsic noise spectrum of the GTJ discussing the sensing limitations due to commonly observed $1/f$ noise spectrum, which we attribute to the effect of fluctuating charge traps at the graphene-substrate interface. Further we show influence of water environment on noise behaviour.

TUE 8

Investigation of the electrophysical properties of novel composite materials based on polyethylene and multi-walled carbon nanotubes modified with magnetic nanoparticles Fe3O4

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Multi-walled carbon nanotubes (MWCNTs) have been widely regarded as an attractive candidate to be used as fillers in the composite materials due to their unique mechanical properties, large surface area, high electrical and thermal conductivity, and chemical stability. The development of new composite materials based on widely used polymers and MWCNTs is one of the promising ways of modern material science. The addition of a small amount of the MWCNT to the polyolefins pro-

vides significant improvement of their mechanical and electrical properties. Adding another component such as magnetic nanoparticles in the material at the preparation stage potentially allows controlled changing of the electromagnetical properties of the composite material by varying dielectric properties of MWCNT and magnetic properties of magnetic nanoparticles. In this work, the special attention has been paid to the issue of how the concentrations of Fe3O4 and MWCNT and their uniformity distribution in the polyethylene (PE) matrix influences on the electrophysical properties of the triple composite materials.
The reported study was funded by RFBR, according to the research project No. 16-32-60046 mol_A_dk.

TUE 9
Engineering excitons at the interface of two dimensional semiconductors

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Our goal is to investigate the interaction of excitons in two-dimensional semiconductors (2DSCs) with their external, modified microenvironment. Here, we report how excitons in 2DSCs may be engineered with gas molecules deposited onto the surface of the 2D material. To accomplish this, we developed a setup capable of i) localized high-temperature annealing of 2DSCs kept in cryogenic vacuum, ii) in-situ deposition of gas molecules atop the 2DSCs, and iii) in-situ Raman and Photoluminescence (PL) measurement. We observed a new defect-like PL peak arising upon deposition of sub-monolayers of oxygen or air onto 2DSCs and disappearing after desorption of molecules by thermal annealing. We suggest that this peak results from binding of an exciton to a charged molecule forming an "out-of-plane" trion. The measured binding energy of such a state ($\approx$ 100eV) is consistent with the variational estimate of exciton-charge distance $\approx$ 0.8nm. Interaction of excitons in 2DSCs with charges at the interface may potentially be used to engineer and modify complex excitonic states and realize a novel sensing mechanism.

TUE 10
Raman spectroscopy and graphene-based FET for highly sensitive detection of carbon quantum dots

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Possessing such superior properties as low toxicity and good biocompatibility renders carbon quantum dots (CQDs) favourable materials for applications in bioimaging, biosensor and drug delivery. We present detection of CGDs by Raman spec-

troscopy and functionalized mechanically exfoliated graphene by means of FET. Mechanically exfoliated graphene flakes were placed onto Si/SiO2 substrate and graphene FET was fabricated by optical lithography. Afterwards a controlled ozone treatment was utilized to create hydroxyl groups onto graphene surface without significant degradation of electron transport properties. Subsequently incubation in APTES solution was used to attach amino groups on the graphene surface. The affinity of negatively charged GQDs carboxyl groups towards the positively charged amino-functionalized graphene allows high sensitive detection based on alteration of FET conductivity. Evidence for charge-transfer involving graphene is also clearly visible by the observation of G peak shift in Raman spectra. We used mapping of G peak for 10x10um area of mechanically exfoliated graphene as a sensitive probe to examine doping of functionalized graphene by carbon quantum dots.

TUE 11
Towards gate-controlled photoluminescence of hexagonal boron nitride quantum emitters

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In the past few years, quantum emission from defect states embedded in crystalline structures has attracted increasing interest due to its promising applications in future quantum information technologies. While the properties of color centers in large band-gap 3D semiconductors like diamond or 4H-SiC are well-established, more recently attention is directed toward quantum emission from 2D systems. Along these lines, hexagonal boron nitride (hBN) has recently emerged as a very attractive 2D platform to host robust, visible light single photon emitters. Here, we report our experiments that address the possibility to control the quantum emission from hBN monolayers through electrostatic gating. To this end, we use confocal microscopy to probe the lifetime and intensity of the light emission from hBN quantum emitters within hBN/graphene vertical heterostructures as a function of temperature and back gate voltage. Moreover, through complementary Raman mapping, we demonstrate the importance of the hBN and graphene layer thickness, as well as the quality of the interface between the layers.

TUE 12
Unravelling the properties of filled carbon nanotubes

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In this contribution I will present recent progress in the synthesis of novel materials based on filled carbon nanotubes followed by nanochemical reactions. This covers the bulk growth metallocenes inside single walled carbon nanotubes and

the bulk growth of metal chains and of linear carcarbyne inside double walled carbon nanotubes. I will show progress on unraveling the influence of charge transfer, local strain and hybridization on their electronic transport properties As selective examples I will present a gas sensing model based on intrinsic functionalization and show how the interaction with reactive gases like nitric oxides can be tailored by advanced filling reactions with metallocenes and metalacetylacetonates towards room temperature selectivity and sensitivity. As a last example I will review how stabilized carbyne chains exhibit novel electronic and optical properties such as a huge resonance Raman signal and act as functional elements enhancing the photoluminescence of inner tubes. This environmental dependence of the chains also allows band gap engineering of these materials towards application in optoelectronics
Work supported by the FWF and EU project 2D-INK

TUE 13
Exploring the role of spin-orbit coupling in transport properties of heteroatom substituted graphene-like molecules

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Design principles for controlling quantum interference in single molecules and exploiting such effects in nanoscale devices and thin-film materials are a long-sought goal of material science. When the core of a graphene-like polyaromatic hydrocarbon (PAH) is weakly coupled to external electrodes, the single-molecule electrical conductance depends on the choice of the connecting atoms. Conductance ratios corresponding to different connectivities are determined by quantum interference within the PAH core. In the present work, to examine the role of the spin-orbit coupling (SOC) in single-molecule transport, we explore how these conductance ratios change when one of the carbon atoms within the 'parent' PAH core is replaced by a heavy heteroatom to yield a 'daughter' molecule with strong SOC. Our results are verified by comparison with density-functional calculations on Bismuth-based PAH.

TUE 14
Origin of Surface States in ZrSiS and Related Compounds

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Three-dimensional Dirac semimetals, which accomodate massless Dirac and Weyl fermions, show exotic physical properties, e.g. an extremly high mobility and giant magnetoresistance. Compounds that comprise nonsymmorphic symmetries are especially interesting as the band crossings that are protected by the symmetry, are

not effected by SOC. ZrSiS, hosting a square lattice of Si atoms, has shown normal, as well as, nonsymmorphically protected 3D Dirac crossings at and close to the Fermi level [1]. ARPES measurements showed additional surface states crossing the bulk bands, which do not fit in the current scheme of surface states. Here, we analyze their origin by comparing ARPES data with DFT and tight-binding calculations. We present the idea of a selective symmetry breaking through the surface that lifts the nonsymmorphic degeneracy at the X point and leads to the formation of these surface states.
[1] L. M. Schoop *et al.*, Nat. Comm. 7, 11696 (2016).

TUE 15
Disclosing the Electron Doping Process in Single-Walled Carbon Nanotubes

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Here we present a systematic in-situ Raman study of the electron doping in enriched metallic and semiconducting HiPCO single-walled carbon nanotubes (SWCNTs). A detailed monitoring of this process was achieved via a controlled time-dependent potassium evaporation under ultra-high vacuum conditions. Our study was focused on a detailed analysis of the radial breathing modes (RBM), which can be correlated to diameter-dependent changes during the charging process, and the G-line development as a function of electron doping. We were able to record different charging steps showing that:
1) The RBM intensity of the largest-diameter CNTs decreases first with increasing doping level.
2) In contrast to semiconducting CNTs, in which no G-line shift can be obtained before reaching their final doped state, the G-line of the metallic ones first upshifts to higher wavenumbers. After reaching a specific doping level the G-line starts to downshift until it reaches its highly doped state.
The specific characteristics of the samples, and our built-in-purpose setup allowed us to track for the first time these differences in the charging process between semiconducting and metallic nanotubes.

TUE 16
A fiber-based microcavity setup for cavity nano-optomechanics with 2D materials

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Cavity optomechanics studies the parametric interaction of light and mechanical motion mediated by dynamical backaction. In this work we will first present our optomechanical setup: a fiber-based near-infrared microcavity in which we insert the mechanical object. The cavity is formed by two opposing glass fibers whose ends are CO2 laser ablated and Bragg-coated, resulting in two concavely shaped, highly reflective mirrors. This configuration leads to small cavity mode volumes and finesse exceeding 100,000. Secondly, we will present our design and fabrication of 2D materials as mechanical resonators. They will be ultra-thin drums made from 2D van der Waals materials presenting a bandgap and low absorption in the wavelength range of interest, e.g. hexagonal boron nitride. On the one hand, the low mass of these 2D materials results in high resonance frequencies in the MHz regime and large zero-point fluctuations, ideal for optomechanics experiments. On the other hand, their thin dimensions make them perfect samples for the geometrical restrictions that our small cavity imposes.

TUE 17
All-electrical piezoresistive AFM for controllable straining of 2D materials

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Single photons are extremely important for quantum information applications and can most probably be the best building block for future quantum communication. In the past years, several works discovered that defects in 2D materials such as WSe_2 and hBN can emit single photons. Single photon emitters in 2D materials are very promising as they can be easily integrated on chips and can be rather easily manipulated. Moreover, it seems that the strain profile of the 2D materials is dominant in the control over the physical properties of the single photon emitters. Still, no experimental confirmation was made of how controlling the localized strain in the vicinity of the defects affects single photon emitters.

In this work, we develop an approach to apply and control localized mechanical strain both at room and cryogenic temperatures while measuring the optical properties of the strained material. Our experimental setup is composed of an all-electrical home-built piezoresistive AFM system that operates inside an optical cryostat. With this system we are able to strain the materials both in room and cryogenic while recording photoluminescence, including single photon emission.

TUE 18
Direct observation of defect evolution in 2D single layer tungsten diselenide by low voltage high resolution transmission electron microscopy

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Defects in two-dimensional transition metal dichalcogenides (TMDs) have received increasing attention in recent years due to their influence on their extraordinary mechanical, electrical, magnetic and optical properties. By controlled electron irradiation under the transmission electron microscope, such defects may tailor a material's unique properties. [1,2]
In this work, defect evolution in WSe_2 was observed in real time using our novel C_c- and C_s - corrected SALVE (Sub Ångström Low Voltage Electron microscopy) instrument [3] with atomic resolution. The combination of high time- and spatial resolution enabled the observation of many intermediate states, atom-by-atom and provides deeper understanding of its formation dynamics.
[1] Y.-C. Lin *et al.*, Nat. Commun. 6, 6736 (2015)
[2] H.-P. Komsa and A. V. Krasheninnikov, Adv. Electron. Mater. 3, 1600468 (2017)
[3] M. Linck *et al.*, Phys. Rev. Lett. 117, 076101 (2016)

TUE 19
Influence of thin film morphology and stacking sequence on nickel-catalyzed graphitization of thin amorphous carbon films

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Metal-induced crystallization with layer exchange (MIC w LE) reduces the crystallization temperature of group 14 elements significantly. This is especially interesting for device fabrication on substrates with limited thermal stability. In this contribution, MIC w LE is applied on Ni and C thin film stacks with different stacking sequences. The influence of the thin film morphology and stacking on the layer exchange degree αLE and the graphitic ordering is studied comprehensively in situ and ex situ.
During annealing of the thin films at up to 700 °C, film morphology and stacking sequence had a significant impact on αLE, showing an incomplete LE for the C/Ni stack. The highest αLE of 96 %, determined by RBS and ERDA, was achieved for the smoothest samples and Ni/C stacking sequence. Raman spectroscopy and TEM demonstrated the formation of 2D crystalline carbon structures independently of the stacking sequence, while the degree of graphitic ordering increased with de-

creasing surface roughness. The simultaneous occurrence of LE and graphitization has been demonstrated in situ by RBS and Raman, giving insights into mechanism responsible for carbon crystallization in this system.

TUE 20
Spherical aerogels of multi-walled carbon nanotubes and polarizability models of conducting spheres

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The polarizability of different spheres consisting of low density MWCNT aerogel, metals, and connected wires are compared in the range of 8-12 GHz. Isotropic connected wire medium (with nanosized wire diameters 5.4 nm) has the structure discreteness with very small lattice constants (near 0.0002 wavelength). This leads to a significant drop in the effective conductivity of the wire medium (6 orders) and an increase in the Maxwell charge relaxation time. Due to this, the polarizability of the spheres consist of the cubic lattice of conductors decreases relative to all-metal spheres with the same conductivity by 10 %. The Debye length also grows to macroscopic sizes (up to 0.01 mm) and the static polarizability of the spheres changes due to a change in the charge distribution of the surface. MWCNT aerogels have a structure with non-rectilinear nanowires and a chaotic distribution of contacts. Nevertheless, it can be assumed that physical processes in such a medium are analogous to processes in media formed by regular structures. Indeed, measurements of the polarizability of aerogels support this proposition.
This work is supported by the Russian Science Foundation (grant 17-73-20293).

TUE 21
Direct observation of intravalley spin relaxation in single-layer WS_2

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In monolayer Transition Metal Dichalcogenides (TMDs) the valence and conduction bands are spin split because of strong spin-orbit interaction. In addition, in tungsten-based TMDs the peculiar spin-ordering of the conduction band gives rise to so-called dark exciton states lying at a lower energy than the optical gap. Photoluminescence experiments have provided an indirect evidence of these dark excitonic states but up to now a direct study of the relaxation dynamics between bright

and dark exciton is still missing. Here we exploit the valley selective optical selection rules and use two-color helicity-resolved pump-probe spectroscopy to directly measure the intravalley spin-flip relaxation dynamics of electrons in the conduction band of single-layer WS2. We find that this process occurs on a sub-picosecond time scale and is significantly depending on the temperature, strongly pointing to a phonon-assisted relaxation mechanism. These experimental observations are supported by time-dependent ab-initio calculations. Our findings provide additional parameters for studies of dark excitons and the applications in spintronics or valleytronics in single-layer TMDs.

TUE 22
Band Structure and Layer Interactions in Van der Waals Materials

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In many Van der Waals materials, the layer number strongly affects the material's band structure, e.g., the transition from a direct to an indirect semiconductor in MoS_2. Although detailed information of these band properties is crucial – particularly in artificial heterojunctions – the small size of the crystals make most techniques unfeasible for band structure measurements. Here, we present a comprehensive overview of the band structure effects in graphene, hexagonal boron nitride and various transition metal dichalcogenides. To this end, we employ angle-resolved reflected-electron spectroscopy (ARRES), which allows us to measure the unoccupied bands from areas as small as $\sim$10 nm. We discuss the effects of inter-layer interaction in Van der Waals homo- as well as heterojunctions.

TUE 23
Vibrational properties of misfit-layer compound nanotubes from CrS_2

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Misfit layer compounds (MLC) offer an interesting approach towards synthesis of novel one-dimensional nanostructures and two-dimensional materials. Understanding their structure and their physical properties has been subject to intense scientific research. The MLCs described by the formula MX-TX_2 consist of a transition metal dichalcogenide (TMD) layer TX_2 and an intercalation layer MX with distorted rock-salt structure. Here M denotes a metal, X is one of the elements S or Se, and T is of the group of transition metals. In our study the TMD layer CrS_2 is intercalated by either LaS-, CeS- or GdS- layers. Upon formation of the MLC charge transfer between the sublayers and deformation of the intercalation layer stabilize the otherwise metastable CrS_2. Due to the misfit between the sublayers in at least one direction and the seaming of dangling bonds at the rim atoms, the synthesis of nanotubes and -scrolls is favored. We investigate the vibrational properties of MLC nanotubes via Raman spectroscopy and density-functional theory. The results are discussed regarding previously published TEM methods.

TUE 24
Unusual silicon oxidation under carbon nanotube films

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The interfacial chemistry of oxide formation is critical to the performance of carbon nanotube-silicon heterojunction solar cells and photodetectors.[1] Under certain oxidation conditions a predominance of silicon suboxides form underneath carbon nanotube films and it has been shown that these suboxides can significantly impact device performance.[2,3] Further, it has recently been suggested the possibility of direct C-O-Si bond formation[4] and that these hybridised states are beneficial to performance. Considering the ongoing efforts to incorporate carbon nanotubes into established silicon microelectronics these issues have far reaching implications. We report the results of our investigations into trying to determine more conclusively, a) what is the effect of the suboxides on device performance, b) what is the microscale origin of the suboxide formation and, c) whether or not there is indeed the formation of C-O-Si bonds.

[1] D. Tune and B. Flavel, Advanced Energy Materials (2018)
[2] Pintossi et al., J. Phys. Chem. C (2013)
[3] Hiroyuki et al., In preparation (2018)
[4] Ponzoni et al., ACS Applied Materials & Interfaces (2017)

TUE 25
^{12}C - ^{13}C isotopic graphene interfaces studied by Tip-enhanced Raman spectroscopy

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By the intentional periodic manipulation of the ^{13}C and ^{12}C precursors, the growth of the graphene flakes can be engineered by creating concentrically arranged rings of ^{13}C and ^{12}C [1]. The two isotopic graphene regions own, in first approximation, the same electronic properties while the phonon frequencies are modified. With tip-enhanced Raman spectroscopy we are able to probe the phonon frequencies locally at the interface between ^{12}C and ^{13}C and map, with high resolution, the propagation of one phonon into the different isotopic region. Depending on the growth conditions, different types of interfaces and phonon mixing are detected.
[1] E. Whiteway, W. Yang, V. Yu, and M. Hilke, Carbon N. Y., 111, 173 (2017).

TUE 26
Correlative Raman-SEM imaging for material characterization

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Rapid advances in nanotechnology have increased the need for precise characterization at nanoscale. The morphology of different materials including several carbon forms can be visualized employing scanning electron microscope (SEM). The chemical quality of these materials can be distinguished using Raman spectroscopy. However, the morphological character of assigned material/carbon surface features could be misleading due to limited resolution of Raman optical microscopy. Combined Raman-SEM imaging within one hybrid instrument, known as RISE microscopy (i.e. correlative Raman Imaging and Scanning Electron microscopy), can provide comprehensive sample characterization in the same sample area. In other words, the overlaid SEM image with color-coded Raman map link structural surface properties of the investigated material with its molecular compound information. Here we present the RISE microscopy of different carbon materials (e.g. diamond, carbon nanotubes and graphene) in their individual or heterostructure forms. We also show their structural degradation after electron beam or Raman laser irradiation at higher voltages/powers.
This work was supported by the grant P108/12/G108.

TUE 27
Selective covalent functionalization of carbon nanotubes activated by light

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The diazonium reaction on nanotubes has recently attracted attention due to the ability of forming bright, fluorescent quantum defect states, by a specific conversion of the sp^2 to sp^3 bonds. The resonant light has been reported to accelerate and tune the reaction velocity. The latter is proportional to the energetic difference between transition energy and incident light. In our study, we demonstrate how a single chirality can be preferably functionalized by tuning optical excitation. We have performed the functionalization on a mixed chirality sample, resonantly exciting one of the nanotube chiralities [(9,7) tube]. The nanotubes were deposited on the substrate and locally exposed to the laser light at 1.58 eV. We monitored the reaction in situ via Raman spectroscopy. A dramatic difference between dark and illuminated areas in the functionalization degree was observed. The material outside the active spot did not demonstrate any changes from the pristine sample. The successful functionalization of the illuminated material was confirmed by resonant Raman scattering. Devices made of functionalized material show modified electroluminescence spectra as compared to pristine tubes.

TUE 28
Towards 2D Topological Insulator Devices

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Spintronics requires the efficient generation, manipulation and detection of spin currents. Graphene has been demonstrated to be a high performance spin transport material, but generation and control of the spin polarization by electrical means is difficult. Promising spin generators are the topological insulators (TIs). One intriguing strategy is to locally decorate graphene by a 3D TI in order to create spin generator regions that could be smoothly integrated with laterally adjacent, bare graphene regions as spin transport channels. Along these lines, it is relevant that theory predicts that the interface-induced spin-orbit coupling (SOC) imparted by the 3D TI is able to increase the band gap of the 2D TI graphene. Here, we report the gate-dependent, low temperature charge transport properties of vertical heterostructures composed of graphene and a thin layer of Bi2Te2Se as 3D TI. By using different contact configurations, we explore the extent to which the presence of the Bi2Te2Se top layer modulates the magnetotransport properties of graphene, and furthermore whether signatures of charge transport through helical 1D edge channels within the graphene can be detected.

TUE 29

Comparison of flat, structured and catalytically-modified boron doped diamond electrodes for electrochemical detection of contaminants in water

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We studied electrochemical detection of metal ions (Cd^{2+}, Pb^{2+}, Cu^{2+}) using boron doped diamond (BDD) electrodes in sense of reproducibility and sensitivity. Three different BDD electrode materials were used: i) flat (as-grown) BDD, ii) structured BDD (nanocones obtained by reactive ion etching using gold nanoparticle's mask) and iii) catalytically-modified BDD electrodes (prepared by annealing of Ni-coated BDD).
We found that standard cyclic voltammetry is not sensitive enough to detect 0.1 mM Cd^{2+} in 0.1 M HCl, however by using differential pulse voltammetry we detected Cd^{2+} even at such low concentrations. Moreover, the BDD recognized individual contaminants in a complex solution consisting of three contaminants (Cd^{2+}, Pb^{2+} and Cu^{2+}). Here, the detection limits were influenced by overlapping or by splitting of voltammetric peaks (i.e. effect of underpotential deposition of metal ions on BDD). In contrast to flat BDD electrodes, the nano-structured or catalytically-modified electrodes improved the limit of detection (LOD).
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TUE 30

Horizontally and vertically aligned thin MoS_2 films: a GIWAXS and optical study

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Sulfurisation of predeposited Mo films is one of the key approaches for growing very thin layers of MoS_2. Depending on the Mo film thickness and growth conditions, the orientation of an as-grown MoS_2 layer may be either parallel to the substrate or perpendicular to it. So far, the transmission electron microscopy and electron diffraction have been used for detection of the MoS_2 layer alignment. Here, we show that grazing incidence wide-angle X-ray scattering (GIWAXS) is a straightforward method not only to analyse the orientation but also to estimate other properties of MoS_2 layers, for instance, a ratio of a crystalline to amorphous MoS_2 phase. We analyse in a detail how the MoS_2 layer alignment depend on the temperature, Mo thickness and other parameters of the growth procedure. However, the instrumentation for GI-

WAXS is rather expensive making the method not widely distributed in laboratories. Therefore, we correlate the GIWAXS results with those gathered by more accessible methods like AFM, Raman and optical spectroscopy to get information on the layer orientation.

TUE 31
Investigating the electrical properties of Graphene/$CoFe_2O_4$ nanocomposties prepared in the autoclave

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Graphene seems to be an ideal material as a nanocomposite substrate for applications in electronics due to its very good electrical and thermal conductivity, excellent mechanical properties, optical and electrochemical properties. Pure graphene is a non-magnetic material. Materials like soft ferrites have the most attractive magnetic properties for many applications. Therefore, combination of very good electrical properties of graphene and magnetic properties of metal oxides can create attractive nanocomposites with good conductance and improved magnetic properties. In this work we present the preparation graphene/$CoFe_2O_4$ nanocomposites using an autoclave. We used X-ray diffraction (XRD) to determine the phase composition of the nanocomposites. Thermal properties were determined with the use of thermogravimetric analysis. Additional morphology studies were performed using high resolution transmission electron microscopy (HR-TEM). Electrical properties were determined by measuring the resistivity of thin layers of composite materials over SiO_2/Si substrates.

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TUE 32
Electrochemical Exfoliation of Black Phosphorus

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Black phosphorus (BP) has recently attracted great attention due to its tunable, layer-dependent bandgap, high carrier mobility, good current on/off ratio, as well as unique in-plane anisotropy, which renders the material attractive for nanoelectronic, thermoelectric and photonic devices.[1] The major challenge for a successful application lies in the fabrication of few- or single layer nanosheets of BP. Several methods have been developed, while mechanical and liquid exfoliation of the bulk crystals figure amongst the most prominent ones.[2] However, large-scale exfoliation leading to uniform and stable dispersions in high yield remains a challenge.

Herein, we present a screening of different solvents and anodic/cathodic conditions for the electrochemical exfoliation of BP nanosheets of good quality and in high yields. The technique is not limited to aqueous systems[3] but has also been reported for organic solvents and ionic liquids, which have an outstanding protective effect in BP.[4]

[1] Angew. Chem., Int. Ed., 2017, 10.1002/anie.201708211

[2] Nat. Commun., 6, 8563 (2015)

[3] Angew. Chem., Int. Ed., 56, 10443 (2017)

[4] JACS, 139, 10432 (2017).

TUE 33

Record Low Thermal Conductivity of Polycrystalline MoS_2 films: Tuning the Thermal Conductivity by Grain Orientation

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Recent advances in two-dimensional (2D) material science have shown the importance of phonon thermal transport in managing heat in future devices. In particular, the understanding of how the thermal conductivity of polycrystalline 2D materials scales with grain sizes has become a key information for engineering efficient and scalable materials towards applications.
In this work we report a record low thermal conductivity in polycrystalline MoS_2 obtained by varying grain sizes and orientations in ultrathin films. By optimizing the sulphurisation parameters of nanometre-thick Mo layer, we could grow MoS_2 films with tuneable morphologies. The thermal conductivity is extracted from a Raman laser power-dependent study on suspended samples. The lowest value of thermal conductivity of $0.27\,Wm^{-1}K^{-1}$ is obtained in a polycrystalline sample formed by a combination of horizontally and vertically oriented grains, with respect to the bulk (001) monocrystal. Analysis by means of molecular dynamics and finite element method simulations confirm that such grain arrangement leads to lowest grain boundary conductance.

TUE 34
Local Photovoltaic Properties of 2D-3D Heterojunctions

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Interfacing of materials with different dimensionalities becomes increasingly relevant for many applications which can utilize the exceptional properties of low-dimensional materials on one hand, and build-up on the existing production know-how for bulk (3D) materials on the other. Numerous appealing possibilities are offered by such combinations. In this work we focus on 2D-3D heterostructures composed of mechanically exfoliated single- and few-layer layer graphene (Gr) or WS_2 coupled to n- or p-doped silicon, respectively. As we have shown recently [1], it is possible to correlate photovoltaic (PV) characteristics of such junctions measured at macroscopic (solar simulator) and microscopic (conductive AFM under light/dark) scales. Therefore we set out to investigate in detail the influence of the layer number, local topography, defects, etc., on local PV properties of the p-Gr/n-Si Schottky junctions and n-WS_2/p-Si p-n junctions. The study is further extended to include the local effects of ionic doping of graphene to enhance increase its conductivity.
[1] Hajkova *et al.*, Chem.Phys.Lett. 676, 82 (2017).

TUE 35
Switching the spin helix direction by magnetic field

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We report the theoretical and experimental study of the spin diffusion and spin drift of electrons and the formation of long-lived spin helix in III-V and II-VI semiconductor quantum wells. The emerging spin helix pattern indicates that the spin waves with a non-zero wave vector possess the longest lifetime. In the absence of an external magnetic field, the spin helix in (001) quantum wells is directed along the [110] or [1$\bar{1}$0] axes, depending on the spin-orbit splitting anisotropy. We demonstrate that the strong enough magnetic field applied in the quantum-well plane alters the spin diffusion pattern and can even switch the spin helix direction. The experimental maps of spin diffusion measured with spatial and temporal resolutions for two orthogonal magnetic field orientations enable us to directly determine the Dresselhaus and Rashba spin-orbit constants.
[1] A.V. Poshakinskiy and S.A. Tarasenko, Phys. Rev. B 92, 045308 (2015).
[2] S. Anghel, F. Passmann *et al.*, arXiv:1708.09150 (2017).

TUE 36
Raman and infrared active rigid layer modes in quasi-two-dimensional crystal structures

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Universal condition under which acoustic modes of arbitrary dynamical subsystems combine into the normal modes of the entire system is formulated. Developed is the formalism of studying such modes and symmetry based analysis of Raman and infrared activity of these, rigid layer modes in quasi-two-dimensional crystal structures is performed. Effective Hessian matrices of interlayer interaction are studied and it is shown that within nearest neighbor approximation rigid layer dynamics can be reduced to simple model of either uniform or alternating linear chain, where each element of the chain represents an atomic monolayer or a set of suitable chosen atomic monolayers. Analytical solution of the alternating chain model is discussed and the modes with dominant displacements of the outer surface layers are shown to be equivalent to the topological boundary modes.

TUE 37
The effects of defects and disorder on the electronic structure of graphene

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We use a real-space nearest neighbor tight-binding model to study the effect of defects on the band dispersion of graphene. We find that defects in graphene either generally preserve the canonical band structure, or disrupt it by separating the two cones creating an "'elongated"' Dirac point. This second structure greatly resembles the band dispersion of experimentally measured epitaxial graphene. By using a

self consistent T-matrix approximation we find the reason why defects create two distinctly different band structures, by showing that point defects are either resonant or non-resonant in graphene. Adding all these pieces together, we conclude on the cause of “elongation” in epitaxial graphene and the nature of the electronic structure in the “elongated” region finding that this region can not be considered a gap.

TUE 38

Observation of unusual Fabry-Perot interferences in a ultra clean carbon nanotube

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Carbon nanotube CNT)is interesting that its electron transport properties is strongly dependent on electrical contacts. For low transparency contacts it is usually in Coulomb blockade regime where charging effects take place, while for high transparency contacts it will be dominated in Fabry-Perot regime. Here we present a study of Fabry-Perot interference in a ultra clean CNT. We observed a very nice pattern of Fabry-Perot oscillations. The pattern consists of a fast oscillation (normal) and an unusual slow secondary oscillation. The slow oscillation is also vividly revealed in the color mapping of dI/dV with respect to gate voltage and source-drain bias. Moreover, we found that the sequentially filling of 4 electrons in one shell is broken at the gate voltage where the minimum or maximum of the slow oscillation occurs, and additional two electrons are added.

TUE 39

Spin-relaxation in superconducting graphene: roles of local magnetic moments and spin-orbit coupling

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The unique electronic band structure of graphene allows formation of resonant states. Resonant impurities enhance spin relaxation of graphene electrons via adatom induced local magnetic moments [1, 2], or locally induced spin-orbit coupling (SOC) [3-5]. Superconducting graphene offers a unique possibility to explore and disentangle those two contributions to the spin relaxation. The proximity induced gap significantly affects the formation of resonances; the presence of local magnetic moments would cause "‘resonant-to-bound state"’ transition by forming Yu- Shiba-Rusinov states. Those can be detected and analyzed by STM experiments [dI/dV versus Fermi energy]. We discuss the formation of such bound states, their fragility with respect to local SOC and their impact on the spin relaxation in superconducting graphene.

[1] D. Kochan, M. Gmitra, J. Fabian, PRL 112, 116602, (2014)
[2] D. Kochan, S. Irmer, M. Gmitra, J. Fabian, PRL 115, 196601, (2015)
[3] M. Gmitra, D. Kochan, J. Fabian, PRL 110, 246602, (2013)

[4] J. Bundesmann, D. Kochan, F. Tkatschenko, J. Fabian, K. Richter, PRB 92, 081403(R), (2015)
[5] D. Kochan, S. Irmer, J. Fabian, PRB 95, 165415, (2017)

TUE 40
Optical inspection of carbon nanotube hybrids towards bio-applications

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Single walled carbon nanotubes (SWCNTs) are ideal candidates for biological sensing applications, since they are strong photoluminescence (PL) emitters in the optical region where biological tissues are transparent. The optical response of SWNTs is strongly dependent on the environment surrounding them and it is therefore important to find pathways to tune their optical properties. Among these methods functionalization of the outer wall of the tubes has been thoroughly investigated and much less has been done with the hollow core, which can host molecules and nanostructures also capable of gaining control of the optical properties. Here we explore two new ways of functionalization of SWCNTs: First, filling SWCNTs with Carbon chains and, second, with on wall doping with Boron. The first were produced by extracting Carbon chain filled inner tubes from DWCNTs via density gradient ultracentrifugation. The B-doped tubes are CVD material with a narrow diameter distribution with record dopant concentrations. The results of both of these hybrid nanotube materials investigated using PL and optical absorption spectroscopies are here presented.

TUE 41
Electrical properties of printed electrolyte-gated tungsten disulphide nanosheet thin film transistors produced from aqueous inks

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A wide range of layered semiconductors (especially the transition metal dichalcogenides) possess exciting functional properties suitable for numerous electrochemical applications including energy storage and conversion, optoelectronics and sensing. In particular, when processed from the liquid phase they are exceptional candidates for use in emerging device configurations that are flexible and/or wearable.
Here we demonstrate the production of printed electrolyte-gated transistors prepared from tungsten disulphide nanosheet dispersions produced by liquid phase exfoliation. The thin film devices are produced at low temperatures (less than 120 °C) in ambient atmosphere and from aqueous inks. We demonstrate state-of-the-art performance for TMD-based thin film transistors as well as outline processing re-

quirements that enable the realisation of ambipolar (i.e. both p and n type) device operation for the first time.

TUE 42
Revealing the 3D structure of graphene defects

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Electron tomography is a powerful technique to determine three-dimensional structures down to atomic resolution. It requires, however, that they remain unchanged under the continuous electron irradiation while acquiring multiple images at different tilting angles. Here we demonstrate a method that reveals the three-dimensional structure around defects in graphene from only two transmission electron microscopy images recorded at different angles. This is possible for structures for which the location of each atom as well as their connections (ie, nearest neighbors) can be discerned from each image. The structure is obtained through an optimization process where both the atomic positions as well as the simulated imaging parameters are iteratively changed until the best possible match to the experimental images is found. We first demonstrate that this method works using an embedded defect in graphene that allows direct comparison to the computationally predicted three-dimensional shape, and then move on to reconstruct the shapes of several experimentally observed grain boundaries. Our results provide deep insights into the three-dimensional structure around defects in graphene.

TUE 43
Giant intravalley scattering on pseudo-magnetic fields in crumpled graphene

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Mechanical strain in graphene can be described as a pseudo-magnetic field which can have dramatic consequences on the behavior of electrons and holes. Here we show that pseudo-magnetic field fluctuations present in crumpled graphene can induce significant intravalley scattering of charge carriers. We detect this by measuring the confocal Raman spectra of crumpled areas, where we observe an anomalously high intensity of the D' peak with respect to the D peak ($I_{D'}/I_D \approx 30$). We reproduce the high D' intensity by numerical calculation of the double resonant Raman spectra. We interpret our results as experimental evidence of the phase shift suffered by Dirac charge carriers in the presence of a pseudo-magnetic field, al-

lowing for complete backscattering. These measurements are the first example of defect-induced Raman scattering on perturbations that are smooth on the atomic scale.

TUE 44
Hiqh-quality dry transferred CVD bilayer graphene

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For years, the electronic properties of chemical vapor deposition (CVD) grown single and bilayer graphene (BLG) could hardly compete with high-quality mechanically exfoliated samples from natural graphite. Here, we report on the fabrication and characterization of high-quality CVD BLG, applying a dry transfer technique to directly pick-up CVD-grown BLG from the metal surface by hexagonal boron nitride (hBN) crystals [1]. Using Raman spectroscopy we reveal an AB-stacking order of the BLG crystals and a high structural quality. From transport measurements on encapsulated hBN/BLG/hBN Hall bar devices we extract charge carrier mobilities of up to 180,000 cm^2/(Vs) at 2 K and up to 40,000 cm^2/(Vs) at 300 K, outperforming state-of-the-art CVD bilayer graphene devices. Moreover, we show an on-off ratio of more than 10,000 and a bandgap opening with values of up to 15 meV for a displacement field of 0.2 V/nm wich is in good agreement with theory. Our findings thus open the route towards a scalable fabrication process which leads to high-quality CVD BLG devices [2].
[1] L. Banszerus *et al.*, Sci. Adv. 1, e1500222 (2015)
[2] M. Schmitz *et al.*, Appl. Phys. Lett. 110, 263110 (2017)

TUE 45
Gate-Defined Quantum Confinement in InSe-based van der Waals Heterostructures

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Two-dimensional (2D) layered materials, such as transition metal dichalcogenides (TMDCs), are promising materials for electronic and optical applications due to their unique properties. One such material is Indium Selenide (InSe). It stands out from other layered materials due to having a large mobility $\sim 10^4$ cm^2/Vs and a bandgap dependent on the number of atomic layers [1]. However, InSe degrades in ambient

conditions, meaning that to study low dimensional transport; devices have to be fabricated avoiding exposure to air.
Here we report the first low dimensional InSe devices defined by local electrostatic gating fabricated in a pure Argon environment. We present our results on electronic transport in 1D quantum confined systems and 2D quantum dots. Multiple steps in conduction due to quantum confinement have been observed over different carrier concentrations, for several devices, consistent with theoretical predictions. These results could be used to gain insight into the fine electronic structure of InSe and could lead to applications in quantum computing.
[1] D. Bandurin *et al.* Nature Nanotechnology (2016).

TUE 46
A novel direct and cost-effective growth of III–V semiconductors on 2D layered materials

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III-V materials and devices play an increasingly important role in a variety of electronic and photonic systems. However, the production of high quality III-V materials requires very complex fabrication processes, which makes them very costly and limits their extension to common applications. Moreover, their current conventional heteroepitaxial growth methods, on various semiconductors including metal-oxides, still have tremendous complexity and suffer from various lattice and thermal expansion mismatches. New and alternative fabrication methods are necessary to restrict inherent lattice matching to favor widespread applications. Here, we demonstrated a new cost effective and simple method to synthesize III-V and III-VI semiconductors directly on top of layered materials. In this method, an active nucleation material is sandwiched between 2D layered materials, such as hexagonal boron nitride (h-BN), to produce a stacked structure. Thus, III-V or III-VI materials can grow and diffuse without aforementioned constraints. This method also paves the way towards developing unique nano-engineered super-lattices.

TUE 47
Capacitive pressure and touch sensors with suspended graphene-polymer heterostructure membranes

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We present the fabrication and characterization of a suspended graphene/polymer heterostructure membrane spanning a large array of micro-cavities each up to 30 μm in diameter with 100 % yield.[1]
Such membrannes are then employed in a capacitive pressure sensor covering an area of just 1 mm^2, showing reproducible pressure transduction under static and dynamic loading up to pressures of 250 kPa, and in good agreement with calcula-

tions. Next, we demonstrate a novel strained membrane transfer and optimizing the sensor architecture. This enables suspended structures with less than 50 nm of air dielectric gap, giving a pressure sensitivity of 123 aF/Pa per mm^2 over a pressure range of 0 to 100 kPa.[2]
Lastly, we demonstrate a touch-mode capacitive pressure sensor (TMCPS) incorporating a SU-8 spacer grid structure.[3] This results in a partially suspended membrane configuration, which produces reproducible deflection, even after exposing the membrane to pressures over 10 times the operating range. The device shows a pressure sensitivity of 27.1 ± 0.5 fF/Pa over a pressure range of 0.5 kPa to 8.5 kPa.
[1] Berger Nanoscale (2016)
[2] Berger Nanoscale (2017)
[3] Berger 2D Materials (2017)

08:30 – 09:30 TUTORIAL: J. Zaumseil, Heidelberg
Optical and Charge Transport Properties of Dense Films of Semiconducting Carbon Nanotubes

09:30 – 10:00 C. Voisin, Paris
Bright and tunable single-photon source with carbon nanotubes

10:00 – 10:30 coffee break

10:30 – 11:00 R. Senga, Tsukuba
Direct measurement of a locally modulated gap transition at defects in carbon nanotubes

11:00 – 11:30 W. Wenseleers, Antwerp
Diameter-controlled stacking of functional molecules in single wall carbon nanotubes

11:30 – 12:00 L. G. Cancado, Minas Gerais
Monopole nanoantennas for near-field scanning optical microscopy

12:00 – 17:00 mini workshops

17:00 – 18:30 Dinner

18:30 – 19:00 E. Joselevich, Rehovot
Coiling and twisting nanotubes

19:00 – 19:30 K. Bolotin, Berlin
Excitons in two-dimensional semiconductors "talking" to their environment

19:30 – 20:00 L. Baszerus, Aachen
Van-der-Waals heterostructures based on dry transferred high-mobility CVD graphene

20:00 – 20:30 F. Koppens, Barcelona
Polaritons in layered two-dimensional materials

08:30
TUTORIAL: Optical and Charge Transport Properties of Dense Films of Semiconducting Carbon Nanotubes
Jana Zaumseil[1]
[1]Angewandte Physikalische Chemie, Universität Heidelberg, Heidelberg

Large volumes of highly purified dispersions of monochiral semiconducting single-walled carbon nanotubes are readily available through polymer-wrapping and shear-force mixing. They enable the deposition (e.g. by aerosol jet printing or filtration) of semiconducting layers of variable thickness from sparse networks to 300 nm thick films with large optical density. These layers can be applied in lateral and vertical field-effect transistors with excellent device performance but also as electrochromic notch filters, for organic light-emitting diodes in the near-infrared or for the demonstration of trion-polaritons in microcavities. Here, we present examples of such applications and investigate the impact of novel n-dopants on nanotube networks, temperature-dependent charge transport within monochiral and mixed layers and their optical properties at different charge carrier densities.

09:30
Bright and tunable single-photon source with carbon nanotubes
Christophe Voisin[1], Jakob Reichel[2], Adrien Jeantet[1], Théo Claude[1], Yannick Chassagneux[1]
[1]Laboratoire Pierre Aigrain, Ecole Normale Supérieure, Université Paris Diderot, Paris
[2]Laboratoire Kastler-Brossel, Ecole Normale Supérieure, UPMC, Paris, France

Carbon nanotubes (CNTs) have unique properties (telecom wavelength emission, room-temperature operation,..) to tackle the challenges awaiting single-photon sources for secure quantum telecommunications. Nevertheless, the broad variety of species and local environment in a typical sample strongly hampers their integration in photonic devices. We designed an open micro-cavity engineered at the apex of an optical fiber to induce cavity quantum electrodynamical (CQED) effects on a single carbon nanotube. The geometry allows us to achieve an optimal spatial and spectral matching, reaching an unprecedented precision in measuring the CQED effects with CNTs. We show that the spontaneous emission diagram is strongly modified by the cavity, with a Purcell factor of 70, reaching an effective luminescence quantum yield of the order of 30 %, an extraction efficiency better than 95 % and a single-photon purity better than 97 %. In addition, we exploit the longitudinal tuning capability to drive the emitter in the so-called cavity feeding regime, where the side-band emission is enhanced far beyond simple spectral filtering, thereby providing an original, bright and tunable single-photon source.

10:30

Direct measurement of a locally modulated gap transition at defects in carbon nanotubes

Ryosuke Senga[1], Thomas Pichler[2], Kazu Suenaga[1]
[1]AIST, Japan
[2]University of Vienna

Defect-related exciton governs the optical properties of semiconducting carbon nanotubes. The light-probe emission/absorption spectroscopy usually has the inferior spatial resolution to assign an individual defect and therefore the direct correlation of exciton peaks with the atomic structures of defects is hardly possible. In this study, we measured the optical gap transitions of an individual semiconducting carbon nanotube with defects by using a monochromated electron microscope. The optical conductivity extracted from an electron energy-loss spectrum for a certain type of defect presents a characteristic modification near the lowest excitation peak. The line-width of exciton peak shows a variety of broadening at different defect sites and suggests different degrees of shortening of its lifetime. Such a direct correlation between absolute optical constants and atomic structures in a quantum object would be useful for further study to quantify the optoelectronic behaviors of nanoscale devices.

11:00

Diameter-controlled stacking of functional molecules in single wall carbon nanotubes

Wim Wenseleers[1], Stein van Bezouw[1], Sofie Cambré[1], Jochen Campo[1], Joeri Defillet[1], Dylan H. Arias[2], Rachelle Ihly[2], Andrew J. Ferguson[2], Justin C. Johnson[2], Jeffrey L. Blackburn[2]

[1]Physics Department, University of Antwerp, Antwerp

[2]Chemistry & Nanoscience Center, National Renewable Energy Laboratory, Golden, Colorado 80401, United States

The well-defined and variable diameters of single-walled carbon nanotubes (SWCNTs) provide an ideal template for creating unique one-dimensional structures by encapsulation of various molecules. We have previously shown that SWCNTs exactly fitting a single file of dipolar molecules can be used to naturally align them in a polar, head-to-tail fashion, coherently adding their nonlinear optical responses. Here, we show that encapsulating a quadrupolar dye results in highly diameter-dependent dye absorption and subsequent excitation energy transfer (EET), due to the diameter dependent stacking and hence inter-molecular interactions. The unique and variable electronic properties of the SWCNTs also make them the ideal vehicle to probe such effects spectroscopically. We studied the systems in detail by optical absorption, 2D fluorescence-excitation, Raman, and transient absorption spectroscopy. In addition, we find that SWCNT filling does not limit the selectivity of subsequent chirality separation protocols. These systems, with tunable dye absorption, fast and efficient EET, and possibilities for subsequent separation, demonstrate potential for implementation in photo-conversion devices.

11:30

Monopole nanoantennas for near-field scanning optical microscopy

Thiago L. Vasconcelos[1], Cassiano Rabelo[2], Bráulio S. Archanjo[1], Carlos A. Achete[1], Ado Jorio[2], Luiz Gustavo Cancado[2]
[1]Divisão de Metrologia de Materiais, Instituto Nacional de Metrologia, Qualidade e Tecnologia (INMETRO), Duque de Caxias, RJ 25250-020, Brazil
[2]Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, MG 30123-970, Brazil

This talk presents a new scattering-type near-field probe formed by a micro–pyramidal body whose length L is scalable to fine-tune LSPR modes, giving rise to a plasmon-tunable tip pyramid (TTP). The local surface plasmon (LSP) modes were studied by electron energy loss spectroscopy (EELS), and the results reveal that TTPs act as monopole antennas. The monopole character of the TTP is a consequence of its geometry: the nanopyramidal part is electrically grounded on a flat metallic plateau that acts like a mirror providing the monopole's image that closes the dipole system. Simulations based on the boundary element method (MNPBEM) were performed to determine a linear relation describing the resonance match between the TTP characteristic length L and the wavelength of the coupled radiation field. The efficiency and reproducibility of the TTPs were tested in tip-enhanced Raman (TERS) experiments performed in single-layer graphene (SLG) and single-walled carbon nanotubes (SWCNT) samples. The results prove the realization of ultra–high enhancement factor (in the order of 1.6×10^4) with excellent yield (> 90 %).

18:30
Coiling and twisting nanotubes
Ernesto Joselevich[1]
[1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot 76100, Israel

Coils play important roles in electricity generation, electronics, magnetic devices and motors. Carbon nanotube (CNT) coils would thus be desirable structures for nanoelectronics and nanoelectromechanical systems. Following the observation of CNT serpentines several years ago, we recently demonstrated the self-coiling of single-wall CNTs into defect-free coils of up (NEMS) to more than 70 turns. Magnetic measurements show that the coils are highly conductive, but shorting between turns degrade their inductive behavior. Few-wall CNT coils could provide sheathing to enable functional inductive devices, such as electromagnets, dynamos, transformers and motors.

What happens when you twist a nanotube? We studied the mechanical and electrical response to torsion of nanotubes of different materials (C, WS_2, BN and BCN), and found intriguing differences between all of them. Recently, we have been able to create torsional resonators based on inorganic nanotubes, and found them to have higher resonant frequencies and quality factors than those based on carbon nanotubes. This demonstrates that inorganic nanotubes could be attractive building blocks for NEMS, including nanogyroscopes.

19:00

Excitons in two-dimensional semiconductors “talking” to their environment

Kirill Bolotin[1]
[1]Physics, Freie Universitat, Berlin

Every atom in two-dimensional semiconductors from the group of Transition Metal Dichalcogenides (TMDs) belongs to the surface. Because of that, TMDs are strongly affected by their microenvironment. In this talk we show that TMD excitons can serve as exquisite probes of the physical and chemical properties of that microenvironment.
First, we show that TMD excitons are strongly screened by nearby dielectrics. In suspended TMD, the behavior of pristine material is approached. We also examine frequency-dependent screening of excitons in TMDC and show that the frequency-dependent dielectric function of the environment can be effectively “sampled” by examining spectral shifts and intensity redistribution between neutral, charged, and defect-bound excitons. Second, we examine near-field energy transfer between TMDs and nanoscale quantum emitters (semiconductor quantum dots or dye molecules) near it. We show that such energy transfer is very efficient, and that its rate can be controlled through electrical gating. Finally, we examine binding of excitons in TMDs to charged molecules on their surface. We demonstrate new molecule-specific excitionic species produced by such binding.

19:30

Van-der-Waals heterostructures based on dry transferred high-mobility CVD graphene

Luca Banszerus[1,2]
[1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany
[2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Chemical vapor deposition (CVD) is a promising route towards upscaling graphene and other 2D materials, for making van-der-Waals (vdW) solids on industrial scales. Using a contamination-free dry transfer technique we fabricate vdW heterostructures based on CVD graphene with electronic properties indistinguishable from those of exfoliated graphene. The devices show mobilities exceeding 100,000 $cm^2/(Vs)$. In addition to the diffusive transport, we show an elastic mean free path exceeding 1 μm at temperatures of up to 200 K using Hall cross devices. By investigating large samples we conclude that the mean free path can exceed 28 μm at 2 K [2]. Importantly, we demonstrate not only hexagonal boron nitride as a suitable substrate for high mobility graphene devices, but also show that WSe_2 allows for ultrahigh mobility graphene at room temperature. Thus, we show that by choosing the right substrates [3] the electronic properties of CVD grown graphene match those of ultrahigh-mobility exfoliated natural graphene.

[1] L. Banszerus *et al.*, Sci. Adv. 1, e1500222 (2015)
[2] L. Banszerus *et al.*, Nano Lett. 16, 1387 (2016)
[3] L. Banszerus *et al.*, 2D Mat. 4, 025030 (2017)

20:00
Polaritons in layered two-dimensional materials
Frank Koppens[1]
[1]Quantum Nano-Optoelectronics, ICFO - The Institute of Photonic Sciences, Castelldefels - Barcelona

Heterostructures of graphene and related two-dimensional materials are a promising new material system with virtually unlimited possibilities. Van der Waals heterostructrures are constructed by vertically stacking atomically thin materials, selected from a rich palette of thousands of materials that can be semi-conducting, insulating, superconducting, metallic or magnetic. These are key enablers for tailoring new and unique electronic, optical and opto-electronic properties.
This platform has also emerged as a toolbox for in-situ control of a wide range of polaritons: plasmons, excitons and phonons. In this talk, we will show several examples of 2D material heterostructure devices with novel ways of exciting, controlling and detecting polaritons. We challenge the limits of quantum light-matter interactions and study the fundamental limits of optical field confinement, at the length-scale of single atoms.

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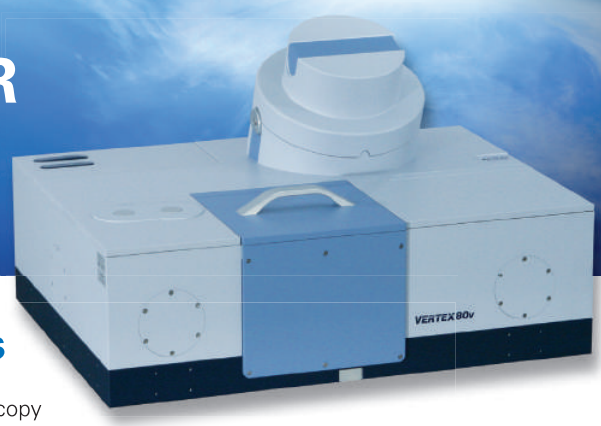

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FT-IR

Innovation with Integrity

08:30 – 09:30 TUTORIAL: S. Louie, Berkeley
Interaction and Topological Effects in Atomically Thin Two-dimensional Materials

09:30 – 10:00 M. Kroner, Zurich
Realization of an Electrically Tunable Narrow-Bandwidth Atomically Thin Mirror Using Monolayer $MoSe_2$

10:00 – 10:30 coffee break

10:30 – 11:00 C. Schneider, Würzburg
Light-Matter coupling in two dimensional materials

11:00 – 11:30 Y. Jiang, Piscataway
Tuning a Circular p-n Junction in Graphene from Quantum Confinement to Optical Guiding

11:30 – 12:00 I. Grigorieva, Manchester
Graphene as a 'tunneling barrier' in vertical magneto-resistive junctions

12:00 – 17:00 mini workshops

17:00 – 18:30 Dinner

18:30 – 19:00 A. Popov, Dresden
Endohedral metallofullerenes as robust single molecule magnets

19:00 – 19:30 M. Ganzhorn, Zurich
Molecular quantum spintronics

19:30 – 20:00 L. Forró, Lausanne
Photovoltaic perovskite nanowires: from fundamental aspects to applications

20:00 Poster Session III

08:30
TUTORIAL: Interaction and Topological Effects in Atomically Thin Two-dimensional Materials

Steven G. Louie[1,2]
[1]Department of Physics, University of California at Berkeley, Berkeley, CA 94720 U.S.A
[2]Lawrence Berkeley National Lab, Berkeley, CA 94720 U.S.A.

Symmetry, interaction and topological effects, as well as environmental screening, dominate many of the quantum properties of reduced-dimensional systems. These effects often lead to manifestation of counter-intuitive concepts and phenomena that may not be so prominent or have not been seen in bulk materials. In this talk, I present some fascinating physical phenomena discovered in recent studies of atomically thin two-dimensional (2D) materials and their nanostructures. A number of highly interesting and unexpected behaviors have been found – e.g., strongly bound excitons (electron-hole pairs) with unusual energy level structures and new topology-dictated optical selection rules; massless excitons; tunable magnetism and plasmonic properties; electron supercollimation by disorders; and novel topological phases – adding to the promise of these 2D materials for valuable applications.
This work was supported by the U. S. Department of Energy, National Science Foundation, and Office of Naval Research.

09:30

Realization of an Electrically Tunable Narrow-Bandwidth Atomically Thin Mirror Using Monolayer $MoSe_2$

Martin Kroner[1], Patrick Back[1], Sina Zeytinoglu[1], Livio Ciorciaro[1], Atac Imamoglu[1]
[1]Institute of Quantum Electronics, ETH Zürich, Zürich

Advent of new materials such as van der Waals heterostructures, propels new research directions in condensed matter physics and enables development of novel devices with unique functionalities. In my presentation, I will show experimental results that a monolayer of $MoSe_2$ embedded in a charge controlled heterostructure can be used to realize an electrically tunable atomically thin mirror, that effects 87 % extinction of an incident field that is resonant with its exciton transition. The corresponding maximum reflection coefficient of 41 % is only limited by the ratio of the radiative decay rate to the linewidth of exciton transition. The reflectivity of the mirror can be drastically modified by applying a gate voltage that modifies the monolayer charge density. Finally, I will introduce some preliminary results on Kerr rotation obtained from the charge tunable $MoSe_2$ heterostructure in magnetic field.

10:30
Light-Matter coupling in two dimensional materials
Christian Schneider[1]
[1]Technische Physik, University of Wuerzburg, Wuerzburg

Monolayers of transition metal dichalcogenides (TMDC) are an emergent class of nanoscale materials, which are close-to-ideal to study excitonic effects, spin-related phenomena and fundamental light matter coupling in condensed matter systems. Their strongly pronounced exciton and trion resonances make them highly suitable to study advanced light-matter interaction phenomena, such as strong coupling between excitons and photons, even at room temperature.
I will discuss the formation of exciton-polaritons in microcavity systems with embedded TMDC monolayers. Polaritonic modes manifest in their characteristic dispersion relation of the emitted light from such a microcavity system. Furthermore, I address peculiarities associated with the polarization of the emitted radiation from such a strongly coupled system, where effects of spin-valley coupling are retained up to room temperature.

11:00

Tuning a Circular p-n Junction in Graphene from Quantum Confinement to Optical Guiding

Yuhang Jiang[1], Jinhai Mao[1], Dean Moldovan[2], Massoud Ramezani Masir[2,3], Guohong Li[1], Kenji Watanabe[4], Takashi Taniguchi[4], Francois M. Peeters[2], Eva Y. Andrei[1]

[1]Physics Department, Rutgers University, USA
[2]Departement Fysica, Universiteit Antwerpen, Belgium
[3]Department of Physics, University of Texas at Austin, USA
[4]Advanced Materials Laboratory, National Institute for Materials Science, Japan

Owing to their ultra-relativistic nature, electrons in graphene are notoriously difficult to control. We show that a tunable circular p-n junction makes it possible to confine and guide the electronic trajectories in graphene [1]. By using a dual gate configuration the junction size can be continuously tuned from the nanometer-scale, where quantum effects are dominant, to the micrometer scale where optical-guiding takes over. In the nanometer-scale junction, electrons are trapped in quantum-confined states that resemble atomic-collapse at a supercritical charge [2]. In this regime, electrons can be captured or released by varying a gate voltage. As the junction-size increases, we observe a transition to optical-guiding which is signaled by the emergence of whispering-gallery modes and Fabry-Perot interference. In this regime, the junction acts on the electronic trajectories like a lens with a tunable focal length.

[1] Yuhang Jiang et al. Nature Nanotechnology 12, 1045 (2017)
[2] Jinhai Mao et al. Nature Physics 12, 545 (2016)

11:30

Graphene as a 'tunneling barrier' in vertical magnetoresistive junctions

Irina Grigorieva[1]

[1]University of Manchester, Manchester, UK

Graphene is hailed as an ideal material for spintronics due to weak intrinsic spin-orbit interaction that facilitates lateral spin transport and tunability of its electronic properties. Another promising application of graphene is related to its use as a spacer separating ferromagnetic metals in vertical magnetoresistive devices (magnetic tunnel junctions). In particular, few-layer graphene was predicted to act as a perfect spin filter. I will review our recent work where we have investigated magnetoresistance (MR) in vertical Co-graphene-NiFe junctions with 1 to 4 graphene layers separating the ferromagnets. We found that the role of graphene in such devices is different from the earlier predictions and determined by proximity-induced spin splitting and charge transfer with adjacent ferromagnetic metals, making graphene a weak ferromagnetic electrode rather than a spin filter. In the particular case of Co and NiFe, the sign and magnitude of MR is determined by spin transport between weakly doped and differently spin-polarized layers of graphene. Our results suggest a new architecture for vertical devices with electrically controlled magnetoresistance.

18:30

Endohedral metallofullerenes as robust single molecule magnets

Alexey Popov[1]
[1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

Encapsulation of metal clusters within the fullerene cage has multiple structural and physical consequences for the properties of endohedral metallofullerenes (EMFs). When encapsulated metals are lanthanides, unusual magnetic properties can be achieved. Interaction of lanthanide ions with negatively-charged non-metals (nitride, carbide, sulfide) create large magnetic anisotropy, which facilitates single molecule magnetism (SMM) in EMFs. On the other hand, fullerene cage protects endohedral species from the environment allowing formation of rather exotic species, such as lanthanide dimers with single-electron metal-metal bond. Such dimer have three-center spin system, e.g. [Dy–e–Dy], with giant exchange coupling between localized magnetic moment of lanthanide centers and the spin of unpaired electron. This contribution will present an overview of the recent developments in the single-molecule magnetism of EMFs. EMFs can be sublimed under UHV conditions and deposited on different substrates without losing their chemical integrity. Monolayers of $Dy_2ScN@C80$ on metallic substrates and their studies by STM and XMCD techniques will be also discussed.

19:00
Molecular quantum spintronics
Marc Ganzhorn[1], Svetlana Klyatskaya[2], Mario Ruben[2], Wolfgang Wernsdorfer[2]
[1]Quantum Technology, IBM Research, Rueschlikon
[2]Karlsruhe Institute of Technology, Germany

The field of quantum electronics is driven by one of the most ambitious technological goals of today's scientists: the realization of an operational quantum computer. Within that framework a new research field has emerged, which combines the concepts of spintronics, molecular electronics and quantum computing: Molecular Quantum Spintronics. The building blocks are magnetic molecules, i.e. well-defined spin qubits. Various research groups are currently developing low-temperature scanning tunneling microscopes to manipulate spins in single molecules, while others are working on molecular devices (such as molecular spin-transistors, spin valves and filters, and carbon-nanotube based devices) to control the spin state. As a very first step towards the implementation of a quantum computer, we will show how to read out and manipulate the electronic or the nuclear spin of such magnetic molecules. We will furthermore discuss the open challenges and requirements to construct a quantum computer based on single molecule magnets.

19:30

Photovoltaic perovskite nanowires: from fundamental aspects to applications

László Forró[1]
[1]EPFL, Lausanne

Recently, we discovered that this photovoltaic perovskite could be synthesized in a nanowire (NW) form [1,2]. It has turned out that these crystalline structures have an excellent performence in photodetectors. Combined with graphene or carbon nanotubes, the devices [3, 4] show outstanding responsivity, as high as 106 A/W [2]. Moreover, at nanoscale one can achieve much better functional integration of CH3NH3PbI3 than with granular thin films of the same material, which altogether promise a wider range of applications such as heterojunctions, tandem solar cells, LEDs and other optoelectronic devices. In this presentation, the synthesis of NWs, their basic physical characterization and representative applications will be reported. Acknowledgment: The work has been performed in collaboration with Endre Horváth, Márton Kollár, Alla Arakcheeva, Andrea Pisoni, Xavier Mettan, Bálint Náfrádi, Károly Holczer, László Mihály, Hugo Dil. The research is supported by the ERC Advanced Grant (PICOPROP).

[1] E. Horváth *et al.*, Nano Letters 14, 6761 (2014)
[2] M. Spina *et al.*, Sci. Rep, 6, 1 (2016)
[3] M. Spina *et al.*, Nanoscale, 8, 4888 (2016)
[4] M. Spina *et al.*, Small, 11, 4824 (2015)

THU 1
Spontaneous breakdown of topological protection in two dimensions

Yigal Meir[1]
[1]Department of Physics, Ben Gurion University of the Negev, Beer Sheva

Topological insulators are electronic materials characterized by a bulk band gap and protected conducting states on their edges or surfaces. In two dimensions these are one-dimensional helical edge modes that, due to time-reversal symmetry (TRS), come in counter-propagating pairs. The TRS protection of these modes has led to a plethora of proposed applications, ranging from spintronics to quantum computation. Here we show that, unlike the infinitely sharp edge utilized in traditional calculations, employing an experimentally more realistic smooth edge gives rise to edge reconstruction and spontaneous TRS breaking. We demonstrate that such edge reconstruction may lead to a breaking of the expected perfect conductance quantization, to finite Hall resistance at zero magnetic field, and possible spin current. This calculation underpins the importance of the shape of the boundary on the robustness against breaking TRS, of importance in proposed applications of topological insulators.

THU 2
2D metal oxide films. Theoretical predictions and experimental evidences

Pavel B Sorokin[1,2,3], Dmitry G Kvashnin[1,3], Konstantin V Larionov[1,2], Leonid A Chernozatonskii[3]
[1]National University of Science and Technology MISIS, Moscow, Russian Federation
[2]Technological Institute for Superhard and Novel Carbon Materials, Moscow, Russian Federation
[3]Emanuel Institute of Biochemical Physics, Moscow, Russian Federation

We studied properties of a novel family of 2D transition metal oxides (TMO) by theoretical methods and supported them by available experimental results. In particular, observed structure of 2D CuO agrees very well with our predictions [Nanoscale 9, 3980 (2017)]. DFT allowed to elucidate the nature of the stability of the observed nanofilms. It was defined a critical role of the oxygen impurity atoms in the formation of stable 2D CuO cluster with unexpected orthogonal lattice. It was found that the structure and stability of 2D CuO clusters strongly depends on the concentration and relative arrangement of oxygen impurities. Number of oxygen configurations was analyzed and the stable configuration was found which corresponded well with experimental data.+

We predict that 2D TMO sheets have unusual electronic and magnetic properties depending on the composition. We study of stability of such films and its stabilization in the graphene 2D matrix. We combine crystal growth theory and atomistic computations for the prediction of the energy favorable structure of 2D TMO/graphene composite.

The reported study under support of the RSF grant No 17-72-20223.

THU 3

High temperature synthesis and electrical properties of composite materials based on MoS_2/graphene nanostructures

A. Okotrub[1], S. Stolyarova[1], A. Romanenko[1], E. Nikulina[2], A. Chuvilin[2], L. Bulusheva[1]
[1]Nikolaev Institute of Inorganic Chemistry, Novosibirsk
[2]CIC NanoGUNE Consolider, San Sebastian

The composite material based on MoS2 and graphene was obtained from amorphous MoS3 with a controlled addition of detonation nanodiamonds (ND) as a result of heating at a temperature of 1400 °C. The MoS2 micro- and nanoparticles coated and permeated with graphene layers were formed. The produced materials were characterized by scanning and transmission electron microscopy, Raman spectroscopy, XPS and XANES. The specific electric conductivity of composites with different carbon content was measured and the percolation transition concentration was determined. Specific conductivity of the composite increases sharply with the addition of 0.3-0.4 % ND and practically does not change at a carbon concentration above 10 %. The temperature dependences of the conductivity are measured, which is described in the model of charge carriers tunneling between conductive crystallites separated by dielectric barriers. The width of the energy gap of a composite material with about percents of carbon content was determined within the flotation conductivity model and amounted to about 0.2 eV.

THU 4

Low wear coating that improves metal-on-metal human prostheses performance

Núria Ferrer-Anglada[1], David Arcos[1], Dani Gabriel[1], Joan Esteve[2]
[1]Physics Department, Universitat Politècnica de Catalunya, Barcelona
[2]Materials Dept. Física Aplicada i Òptica, Universitat de Barcelona. Barcelona 08028, Catalunya

Nowadays, a big challenge in the orthopedics sector is the durability problems that show the joint prosthesis based in Metal-on-Metal contacts. We have developed a carbon-based coating intended to improve the wear shortcomings found in the classical coatings. Our coatings were deposited with a specific graded composition which changes from highly metallic at the interface, to obtain good adhesion and low stresses, up to a high carbonaceous DLC at the sliding contact region. The coatings show very good wear performance results when they are tested either in a highly humid air atmosphere, or in simulated body fluid (SBF) immersion. The friction coefficients of the DLC coating versus DLC pair are always less than 0.1. Wear rates, were extremely low, lower than $2.5 \cdot 10^{-8}$ mm^3/Nm, and produces highly polished surfaces. Compressive stresses are always lower than 1.5 GPa. These low

stresses, combined with the good interface adhesion to the metal substrates, make these coatings very resistant to delamination by contact fatigue. Raman analyses confirm that no tribomechanical reactions occur on the coating.
We acknowledge financial support, project MAT2015-67103-C4-3-R(MINECO/FEDER)

THU 5
High-resolution mapping of defect modes in boron nitride nanostructures

Daniel Datz[1], Gergely Németh[1], Áron Pekker[1], Katalin Kamarás[1]
[1]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, HAS, Budapest

Probing the optical properties of a single nano-object is a challenging task due to the diffraction limit. One way of solving this problem is by utilizing the near-field interaction between an illuminated AFM tip and the nano-object. The interaction modifies the scattered electromagnetic waves which makes it possible to create optical maps with down to 10 nm spatial resolution, independent of the illumination wavelength.
Optical maps of individual multi-walled boron nitride nanotubes (2-6 nm in diameter) were taken at different wavelengths before and after a chemical cleaning and opening procedure. An absorption peak at 1375 cm^{-1} is well known to be a phonon polariton mode of the nanotubes, and is present uniformly along the nanotubes both before and after the chemical modification. However, additional localized peaks are present in the chemically modified sample due to local defects, thus local defect structure of single nanotubes can be visualized. Similar measurements were done on two-dimensional hexagonal boron nitride (hBN) samples. The goal is to follow the chemical manipulation of an intact hBN surface by mapping localized phonon polariton modes around defect sites.

THU 6
Tracing growth process of horizontal arrays of single-walled carbon nanotubes by digital isotope coding

Keigo Otsuka[1], Shun Yamamoto[1], Taiki Inoue[1], Rong Xiang[1], Shohei Chiashi[1], Shigeo Maruyama[1,2]
[1]Department of Mechanical Engineering, The University of Tokyo, Tokyo
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Single-walled carbon nanotubes (SWNTs) attract attentions as an alternative of Si for high-performance electronics if those with semiconducting properties are prepared in a dense array structure. Despite significant progresses in controlled synthesis of SWNTs, the growth process remains a mystery due to their size and variety. Here we present a method for tracing the time-resolved growth process of individual SWNTs with length of 10–250 μm by embedding digital-coded isotope la-

bels. SWNTs were grown from Fe catalysts patterned in stripes on r-cut quartz substrates. Binary-like codes were embedded in SWNTs by periodically introducing the pulse of 13C ethanol with three different ratios, and then detected by ex situ Raman mapping. We found that after various lengths of incubation, SWNTs elongated at constant rates until abrupt termination.The chirality rarely changed along SWNTs, resulting in sudden modulation of growth rate. Such junctions could provide unique insights on intrinsic chirality-dependences. Similar analyses for the growth from a variety of catalysts and conditions in combination with other characterizations would lead to a quantum leap in the controlled growth.

THU 7

Carbon nanotube chirality determines properties of encapsulated linear carbon chain

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Long linear carbon chains encapsulated inside carbon nanotubes are a very close realization of carbyne, the truly one-dimensional allotrope of carbon [1]. Here we study individual pairs of double-walled carbon nanotubes and encapsulated linear carbon chains by tip-enhanced Raman scattering [2]. We observe that the radial breathing mode of the inner nanotube correlates with the frequency of carbon chain's Raman mode revealing that the nanotube chirality determines the vibronic and electronic properties of the encapsulated carbon chain. We provide the missing link that connects the properties of the encapsulated long linear carbon chains with the structure of the host nanotube.

[1] L. Shi, P. Rohringer, K. Suenaga, Y. Niimi, J. Kotakoski, J.C. Meyer, *et al.*. Confined linear carbon chains as a route to bulk carbyne. Nature Materials, 15(6), 634–639, (2016).

[2] S. Heeg, L. Shi, L.V. Poulikakos, T. Pichler, L. Novotny, Carbon nanotube chirality determines properties of encapsulated linear carbon chain, arXiv:1711.04753 (2017).

THU 8

Ultra-high vacuum Raman spectroscopy of Cs doped monolayer graphene

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We show that ultra-high vacuum (UHV) Raman spectroscopy is a valuable tool for in-situ characterization of epitaxial graphene on Ir(111) regarding strain, defects and doping level. We study the Cs doping induced changes in the Raman spectrum of epitaxial monolayer graphene for 2x2 and $\sqrt{3}$ x$\sqrt{3}$ Cs adsorption geometries for exciting laser energies in a wide range (325 nm to 633 nm). The combined effects

of lattice expansion and dynamic effects lead to characteristic changes in the Raman spectrum that allow us to identify the charge transfer and the electron-phonon coupling strength from the position, width and asymmetry of the G band Raman line. The electronic and structural characterization of Cs doped graphene is complemented by angle-resolved photoemission measurements and scanning tunneling microscopy on identically prepared samples. The high energy resolution of Raman ($\sim$1 wavenumber) allows for a precise determination of temperature induced strain of epitaxial graphene. Finally, we will show new results regarding the UHV Raman and luminescence characterization of transition metal dichalcogenides grown on graphene/Ir(111).

THU 9
All-printed thin-film transistors from networks of liquid-exfoliated nanosheets

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All-printed transistors consisting of interconnected networks of various types of two-dimensional nanosheets are an important goal in nanoscience. Using electrolytic gating, we demonstrate all-printed, vertically stacked transistors with graphene source, drain, and gate electrodes, a transition metal dichalcogenide channel, and a boron nitride (BN) separator, all formed from nanosheet networks. The BN network contains an ionic liquid within its porous interior that allows electrolytic gating in a solid-like structure. Nanosheet network channels display on:off ratios of up to 600, transconductances exceeding 5 mS, and mobilities of approximately 0.1 cm^2/Vs. These devices also show scaling of on-currents with network thickness and volumetric capacitance. The large double-layer capacitance, while hindering switching speeds, allows these devices to carry high currents at low drive voltages relative to other devices with similar mobility.

THU 10
Waveguide-integrated $MoTe_2$ photodetectors

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Over the last years, two-dimensional (2D) materials have attracted great attention due to their intriguing optoelectronic properties and possible applications. Tremendous efforts have been devoted to the development of photodetectors, a key com-

ponent for optical communication that could pave the way for the integration of 2D materials into photonic circuits.

Here we present photodetectors based on 2D heterostructures integrated into a guided wave silicon photonics platform. By making use of the layer-dependent bandgap of $MoTe_2$ we achieve highly sensitive photodetection across the entire O-band of the telecommunication wavelengths. By design, our photodetectors have no trade-off between responsivity and speed, which allows us to achieve a fast photoresponse with a 3-dB cutoff frequency approaching 1 GHz, outperforming those of prior works of photodetectors based on transition metal dichalcogenides (TMDCs) photodetectors. Data transmission experiments showed wide eye opening for data streams of up to 1 Gbit/s. This proves the viability of our devices for telecommunication applications and highlights the potential of integrating TMDCs with existing silicon technology.

THU 11
Fabrication of MoS_2 films on different substrates

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Among metal dichalcogenides, molybdenum sulfide (MoS_2) has been extensively investigated for its interesting properties including enhanced optical absorption, thermoresponsive photogeneration, efficient hydrogen evolution reaction capability, valley polarization and high on/off ratio with low subthreshold swing. A large effort has been made to develop methods for growing high quality films. Recently, methods of physical vapor deposition; especially pulsed laser deposition (PLD) and sulfurization have successfully been used for the fabrication of ultrathin films. Sulfurization is very simple and effective method for the preparation of a few layer films. Here we present fabrication of MoS_2 thin films using sulfurization of Mo films on different types of substrates. Conventional substrates (c-plane sapphire) as well as exotic substrates (GaN, GaP, diamond, B_4C) were used. Prepared films were characterized by number of techniques including XRD, AFM, SEM, Raman, transport and optical measurements. From thorough analyses we can assess the advantages and disadvantages of the substrate on the properties and quality of the final films.

THU 12
Bio-nanostructure for treatment of Klebsiella Pneumoniae infections via nanophotothermolysis

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The aim of this study was to develop a gold based nanostructure as an efficacious pulse laser mode treatment of individual Klebsiella Pneumoniae agents with minimal effects on the surrounding cells, providing highly localized killing effects for the antibody-gold nanoparticle targeted bacteria only. Gold nanoparticles (GNPs) stabilized with chitosan were obtained in the first step. Next, the Epidermal Growth Factor (EGF) was attached to the chitosan coated GNPs via EDC/NHS chemistry. The position of the Surface Plasmon Resonance (SPR) band was determined by UV-Vis spectroscopy while size, surface zeta-potential and polydispersity index was assessed by means of dynamic light scattering. FTIR spectroscopy was used to confirm the success of coupling EGF to the gold nanoparticles. Atomic force microscopy measurements showed that the bio-nanostructure had a spheroidal shape.

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THU 13
On-surface synthesis of covalent architectures for energy conversion chemistry

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Creating nanostructures in a bottom-up approach by using molecular precursors allows for the fabrication of tailored nanomaterials for specific applications such as energy conversion. In particular (metal)organic networks synthesized in UHV on crystalline surfaces can be used as efficient electrocatalysts. Inspired by the photocatalytic hydrogen evolution properties of triazine-containing bulk covalent organic frameworks, we investigate structurally similar 2D networks for their propensity for the hydrogen evolution reaction. In this work we synthesize two-dimensional covalent polymers from 2,4,6-tri-(4-bromophenyl)-1,3,5-triazine on Au(111) and visualize their topography by scanning tunneling microscopy. The polymer-decorated surface shows a promising improvement for the hydrogen evolution reaction compared to bare Au(111) in electrocatalytic experiments. The influence of electrolyte exposure and electrocatalytic conditions on the polymer structure is discussed. These results highlight the capability of single-layer functional 2D polymers for electrocatalysis.

THU 14

Electronic structure studies of various topological quantum materials by angle and spin resolved photoemission spectroscopy.

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Topological quantum materials such as topological insulators, Dirac semimetals, Weyl semimetals, and nodal-line semimetals have attracted considerable interest in solid state physics. Using angle and spin resolved photoemision spectroscopy together with ab-initio band structure calculations, based on the density functional theory, we have studied the electronic structure of various topological compounds. These studies were amended by measurements of transport properties. In particular we report results on the topological metal LaBi, the topological insulator CaAgAs, the Dirac semimetal $PtSe_2$, and the two-dimensional electronic structure of $OsTe_2$.

THU 15

Quantized conductance of graphene constrictions prepared by atomic force microscope-based lithography

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Signatures of quantized conductance have been observed in suspended graphene, with limited control on constriction width [1]. In graphene sandwiched by hexagonal boron nitride evenly spaced modulations, superimposed on the linear conductance, have been identified as size quantization signatures [2]. However, in all these experiments a major bottleneck is the charging of localized states at the rough constriction edges. Therefore, the observation of size quantization in graphene at zero external magnetic field is still challenging. A promising approach to improve the edge quality is to use local scanning probe technique based patterning instead of reactive ion etching. Here we realized the direct cutting of the graphene sheet by Atomic Force Microscope Lithography. We prepare narrow constrictions (50 to 150 nm) showing signatures of size quantization, even on SiO_2 supported graphene. The conductance has been measured as a function of back gate voltage, at a temperature of 1.5 K. We observe plateau-like features which are evenly-spaced by e^2/h at B=0 T.

[1] N. Tombros *et al.*, Nat. Phy. 7, 697-700 (2011)

[2] B. Terrés *et al.*, Nat. Comm. 7, 1-7 (2016)

THU 16
Study of Ni clusters inside single-walled carbon nanotubes by scattering-type Scanning Near-field Infrared Microscopy

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In our measurements, we studied the near-field optical response of metal clusters inside single-walled carbon nanotubes by scattering-type scanning near-field infrared microscopy. The investigated nanotubes were filled with Ni(II) acetylacetonate. An annealing process was performed to make the molecules dissociate in order to form nickel clusters. In our previous experiments [1,2] we have already seen that semiconducting and metallic carbon nanotubes provide different near-field signal contrast compared to the silicon substrate because of the higher free-carrier concentration of the metallic nanotubes. In case of the metal clusters, we were looking for the additional near-field contribution when the nickel clusters are present.

[1] G. Németh, D. Datz, H. M. Tóháti, Á. Pekker, K. Kamarás, physica status solidi (b), 253 (12), 2413-2416 (2016)

[2] G. Németh, D. Datz, H. M. Tóháti, Á. Pekker, K. Otsuka, T. Inoue, S.

THU 17
Atomic resolution imaging of 2D materials in controlled atmospheres

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We have studied the effect of a controlled gas environment in the transmission electron microscope (TEM) on the surfaces and edges of graphene and MoS_2. The Nion UltraSTEM100 instrument in Vienna has been uniquely modified with a leak-valve system that allows to leak small amounts of a desired gas into the microscope column (pressure range of 10^{-10}-10^{-6} mbar), while simultaneously imaging a sample at atomic resolution.

According to density functional theory calculations, the armchair edge in graphene should be more stable than the zigzag edge under an electron beam at typical voltages. However, TEM imaging studies of graphene edges have until now revealed mostly zigzag edges. Through experiments in oxygen atmosphere, we show here that this is due to an electron-beam-driven chemical etching process that preferentially erodes armchair edges, caused by the residual gases in typical (non-UHV) TEM columns. We also show that the leakvalve system can be used to clean graphene surfaces without damaging the pristine lattice due to the higher reactivity of the contamination species.

THU 18
Nano-chemical reactions inside individual carbon nanotube by in-situ laser annealing.

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Double wall carbon nanotubes (DWCNTs) have been studied for many decades. Their most common synthesis methods encompass CVD, or nano-chemical reactions from encapsulated C60 peapods and high-temperature annealing. The inner tube transformation from fullerene coalescence can be monitored by the evolution of the radial breathing mode (RBM) in Raman spectroscopy. These experiments have inspired new methods of or the synthesis of other nano structures inside nanotubes, for example, inner nanotubes, graphene nanoribbons, and linear carbon chains [1]. Based on this concept we have investigated the decomposition and changes of the system inside a SWCNT via temperature or laser irradiation. In this work, we have monitored nano-chemical reactions inside different-diameter SWCNTs by in-situ laser annealing with simultaneous Raman spectroscopy measurements. Interestingly, RBM peaks have been found and additional information about the nano-chemical reaction process as well as the growth mechanisms of the encapsulated nanocompound have been obtained.
[1] Nature Mater. 15, 634 (2016).

THU 19
Ultra-sensitive graphene-based gas sensors for the detection of toxic gases

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Graphene is a very promising material for gas sensing applications. Because it is 2D, gas molecules adsorbed onto a graphene sheet strongly modify its conductance, allowing the detection of individual molecules [1].
The relative change in conductance $(G_{end} - G_{start})/G_{start}$ is often used as the response function for such devices. However, it has been shown in recent studies that graphene-based devices do not reach equilibrium when exposed to a target gas, even after a long time. Because of that, the previous definition seems unsuitable as the end value is arbitrarily chosen. A model of the transient response of the devices is therefore needed in order to derive a relevant response function [2].
In this work, in-situ field-effect measurements are used to probe the interaction between a graphene transistor and nitrogen dioxide molecules. Measurements were performed at very low concentrations and at different temperatures. By modelling the transconductance variation, we were able to extract important adsorption parameters and to propose a new response function for graphene gas sensors.
[1] Schedin *et al.*, Nat. Mat. 6, 652 (2007)
[2] Wen *et al.*, Sens. Act. B, 223, 79 (2016)

THU 20

Calculation of the Josephson current in multiterminal Josephson junctions

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Several schemes for the realization of the quantum two-level systems (qubits) rely on the phase shift of π between the superconducting banks in Josephson junctions (JJ's). However, only a few experimental realizations of the π JJ's have been reported in ferromagnetic systems or in devices driven out from the equilibrium by injection of additional charge carriers.
In this work we studied the Josephson current contributed from the bound and scattering states of a JJ. We showed that there are continuum states in the superconducting energy gap when a normal lead is contacted to the JJ. Furthermore, we developed a model to obtain the Josephson current in a multiterminal setup. Using this model we examine the properties of multiterminal JJ's and the possibility to turn them into a π state regime.

THU 21

Theoretical investigation of new thermoelectric materials, based on fullerites consist of endohedral metallofullerenes

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Potentially new class of thermoelectric materials, fullerites, is proposed and theoretically investigated. These materials consist of the solid phase of fullerenes or endohedral metallofullerenes (EMF), where the molecules are bound by van der Waals forces. Thermoelectric efficiency measured by the figure of merit $ZT = S^2\sigma T/k$, where S is Seebeck coefficient, σ and k are the electrical and thermal conductivities respectively were calculated by the semiclassical approach based on the Boltzmann's equation solution (BoltzTraP package) and by our own model uses calculation of transport properties of weakly interconnected particles.
These materials have narrow electronic bands and band gap varies from 2 eV (C_{60}) to several tenths of eV for different EMF. Using these facts, it is shown that the maximum figure of merit, ZT_{max}, when the electronic contribution to thermal conductivity is in the denominator of ZT, for fullerites consist of EMF molecules, for example $Ti_2C_2@C_{78}$, can reaches 0.5-1. Thus, it was shown that fullerites on the base of the EMFs represent a perspective class of thermoelectric materials.

THU 22

Single-wall carbon nanotube or graphene non-covalently doped with acceptor molecules

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Non-covalent doping is a promising way to reach a high doping level in carbon nanotubes or graphene keeping their crystalline structure. We doped with a gas phase CuCl thin films of single-wall carbon nanotubes or one-layer graphene. The doping level increased with the treatment time and finally saturated (after 12 hours). The Fermi level shift reached 1 eV. The form of optical absorption spectra and a high-frequency shift of Raman tangential mode proved the doping. At high doping levels we observed both exciton and trion PL bands. Their characteristic times were measured by pump-probe. The electrophysical measurements have revealed a low surface electrical resistance and a high optical transparency of doped films. Due to their higher optical transparency in UV range (comparing with ITO) such films are promising for transparent conductive electrodes in solar cells and light-emitting GaN diodes. The test experiments have been performed.
The work was supported by RFBR projects 16-02-00979 and 17-302-50008. P.A.O. thanks RSF project 17-72-10303.
[1] T.V. Eremin, Phys. Stat. Sol. B 255, 1700272 (2018)
[2] M.G. Rybin, Appl. Phys. Lett. (2018)
[3] V.I. Tsebro, Phys. Rev B 94, 245438 (2016)

THU 23

Electronic properties of single-walled carbon nanotubes filled with silver chloride

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Applications of single-walled carbon nanotubes (SWCNTs) require the nanotube samples with tailored properties. The latter can be achieved through chemical functionalization of SWCNTs. Recently, it has been shown that the filling of SWCNT channels is a promising method of fine tuning their physical and chemical properties [1]. In the present work, we perform the filling of internal channels of SWCNTs with silver chloride. We study the influence of the encapsulated compound on the elec-

tronic properties of metallicity sorted semiconducting and metallic SWCNTs as well as metallicity mixed nanotubes of different diameters by Raman and photoemission spectroscopy. We show that the filling of semiconducting SWCNTs leads to modifications of Raman modes of nanotubes. The filling of metallic SWCNTs results in p-doping of nanotubes accompanied by the downshift of their Fermi level and the charge transfer from nanotubes to the encapsulated compound. The filling of SWCNTs with diameters between 1.4 and 1.9 nm leads to similar modifications of their electronic properties.
[1] M.V. Kharlamova, Prog. Mater. Sci. 77, 125-211 (2016)

THU 24
Single-Walled Carbon Nanotubes for Perovskite Solar Cells

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Single-walled carbon nanotubes (SWNT), graphene, and fullerene (C60 and PCBM) can be very efficiently used in lead halide Perovskite solar cells. A film of SWNTs or graphene can be flexible and stretchable transparent-conductive layer. At the same time, this film can be carrier-selective layers, i.e., electron-blocking-layers or hole-blocking-layers. We have demonstrated the replacement of ITO in inverted-type flexible perovskite solar cells [1]. The normal-type perovskite solar cell, composed of ITO/C60/MAPbI3/SWNTs, can achieve a PCE of 17 % with spiro-MeOTAD as dopant to SWNTs [2]. This structure with a perovskite layer sandwiched by C60 and SWNTs can lead to the solar cells without hysteresis and with much improved air-stability [2]. More recent configuration is using a film of SWNTs for both anode and cathode electrode [3].

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[1] I. Jeon et al., J. Phys. Chem. Lett., 8, 5395 (2017)
[2] N. Ahn et al., J. Mater. Chem. A, (2018) [DOI: 10.1039/C7TA09174E].
[3] I. Jeon et al., J. Phys. Chem. C, 121 (2017) 25743 (2017)

THU 25
Synthesis of Low-Dimensional Platinum Compounds inside Carbon Nanotubes

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The preparation of nanomaterials with a desired structure and specific properties requires the ability to control their size, shape and composition. A series of chemical reactions with Pt compounds carried out within single-walled carbon nanotubes (SWNTs) have demonstrated the ability of SWNTs to act as both an effective reaction vessel and a template for the formation of nanocrystals of PtI_2 and PtS_2.
The stepwise synthesis inside nanotubes has enabled the formation of Pt compounds to be monitored at each step of the reaction by transmission electron microscopy (TEM), and by an innovative combination of fluorescence-detected X-ray absorption spectroscopy (FD-XAS) and Raman spectroscopy, monitoring the oxidation states of the platinum guest-compounds within the nanotube and the vibrational properties of the SWNT, respectively. A new approach for nanoscale synthesis in nanotubes developed in this study utilises the versatile coordination chemistry of Pt which has enabled the insertion of the required chemical elements (e.g. metal and halogens or chalcogens) into the nanoreactor in the correct proportions for the controlled formation of PtI_2 and PtS_2 with the correct stoichiometry.

THU 26
Characterizing stacking domains in Van der Waals materials

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In Van der Waals materials, consecutive layers can be stacked in different ways. Energy differences between the different stacking possibilities are often small or even zero. Hence, strain or twist introduced during fabrication can cause different stackings to coexists. The formed domains of different stable stackings, in general, strongly affect the properties of the Van der Waals materials.

Here, we employ Low Energy Electron Microscopy (LEEM) to characterize stacking domains. Breaking the rotational symmetry by tilting the imaging electron beam, a technique called Dark Field LEEM, allows for direct imaging of the domains with a

resolution of 10 nm. The precise stacking of mono-, bi- and trilayer quasi–freestanding graphene grown on 4H-SiC, as well as the stacking of MoS_2 are mapped in detail. For graphene, we identify the local stacking by comparing measured electron reflectivity spectra to theoretical predictions. We identify two physical causes of domain formation: strain and nucleation. Moreover, we discuss the influence of stacking domains on the intercalation of hydrogen between silicon carbide and graphene.

THU 27

Magnetic and electronic properties of alkali-doped black phosphorus probed by NMR, ESR and microwave spectroscopy

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We present results on alkali (A=Na/K/Rb/Cs) intercalated black phosphorus with different A:P ratios. Samples were probed by room temperature ^{31}P NMR, ESR spectroscopy measurements and the microwave conductivity was measured between 3-200 K. All methods are contactless techniques with low energy photons thus well suited to study air sensitive materials. NMR measurements suggest that the electronic neighborhood of the P nuclei change upon A doping and the effect is also strongly A dependent. ESR measurements indicate the presence of newly added electrons in the system and yield an unexpected microwave absorption behavior, that the more alkali is present the less the sample absorbs. The latter is also confirmed by microwave conductivity measurements, which also show that no true metallic phase is formed upon doping, albeit the conducting properties are different from the pristine material. We also note that no traces of bulk superconductivity is found down to 3.5 K, which compared to the SQUID results mean that the SC phase is only formed in small volume near the surface, probably due to the presence of a non-stoichiometric amorphous phase or because of topological effects.

THU 28

Magnetic edge state and coherent manipulation of molecular graphene nanoribbons

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Graphene, a well-defined two-dimensional network of carbon atoms, shows impressive electrical and mechanical properties. By introducing magnetic edges in graphene nanoribbons, ferromagnetic couplings and superior spin filtering are predicted. Conventional techniques such as unzipping of carbon nanotubes, however, do not deliver the necessary degree of purity to design such systems.
By utilising an ultra-clean synthetic approach, we created graphene nanoribbons with great purity, and functionalize them with magnetic nitronyl-nitroxide radicals as magnetic sites. Using electron paramagnetic resonance spectroscopy, we gain a full picture of the interactions between the magnetic radicals. The coherence time reach microseconds at W-band frequencies at liquid nitrogen temperature, and submicroseconds at room temperature. We obtained evidence of the existence of a magnetic edge state in the nanoribbon, a matter predicted 20 years ago and now observed with high resolution. Via double-electron-electron-resonance spectroscopy, we observed a coupling between the edge state and the radical spins, where we determined a two-qubit inversion time of 350 ns, enabling interesting applications.

THU 29
Capacitive behavior of MoS_2/multilayer graphene hybrids in Li-ion batteries

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MoS_2 possessing a theoretical specific capacity of 669 mAh/g is attractive as anode for Li-ion batteries. However, the mechanism of Li interaction with MoS_2 during the battery operation is still under the study. In the present work, we show that the path of the delithiation reaction is dependent on actual structure of electrode material. MoS_2/graphene hybrids were produced by annealing of amorphous MoS_3 deposited on the surface of multilayer graphene flakes in diffusion vacuum at 500 °C, 800 °C, and 1000 °C. XPS confirmed a transformation of MoS_3 to MoS_2 at these conditions. High-resolution transmission electron microscopy and Raman scattering showed a growth of in-plane size of MoS2 nanocrystals with a rise of annealing temperature. Electrochemical tests detected a gradual loss of the specific capacity of the MoS_2/graphene materials prepared at 500 and 800 °C and a stable performance for the material synthesized at 1000 °C even at high current densities.

Based on the initial discharge-charge profiles, we associate this effect with in-plane size of MoS_2 nanocrystals, which should disintegrate more easily when the size is small due to the interaction of lithium with edge sulfur atoms.

THU 30
Characterization of GNRs/Fe_2O_3 nanocomposties prepared by microwave assisted solvothermal method

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Graphene-based nanocomposites have been demonstrated to be promising high-capacity anodes for lithium ion batteries to satisfy the ever growing demands for higher capacity, longer cycle life and better high-rate performance. Here we present studies on the preparation of graphene nanoribbons (GNRs) from multiwalled carbon nanotubes using wet chemistry methods, oxidizing agents like e.g. concentrated acids and high frequency ultrasound homogenization. Consequently GNRs/Fe_2O_3 nanocomposites were prepared using a microwave-assisted solvothermal synthesis. Structural characterization of the obtained samples was measured by transmission electron microscope (TEM), X-Ray Diffraction (XRD), Raman spectroscopy and infrared spectroscopy (FT-IR). A specific surface area of the obtained materials was determined using a low temperature nitrogen adsorption according to the BET (Brunauer-Emmett-Teller) method. Also electrochemical and magnetic performances of the prepared composite samples were examined.
This work was supported by project: LIDER/496/L-6/14/NCBR/2015 financed by The National Centre for Research and Development.

THU 31
μ-Droplet Spectroelectrochemistry of Monolayer MoS_2 and WS_2

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Individual monolayers of transition metal dichalcogenides (MX_2) are nowadays stud-

ied for their remarkable optoelectronic properties applicable in advanced technologies. Raman spectroscopy is one of the most prominent tools for characterization of such materials. Using a combined method of "μ-droplet Raman spectroelectrochemistry" it is possible to characterize isolated 2D crystals during charging and/or strain loading. Controlled doping (shift of the Fermi level) and strain level (breaking the lattice symmetry, changing the chemical potential) can thus be studied on a microscale. In this study, mainly E' and A_1' Raman modes as well as photoluminescence (PL) in the monoloayer MoS_2 (WS_2) were investigated during the electrochemical charging (usually in cycles) with respect to the evolution of intensities, positions and linewidths of those bands. The derived results allow to apply the E'/A_1' vector analysis – similar to the G/2D for graphene – to disentangle strain and doping effect in the layers. Besides pristine dichalcogenides, Raman μ-droplet studies of the MX_2/graphene Van der Walls heterostructures were carried out.

THU 32
Low-Energy Electron Microscopy for Investigation of 2D Material Systems: tSEM and LEND

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State-of-the-art scanning electron microscopes offer a great potential for the in-depth investigation of 2D material systems. Less spatial confinement around the sample and a high versatility allow for the use of a variety of add-on tools for in situ investigations. The reduced electron energy compared to classical TEM offers an increased scattering cross section and therefore a higher contrast especially for light element materials as graphene.
We will present low-energy data acquired from ultra-clean graphene utilizing transmitted electrons (tSEM) for the generation of crystallographic contrast. tSEM imaging at 2 kV and below allows us to image topological defects and can give direct access to the numbers of layers.
Furthermore, we will introduce low energy nanodiffraction (LEND) directly in the SEM which allows for a simultaneous acquisition of information from real and reciprocal space. This methodological development helps to correlate crystallographic (atomic scale) order with real space imaging and was proven to be usable at ultra-low energies of 2 keV and below.

THU 33
Graphene cantilevers: Renormalization of bending rigidity

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Suspended graphene is not flat, but wrinkled due to both dynamic out-of-plane

flexural phonons and static surface corrugations arising from boundary conditions. Theses static and dynamic deformations renormalize every mechanical constant of graphene and strongly affect its electrical transport coefficients. In particular bending rigidity is expected to increase by orders of magnitude compared to values naively calculated from the phonon dispersion relation. Measurements of bending rigidity have been reported, however interpretation of the data remains complicated owing to interaction of graphene with its environment, complex experimental geometries, and interplay between static and dynamic wrinkles. Here we report direct measurements of bending rigidity of singly clamped graphene cantilevers in vacuum from room to cryogenic temperatures. These cantilevers are cut from suspended CVD graphene membranes by a focused beam of Helium ions (Zeiss Orion). We then use sensitive laser interferometry to analyze the bending rigidity and discriminate between contributions from flexural phonons and static wrinkles.

THU 34
Smeared d-Wave Anisotropy and Discrete Andreev States in Monolayer Organic Superconductor

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Epitaxially grown monolayer of organic superconductor, $(BETS)_2GaCl_4$ [where BETS is bis(ethylenedithio)tetraselenafulvalene], on Ag(111) form islands of uniform and mixed stacking of 2-dimensional stripes. A d-wave superconducting gap, of magnitude 14 meV, is ubiquitously measured on uniform islands while been structurally altered on the inhomogeneous islands. Mixing of intra-stripes antinodal states are manifested by smeared anisotropy of the low energy quasiparticle as well as features of multigaps in their density of states. Despite proximal convolution, the pronounced coherence peaks indicate well preserved superconducting state. Robust zero bias peaks are detected only at the edges of isolated stripes indicating tunneling into Andreev bound states. These features broaden significantly away from the edges due to quantum interference with nearby discrete states. The interplay between structural parameters and electronic properties makes single layer $(BETS)_2GaCl_4$ a unique playground to test the effect confinement and symmetry variation on the superconducting ground state.

THU 35
Electron spin detection using a nanotube mechanical resonator

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Micro-scale mechanical resonators are highly sensitive force sensors, enabling the detection of very small ensembles of electron spins. Recently, we showed that mechanical resonators made of suspended carbon nanotubes display outstanding properties, such as quality factors up to 5 million, and force noise as low as 10^{-21} N/Hz$^{1/2}$.
We propose to use this excellent sensitivity capability to detect and manipulate the electron spin of a small number of molecules deposited on top of the carbon nanotube. For this, we use the specific magnetic resonance protocol developed by Nichol (MAGGIC protocol) and a superconducting coplanar waveguide patterned very close to the nanotube to generate both the oscillating magnetic field and the magnetic field gradient, which are needed to manipulate the nuclear spins of the nanotube, and to detect them.

THU 36
Physical Properties of Tubular Structures of Misfit Layered Compounds

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LaS-TaS_2 and other Misfit layered compounds (MLC) nanotubes (NTs), so far exclusively synthesized by Prof Tenne's group, constitute a novel material with potentially interesting 1D electrical characteristics. This research, the first of its type, aims to experimentally reveal the electrical transport characteristics of the material. The main goal of the research was to incorporate single LaS-TaS_2 MLC NTs into electrical devices, using lithographic technics, and to characterize their electrical behavior. First, horizontal laying NTs were analyzed by using SEM, TEM, AFM and EDS. In addition cross-sectional lamellae were prepared by FIB and analyzed too. Then, two and four probe electrical devices were fabricated by advanced lithographic techniques. Measurements at room and at low temperatures were performed, showing a narrow band-gap semi-conductor behavior. Raman measurements with individual NT devices were performed as well. Nowadays we are focusing on the fabrication and measurement of more complex devices which will allow us to perform Hall-Effect measurements and hopefully also to measure and learn about the conductance through a cross sectional device (radial conductance).

THU 37
Single-, Double- and Multi-walled carbon nanotubes dynamically compressed to 50 GPa: a comparative study

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Single (S)- Double (D)- and Multi-walled (MW) carbon nanotubes (CNTs) were dynamically (shock) compressed to about 0.5 MBar. The recovered after shock material was characterized by multi-wavelength Raman spectroscopy and HRTEM. No trace of diamond were found in the samples. DW nanotubes show similar to SWCNTs transformation into a mixture of multilayer graphene (MLG) and two-phase material comprised of disordered carbon and nano-sized graphene clusters after the total collapse and posterior destruction of the tubes under the shock [1]. The coherent scatterers size (La) was estimated at about 30 nm for both SW- and DWCNT-derived MLG material, but with a notoriously higher defects density in the latter case. Remarkably, some of the MWCNTs survived 50 GPa shock compression though severely damaged via tubes "chopping", outer walls "peeling off" and/or "unzipping". We discuss peculiarities of the CNTs transformation into different forms of nanostructured carbon under the shock and its dependence on the nanotubes morphology.
[1] Pablo Botella, et al. phys. stat. sol. b, 254, 11, 1700315 (2017)

THU 38

Femtosecond dynamics of light-matter interaction in the intrinsic cavity of WS_2 nanotubes

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Focusing on the optical properties of semiconducting WS_2 nanotubes, it was shown that these nanostructures exhibit strong light – matter interaction and form exciton – polaritons. These nanotubes readily provide both the electric dipoles in the form of their excitonic resonances, and the optical cavity due to their dielectric constant and cylindrical shape.
Here we investigate the non-equilibrium light-matter interaction in WS_2 nanotubes in the time domain using femtosecond transient absorption spectroscopy. We find that the temporal evolution of the transmission spectrum is governed by the time dependence of four main parameters: the frequency of the two exciton resonances, the coupling strength of the cavity mode to its energetically closest exciton resonance, and the damping of the cavity mode. All four time dependences can be traced back

to the relaxation dynamics of the photoexcited charge carrier populations. The transient spectra of the INT-WS_2, although dominated by the coupling, can be traced back to the electron dynamics in the semiconductor. This will enable future studies of optoelectronic and photonic devices based on TMD NTs.

THU 39

Low-temperature transport in two-dimensional nano-crystal superlattices

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The combination of graphene-like Dirac carriers with a strong spin-orbit coupling (SOC) could open the way to the observation of new topological states of matter. In graphene, however, this cannot be observed due to the small SOC. We use atomically coherent two-dimensional superlattices of semi-conductor nano-crystals that combine the atomic lattice and the geometry imposed by the nanocrystal attachment to form a rich bandstructure. Their geometry can be tuned to form square or honeycomb lattices.[1]
We investigate the transport properties of monolayer superlattices consisting of PbSe building blocks of 5 nm in size in a square geometry. This material was contacted in a four-probe configuration and brought in the electron conduction band using an ionic-liquid gate.[2] The room-temperature mobility reaches 8 cm^2/Vs. Surprisingly and despite the relatively high mobility, the low-temperature transport characteristics show temperature-activated behavior that is well described by variable range hopping models.
[1] W. Evers *et al.*, Nano letters 13.6 (2012)
[2] V.A.E.C. Janssen, *et al.*, Nano letters 17.9 (2017)

THU 40

Mechanisms of graphitization of diamond studied by transmission electron mircoscopy

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A catalytic reaction at the interface between Ni and diamond can lead to the formation of graphene or graphite. Single-crystal diamond (SCD) and nanocrystalline diamond (NCD) were covered with a thin Ni film, annealed at 800 °C, and studied

in cross-sectional geometry using a double-corrected transmission electron microscope. Upon heating of the NCD for 10 min, isolated Ni particles formed by dewetting of the Ni film penetrate into the diamond. Due to the catalytic reaction in front of the particles (i.e. at the Ni-diamond interface) the C atoms become highly mobile. The diffusional flux of C atoms from the Ni-diamond interface to the backside of the Ni particles causes the latter to penetrate into the diamond. At the backside of the Ni particles, the C atoms reorganize forming sp^2-bonded layers. Finally, graphite arises by successive formation of such layers filling the channels behind the moving Ni particles. Frequently, the (0002) planes of graphite are oriented perpendicular to the (111) planes of diamond surrounding the channels. In the case of the SCD annealed for 5 min, the Ni particles move along the free diamond surface and thus convert it into graphite.

THU 41
Negative differential conductance in lateral MoS_2 tunnel junctions defined by photodoping

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The advances in making increasingly complex van-der Waals heterostructures consisting of stacks of different two-dimensional material open the door for investigating mesoscopic transport in semiconducting transition metal dichalcogenides (TMDs), such as MoS_2. Recently, first experiments on broken symmetry states and quantum confinement in one- and zero-dimensional structures have been demonstrated. However, the device quality is still quite limited due to the relatively large amount of intrinsic defects in natural MoS_2.

We present a device scheme to explore the electrical transport through lateral MoS_2 tunnel junctions which enables to study the role of defect induced impurity bands by negative differential conductance measurements at low temperature. Our devices are based on exfoliated MoS_2 flakes encapsulated in hexagonal boron nitride and contacted by few layer graphene [1]. Using metal shadow masks, we define the tunnel junctions through a photodoping technique allowing for well-defined lateral doping profiles.

[1] Epping *et al.*, arXiv: 1612.01118

THU 42
Ultrasharp Polarized Lines of Excitons Bound to 1D Intersection of a Stacking Fault Plane with a Quantum Well

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Stacking faults (SFs) in bulk semiconductors being extremely two-dimensional systems attract growing attention as a source of narrow excitonic lines [1]. We propose theoretically and study experimentally excitons bound to 1D intersection of a SF with a quantum well [2]. As a proof of concept we performed micro-photoluminescence measurements in a ZnSe-based specimen used for prior transmission electron microscopy studies. This approach revealed that exciton polarization is linear and directed along the intersection. The corresponding linewidth is determined by the SF size and can reach 0.15 meV. Theoretical description based on the effective mass approach and the density functional theory showed that the exciton binding energy is determined by an intrinsic electric field inside the SF. As a results an electron and a hole in the bound exciton are spatially separated, which should lead to a strong increase of exciton lifetime. The proposed 1D intersection of natural and artificial 2D objects is a promising playground for many body excitonic effects.

[1] T. Karin *et al.*, Phys. Rev. B 94, 041201 (2016).

[2] D. S. Smirnov *et al.*, Phys. Status Solidi RRL, in press.

THU 43
Linear antenna microwave plasma system for growth of porous diamond structures at low pressure

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Due to an extraordinary combination of intrinsic properties, diamond films become used as the functional layers for various bio-opto-electronic devices. Here, the growth of dimensional forms or porous structures is still a challenge. This study reviews the fabrication of porous diamond structures employing linear antenna microwave plasma over a large area (up to 1 m^2) at low pressure (1 Pa) and low temperature (400 ∘C). It covers the bottom-up and templated growth of high, middle and low density-packed diamond nano- or micro-forms (i.e. diamond plates, dendritic-like geometries, thin-films) which were grown on planar silicon substrates, buckypapers, amorphous silicon oxide mats (fibers) and carbon foams. The low-pressure range and cold plasma conditions facilitated the growth of three-dimensional pre-structured substrates forming self-standing porous diamond coated membranes.

Potential applications of such porous-forms in electrochemistry, gas sensing and life-science will be pointed out.
This work was financially supported by the AZV grant no. 15-33018A.

THU 44
Exfoliation of single layer BiTeI flakes

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Spin orbit interaction can be strongly boosted when a heavy element is embedded into an inversion asymmetric crystal field. A simple structure to realize this concept in a 2D crystal contains three atomic layers, a middle one built up from heavy elements generating strong atomic spin-orbit interaction and two neighboring atomic layers with different electron negativity. BiTeI is a promising candidate for such a 2D crystal, since it contains a heavy Bi layer between Te and I layers. Recently, the bulk form of BiTeI attracted considerable attention due to its giant Rashba spin splitting, however, 2D form of this crystal was not yet created. In this work we report the first exfoliation of single layer BiTeI using a recently developed exfoliation technique on stripped gold. Our combined scanning probe studies and first principles calculations show that SL BiTeI flakes with sizes of 100 μm were achieved which are stable at ambient conditions. The giant Rashba splitting and spin-momentum locking of this new member of 2D crystals open the way towards novel spintronic applications and synthetic topological heterostructures.

THU 45
Dislocation Manipulation and Switching in Bilayer Graphene

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Topological defects known as Dislocations are one of the fundamental Phenomena researched by materials science. They have a tremendous impact on the mechanical, optical and electronic properties of any material. This impact is even more pronounced for 2D Materials, where a single Defect can extend through the whole

volume of the material. For bilayer graphene, the thinnest material to host extend dislocations, it was shown, that dislocations can lead to interesting physical phenomena such as phonon reflection or valley polarized transport. However controlling the occurrence and extent of dislocations has remained elusive so far.
In this work we present a novel way of directly manipulating individual dislocations in situ in free-standing bilayer graphene. This is enabled by a combination of transmission SEM (tSEM) imaging with in situ piezo-controlled micro-manipulation. In our experiments we confirm fundamental dislocation properties, such as line tension and intersection formation. Furthermore a novel switching mechanism was found that allowed us to conceive a topological switch with expected electronic properties.

THU 46
Understanding the fingerprints of SWCNTs in Photoemission

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Establishing the prerequisites for studying the rich low-dimensional physics of pristine vs. functionalized Single-Walled Carbon Nanotubes (SWCNTs) using photoemission spectroscopy has been a significant challenge for many years due to the purity of the starting material available in the past. This poster will focus this discussion on our recent progress towards the identification of the changes in the site selective electronic structure within various types of SWCNTs: metallicity pure tubes, substitutionally doped SWCNTs, and tubes with different fillings. This is a pioneering step towards understanding the changes on the electronic structure of these materials after specific functionalization.

THU 47
Engineering of electronic and magnetic properties of boron nitride with oxygen

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Engineering of optical, electronic and magnetic properties of h-BN nanomaterials via

oxygen doping and functionalization has extensively been studied in theory. However, it is still unclear to what extent these properties can be modulated using such methodology because of lack of significant experimental progresses and systematic theoretical investigations. Therefore, herein, we provide comprehensive theoretical predictions verified by solid experimental confirmations that unambiguously answer this longstanding question. We report on the strong narrowing of the optical band gap in h-BN nanosheets and appearance of paramagnetism after oxygen doping and functionalization. Our systematic theoretical studies have predicted that the electronic properties of h-BN monoatomic sheets are tunable and their band gap can be significantly narrowed through oxygen doping and/or functionalization. These findings pave the new way for h-BN nanosheet optical, electronic and magnetic property engineering, and should breed brand-new applications of layered BN materials in optical, electrical, information and energy-related fields. Results were published in Advanced Materials journal in 2017.

08:30 – 09:00 M. Pumera, Singapore
2D Nanomaterials, Nanomachines and Sensing

09:00 – 09:30 C. Backes, Heidelberg
Liquid exfoliation as versatile technique to study fundamental properties of 2D materials

09:30 – 10:00 A. Kuc, Leipzig
Tuning Electronic Structure of 2D Chalcogenide Materials

10:00 – 10:30 coffee break

10:30 – 11:00 Y. Li, Beijing
Structure Characterization of Catalysts and Single-Walled Carbon Nanotubes in Chirality-Specified Synthesis

11:00 – 11:30 B. Flavel, Karlsruhe
Separation of Double Walled Carbon Nanotubes

11:30 – 12:00 H.-M. Cheng, Shenyang
Size-Controlled Growth of Single-Crystal Graphene Domains by CVD

12:00 – 17:00 mini workshops

17:00 – 17:30 M. Lagos, Hamilton
Phonon spectroscopy of nanomaterials using angstrom-size electron beams

17:30 – 18:00 S. van der Molen, Leiden
Probing interlayer interaction in van der Waals materials

18:00 – 18:30 SUMMARY: C. Stampfer, Aachen
Conference summary

18:30 – 20:00 break

20:00 – 22:00 Bauernbuffet – Farewell dinner

08:30
2D Nanomaterials, Nanomachines and Sensing
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[1]VSCHT Praha, Czech Republic
[2]Nanyang Technological University, Singapore

In this talk I will discuss various uses of nanomaterials for sensing, from 2D and layered materials, through labels to self-propelled autonomous sensing platforms. In detail, I will first focus on 2D materials, such as graphne, transition metal dichalcogenides, black phosphorus, arsenene, antimonene, bismuthene. The electrochemistry of 2D materials is far more interesting and complex than anticipated. This is because the real world 2D materials contain defects, adatoms, and various oxygen functional groups. I will show that many electrocatalytic properties assigned to 2D materials actually originated from the embedded metallic impurities. I will discuss our recent research on the electrochemistry of layered transition metal dichalcogenides, black phosphorus and antimonene, arsenene and bismuthene. In the second section, I will discuss the use of self-propelled micromachines for sensing.

09:00

Liquid exfoliation as versatile technique to study fundamental properties of 2D materials

Claudia Backes[1]

[1]Applied Physical Chemistry, University of Heidelberg, Heidelberg

Liquid exfoliation has become an important production technique to give access to large quantities of two-dimensional nanosheets in colloidal dispersion. In this talk, recent advancements in the liquid exfoliation and optical characterisation of a range of 2D-materials will be summarised including unifying principles among various materials in size selection and optical properties. Materials include transition metal dichalcogenides, GaS, h-BN, black phosphorus, $RuCl_3$ and more exotic candidates ($LaSeTe_2$, $NiPS_3$). All materials can be exfoliated and size-selected in a similar way yielding nanosheet dispersions with well-defined changes in their lateral dimensions and thickness. Optical extinction and absorbance spectra show systematic changes across all material classes giving access to studying fundamental physical properties. In addition, we show that liquid-exfoliated nanosheets are ideal to track degradation due to the reaction with water and oxygen by time dependent optical measurements of the dispersions. This lays the foundation to investigate ways to chemically passivate defect sites, for example by anchoring thiols to sulfur vacancies in TMDs as we show for WS_2 and TiS_2.

09:30

Tuning Electronic Structure of 2D Chalcogenide Materials

Agnieszka Beata Kuc[1]
[1]Faculty of Chemistry and Mineralogy, Leipzig University, Leipzig

In this talk, I would like to present our recent advances in the subject of electronic structure manipulations of 2D chalcogenide materials, for applications in nano(opto)-electronics. In the past years, we have investigated several types of materials, for example, 2H polytypes of Group 6, 1T polytypes of Groups 4 and 10, as well as, some materials from the main group metal atoms (Ga or Tl). More exotic structures, like Haeckelite type, were also taken into account. We were mostly focused on the electronic structures, as well as, magnetic properties of these materials. In several cases, we have investigated these properties together with the experimental groups, what allowed us to gain a deeper understanding of the structures and their properties. In this talk, I will give just a few most interesting examples from our recent research in comparison with experimental data.

10:30
Structure Characterization of Catalysts and Single-Walled Carbon Nanotubes in Chirality-Specified Synthesis
Yan Li[1], Feng Yang[1], Juan Yang[1]
[1]Peking University, Beijing

Single-walled carbon nanotubes (SWNTs) have shown great potentials in various fields attributing to their unique structure-dependent properties, therefore, the structure-controlled preparation of SWNTs is a crucial issue for their advanced applications (e.g. carbon-based nanoelectronics) and has been a great challenge for about two decades. We developed a strategy to produce SWNTs with specific chirality by using tungsten-based intermetallic compound nanocrystals as catalysts. The characterization of catalyst structure is very important to reveal the growth mechanism of SWNTs. We used transmission electron microscopy (TEM) including high-resolution TEM, scanning TEM, as well as image simulation to probe the W6Co7 catalyst structure before and after the SWNT growth. In-situ TEM performed at 1100 °C was used to prove that the W6Co7 catalysts are crystalized and keep stable structure. The chirality characterization is also very important. We found that the electronic Raman scattering (ERS) can offer an accurate chirality assignment for metallic tubes. We also developed a bilayer plot for determining the chiralities of SWNTs under complex environment.

11:00
Separation of Double Walled Carbon Nanotubes
Benjamin Flavel[1]
[1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe

A separation technique capable of sorting double walled carbon nanotubes (DWCNTs) by semiconducting (S) or metallic (M) inner- and outer- wall electronic type is presented. Electronic coupling between the inner- and outer- wall is used to alter the surfactant coating around each of the DWCNT types and aqueous gel permeation is used to separate them. Aqueous methods are used to remove single walled (SWCNT) species from the raw material and prepare enriched DWCNT fractions. The enriched DWCNT fractions are then transferred into either chlorobenzene or toluene using the copolymer PFO-BPy to yield the four inner@outer combinations of M@M, M@S, S@M and S@S.

[1] H. Li, G. Gordeev, S. Wasserroth, V. S. K. Chakravadhanula, S. K. C. Neelakandhan, F. Hennrich, A. Jorio, S. Reich, R. Krupke, B. S. Flavel, Nature Nanotechnology (2017) DOI: 10.1038/NNANO.2017.207.
[2] K. E. Moore, M. Pfohl, D. D. Tune, F. Hennrich, S. Dehm, V. S. K. Chakradhanula, C. Kuebel, R. Krupke, B. S. Flavel, ACS Nano 9 (2015) DOI: 10.1021/nn506.

11:30

Size-Controlled Growth of Single-Crystal Graphene Domains by CVD

Hui-Ming Cheng[1,2]

[1]Shenyang National Lab for Materials Science, Institute of Metal Research, CAS, Shenyang

[2]Tsinghua-Berkeley Shenzhen Institute, Shenzhen 518055, P. R. China

The controlled growth of single-crystal graphene domains with different sizes is desired for device applications and property investigations. The edges of graphene influence the electronic properties and chemical reactivity of graphene, and of course, its growth. We have first synthesized millimeter-size single crystal graphene grains and films on Pt substrates by CVD, and demonstrated the growth of single-crystal graphene domains with controlled edges that range from zigzag to armchair orientations via a growth–etching–regrowth in the CVD process. It was found that the evolution and control of the edge and morphology in single-crystal graphene following the classical kinetic Wulff construction theory. This growth–etching–regrowth CVD can be used to grow high-quality single crystal graphene domains with large sizes. Finally, we have developed a segregation–adsorption CVD method to grow very small graphene domains and well-stitched high-quality monolayer graphene films with a tunable uniform grain size from 200 nm to 1 mm and found that the changes in both thermal and electrical conductivities are directly proportional to the grain size.

17:00

Phonon spectroscopy of nanomaterials using angstrom-size electron beams

Maureen Joel Lagos[1]

[1]Department of Materials Science and Engineering, McMaster University, Hamilton

Recently, instrumental development in monochromators now permits the detection of excitations down to the infrared range using electron microscopes, thus opening up exploration of surface phonon polariton and bulk phonon modes in nanostructures. We present recent progress towards the understanding of phonon excitations in nano-objects using about 0.15 nm probe and 9 meV energy resolution. We will present results about the mapping of bulk and surface phonon excitations in a single nanocube. We detected bulk optical and acoustic modes, containing lattice contributions spanning the whole Brilloiun zone, and located mainly within the inner regions of the nanocube. A large variety of surface phonon modes are excited on the cube surface. We will also present a study of thermal effects on the inelastic electron scattering by phonons. Comparing the energy loss and energy gain scatterings, we are able to measure the local temperature of nanomaterials with good accuracy and sub-nanometer resolution.Our results provide progress in understanding swift electron scattering from vibrational modes, and promise a bright future for wide exploration of highly-localized excitations in nanoscrystals.

17:30

Probing interlayer interaction in van der Waals materials

Sense Jan van der Molen[1], Daniel Geelen[1], Ruud Tromp[1], Johannes Jobst[1]
[1]Institute of Physics, Universiteit Leiden, Leiden

Knowledge on the interaction between layers is crucial to tailor the properties of van der Waals (vdW) materials. We investigate these using newly developed techniques based on low-energy electron microscopy (LEEM). With LEEM, we probe the reflection of electrons as a function of incoming energy (0-100 eV). We have recently extended our instrument to also measure low-energy electron transmission (eV-TEM).
We apply LEEM and eV-TEM to few-layer graphene. With each layer, an unoccupied interlayer state is added, which hybridizes with the other states. In LEEM, the resulting eigenstates appear as minima in the reflection spectrum. In transmission, they show up as maxima. From both functions, we determine the hybridization energies of the interlayer states, which extend in 2D.
Next, we study the 2D-dispersion relations of these states. For that, we have developed angle-resolved reflected-electron spectroscopy (ARRES) [1]. With ARRES, we investigate few-layer graphene, hBN, as well as their combination. For the latter case we find negligible interaction. [2]

[1] Jobst et al., Nat. Comm. 6, 8926 (2015)
[2] Jobst et al., Nat. Comm. 7, 13621 (2016)

18:00
Kirchberg 2018 - Summary
Christoph Stampfer[1]
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Depends; for sure we will see what the Winterschool had to offer.

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