**Name**

IWEPNM 2016

# XXXth
# International Winterschool on Electronic Properties of Novel Materials

## Molecular Nanostructures

## Program

Hotel Sonnalp
Kirchberg/Tirol
Austria

13 - 20 February, 2016

# SUPPORTERS

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

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# LAYOUT

María Machón, Felix Herziger

Logo designed by Artur Kaczmarczyk
The logo shows exfoliated flakes of $MoS_2$ on a transparent polymer observed in transmission mode with an optical microscope.

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Financial assistance from the sponsors and supporters is greatly acknowledged.

Dear Friend:

Welcome to the 30th International Winterschool on:

Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of twenty-nine 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 |
| Amelie Biermann, Hans Tornatzky | finances |
| Asmus Vierck, Harald Scheel | website |
| Roland Gillen | technical assistance, video transfer, sponsoring |
| Felix Kampmann | announcements, website assistance |
| Emanuele Poliani | technical assistance |
| Aurélie Pierret | abstract booklet |
| 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,
Christian, Janina, Andreas, Hans, Stephanie and Siegmar

## Chairpersons

C. Thomsen (Berlin)
J. Maultzsch (Berlin)
A. Hirsch (Erlangen)
H. Kuzmany (Vienna)
S. Reich (Berlin)
S. Roth (Munich)

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C. Thomsen (DE)
A. Zettl (US)

## Scope

This winterschool will provide a platform for reviewing and discussing new developments in the field of electronic properties of molecular nanostructures and their applications. 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 insulators
- Single-molecule experiments

# INFORMATION FOR PARTICIPANTS

## Time and location

The IWEPNM 2016 starts on Saturday, 13 February, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, 20 February, breakfast. There will be a reception party on Saturday, 13 February, after dinner, and a farewell party including dinner on Friday, 19 February.

## 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 2016, Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria
e-mail: info@hotelsonnalp.info, web: www.hotelsonnalp.info

All questions concerning the IWEPNM 2016 should be directed to:
Prof. Dr. Christian Thomsen,
Institut für Festkörperphysik, Technische Universität 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 2016 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. Participants are invited to contribute comments to research and tutorial lectures where 10 minutes for discussion are reserved after each lecture. Video projection will be available for presentations. Presentation of video films needs prearranged confirmation. 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 video of the presentations.**

## Childcare

Childcare is provided by Michaela Kisch and her team (michaela@kitzkids.com, Tel.: 0043-664-5225265). 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 2016 are scheduled for publication in physica status solidi (pss). **Manuscript submission is due on April 15th.** The publication is planned as a special issue with regular articles to be published in the journal pss (b) (Feature Articles/topical reviews, Original Papers) or pss (c). In selected cases articles are highlighted in pss (RRL) (Reviews@RRL, Rapid Research Letters). 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. Do not modify any pre-settings in the style files such as font sizes, margins, and other formats, to avoid an incorrect layout of the publication.
Please **submit one complete PDF- or Word-file for review** (Word or Latex source files are required after acceptance for production).
The submission system is here: http://www.editorialmanager.com/pssb-journal

Select article type "Original Paper" and section "IWEPNM 2016: Electronic Properties of Novel Materials". If you intend to submit a "Rapid Research Letter" or a "Feature Article" manuscript, please consult with the editors.
pss editorial office e-mail: pss@wiley-vch.de

# IWEPNM 2016
# CHAIRPERSONS FOR THE ORAL SESSIONS

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

| | | |
|---|---|---|
| Sunday, 14.02. | morning | Hans Kuzmany |
| | morning, after coffee break | Hui-Ming Cheng |
| | evening | Janina Maultzsch |
| Monday, 15.02. | morning | Paola Ayala |
| | morning, after coffee break | Ermin Malic |
| | evening | Elena Obraztsova |
| Tuesday, 16.02. | morning | Annick Loiseau |
| | morning, after coffee break | Claudia Backes |
| | evening | Andreas Hirsch |
| Wednesday, 17.02. | morning | Otakar Frank |
| | morning, after coffee break | Anna Swan |
| | evening | Ralph Krupke |
| Thursday, 18.02. | morning | Klaus Ensslin |
| | morning, after coffee break | Peter Dinse |
| | evening | Tony Heinz |
| Friday, 19.02. | morning | Christoph Stampfer |
| | morning, after coffee break | Viera Skákalová |
| | evening | Siegmar Roth |

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

Chairpersons please remember:
**You have to ask for questions from the sideroom (bar)!**

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

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

We acknowledge your support. The Organizers

# Final program

| | Sunday, February 14 | Monday, February 15 | Tuesday, February 16 | Wednesday, February 17 | Thursday, February 18 | Friday, February 19 |
|---|---|---|---|---|---|---|
| **Topics** | **TEM - CNT** | **TMDs, nanowires, plasmonics** | **Growth, chemical functionalization, applications** | **Graphene optics and nanomechanics** | **Topological states, magnetic properties, applications** | **Graphene transport** |
| **08:30** | Liquid cells for high-resolution transmission electron microscopy<br>ZETTL | Optical properties of atomically thin semiconductors and heterostructures<br>HEINZ | Growth of transition metal dichalcogenides by thermally assisted conversion<br>McEVOY | Bending, pulling, and cutting wrinkled two-dimensional materials<br>BOLOTIN | Strong, weak, and weak-and-strong topological insulators<br>BROUWER | Measurement back-action in stacked graphene quantum dots<br>ENSSLIN |
| **09:00** | Atomic level studies of defects and dopants in 2D materials<br>WARNER | | Towards integrated manufacturing of 2D materials<br>HOFMANN | Phonons in low dimensional sp2 carbon systems<br>BENDIAB | | Electron-phonon coupling in suspended mono- and bilayer graphene<br>HAKONEN |
| **09:30** | Fabrication and microscopic analysis of defective, amorphous, deformed, strained, and functionalized 2D materials<br>MEYER | Temperature-dependent photoluminescence spectra of $MoS_2$: trion peak asymmetry<br>SWAN | Chemical functionalization of 2D materials<br>ABELLÁN | Raman spectroscopy as probe of nanometer-scale strain variations in graphene<br>NEUMANN | From Floquet to Dicke: quantum spin-Hall insulator in quantum light<br>DORA | Electron-optics in suspended graphene<br>MAKK |
| **10:00** | **Coffee break** | | | | | |
| **10:30** | Structure and energetics of carbon double wall nanotubes<br>LOISEAU | Probing quantum transport in atomically thin transition metal dichalcogenides<br>WANG | CVD Growth of High-Quality 2D Transitional Metal Sulfides and Carbides<br>CHENG | Nanospectroscopy for Functional Nanomaterials<br>ROY | Induced superconductivity and unconventional pairing in HgTe/HgCdTe quantum wells<br>HART | Engineering electron and hole wires in 2D materials through polar discontinuities<br>GIBERTINI |
| **11:00** | Single files of dipoles aligned in carbon nanotubes<br>WENSELEERS | Spintronics with two-dimensional materials and heterostructures<br>DASH | Single layer graphene in water<br>BEPETE | Bright visible light emission from graphene<br>KIM | Imaging currents in 2D quantum materials<br>NOWACK | Symmetry-broken quantum Hall states in bilayer and trilayer graphene<br>SHI |
| **11:30** | Low-dimensional metal-organic nanostructures<br>SHIOZAWA | Electronic and optical properties of monoclinic $MoTe_2$<br>YANG | Graphene in water: Preparation and applications<br>VÁZQUEZ | Topological valley transport at bilayer graphene domain walls<br>JU | Tunable Pseudo-Zeeman field in graphene<br>NEMES-INCZE | |

|  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| **12:00 - 17:00** | Mini workshops | Mini workshops | Mini workshops | Mini workshops | Mini workshops | Mini workshops |
| **17:00 - 18:30** | Dinner |  |  |  |  | 17:00<br>Exciton physics in individual suspended carbon nanotubes<br>KATO |
| **18:30** | Synthesis of single-walled carbon nanotubes with specific structure<br>LI | Microscopic modelling of electrical and optical properties of 2D materials<br>PEREBEINOS | New organic compounds for photovoltaic devices<br>MARTIN | Superconductivity in alkali-metal doped graphene<br>GRIGORIEVA | Photon emission from hBN tunnel junctions<br>NOVOTNY | 17:30<br>Exploring novel 2D elemental materials with group IV elements<br>XIAN |
| **19:00** | Tuning thermoelectric properties of chirality selected single wall carbon nanotubes by electric double layer carrier injections<br>YANAGI | Recent progress in semiconductor nanowire photodetectors for multispectral imaging and in nanoscale sensing using SERS<br>CROZIER | Self-assembled carbon electronics<br>HALIK | Anharmonic matter: charge-density-waves in dichalcogenides and hydrogen sulfide superconductor<br>MAURI | The enabling role of graphene for on-chip photonic systems<br>NEUMAIER | 18:00<br>Conference Summary<br>JORIO |
| **19:30** | Phonons in Free-standing Silicon Membranes: an insight into heat transport in the Nano scale<br>SOTOMAYOR-TORRES | Carpets of ordered organic nanowires by concerted action of molecular self assembly and solvent structure<br>SCALIA | Polymer-SWNT hybrids: toward high performance field effect transistors<br>LOI | Theory of disorder induced magnetotransport in 2D materials<br>ADAM | Energy conversion and storage devices based on graphene and other 2D crystals<br>BONACCORSO | 18:30 - 20:00<br>Break |
| **20:00** | Nanopores in 2D materials<br>RADENOVIC | Poster I<br>Monday | Poster II<br>Tuesday | Two-dimensional heterostructures with spin-orbit coupling<br>ROSSI | Poster III<br>Thursday | Bauernbuffet<br>Farewell |
| **20:30** |  |  |  |  |  |  |
| **Topics** | **TEM - CNT** | **TMDs, nanowires, plasmonics** | **Growth, chemical functionalization, applications** | **Graphene optics and nanomechanics** | **Topological states, magnetic properties, applications** | **Graphene transport** |
|  | Sunday, February 14 | Monday, February 15 | Tuesday, February 16 | Wednesday, February 17 | Thursday, February 18 | Friday, February 19 |

# PROGRAM

# AND

# ABSTRACTS

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Innovation with Integrity

FT-IR

| | |
|---|---|
| 08:30 – 09:00 | A. Zettl, Berkeley<br>*Liquid Cells for High-Resolution Transmission Electron Microscopy* |
| 09:00 – 09:30 | J. Warner, Oxford<br>*Atomic level studies of defects and dopants in 2D materials* |
| 09:30 – 10:00 | J. Meyer, Vienna<br>*Fabrication and microscopic analysis of defective, amorphous, deformed, strained, and functionalized 2D materials* |
| 10:00 – 10:30 | coffee break |
| 10:30 – 11:00 | A. Loiseau, Chatillon<br>*Structure and energetics of carbon double wall nanotubes* |
| 11:00 – 11:30 | W. Wenseleers, Antwerp<br>*Single files of dipoles aligned in carbon nanotubes* |
| 11:30 – 12:00 | H. Shiozawa, Vienna<br>*Low-dimensional metal-organic nanostructures* |
| 12:00 – 17:00 | mini workshops |
| 17:00 – 18:30 | Dinner |
| 18:30 – 19:00 | Y. Li, Beijing<br>*Synthesis of Single-Walled Carbon Nanotubes with Specific Structure* |
| 19:00 – 19:30 | K. Yanagi, Tokyo<br>*Tuning thermoelectric properties of chirality selected single wall carbon nanotubes by electric double layer carrier injections* |
| 19:30 – 20:00 | C. Sotomayor Torres, Bellaterra<br>*Phonons in Free-standing Silicon Membranes: an insight into heat transport in the Nano scale* |
| 20:00 – 20:30 | A. Radenovic, Lausanne<br>*Nanopores in 2D materials* |

### 08:30

### Liquid Cells for High-Resolution Transmission Electron Microscopy

Alex Zettl[1]

[1]Department of Physics, University of California, Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 U.S.A.

Recent instrumentation advances in ultra-high-resolution transmission electron microscopy (TEM) have made it possible to image nanoscale structures in real time and with atomic resolution, including those composed of low-Z elements such as carbon, boron, and nitrogen. Typically this is done in a high-vacuum environment. In order to study various chemical and biological process in liquid environments via TEM, we have developed a graphene liquid cell that uses monolayer graphene windows to hermetically seal a small volume of liquid containing the species of interest. The method has been applied to platinum nanocrystal growth, DNA dynamics, and mineral precipitation. I will describe relevant science and future directions.

### 09:00

### Atomic level studies of defects and dopants in 2D materials

Jamie Warner[1]
[1]Department of Materials, University of Oxford

Defects and dopants influence the properties of 2D materials and it is important to have accurate knowledge about their structure at the atomic level. Aberration-corrected transmission electron microscopy (AC-TEM) can image the structure of 2D materials, such as graphene and MoS2, with spatial resolution approaching 80pm, enabling bond lengths to be measured. I will present results on the various vacancies in graphene and compare them to monolayered transition metal dichalcogenides, discussing migration and aggregation dynamics. The interactions between single metal atoms and metal clusters with graphene and MoS2 surfaces and lattice will also be presented. Atomic models produced from the AC-TEM images can be correlated to predictions from density functional theory to gain insight into the property change from deviations of the pristine structure.

### 09:30

### Fabrication and microscopic analysis of defective, amorphous, deformed, strained, and functionalized 2D materials

Jannik C. Meyer[1], J. Kotakoski[1], C. Mangler[1], B. C. Bayer[1], C. Kramberger-Kaplan[1], T. J. Pennycook[1], V. Skákalová[1], G. Argentero[1], A. Mittelberger[1], S. Hummel[1], K. Elibol[1], R. Mirzayev[1], U. Ludacka[1], A. Grill[1], C. Hofer[1], T. Susi[1]
[1]Faculty of Physics, University of Vienna, Vienna

In this presentation, I will show several recent experiments with 2D materials that have been treated for the generation of defects, synthesized in amorphous form, deformed and strained via local probes, or decorated with molecules. The first part concerns the study of these systems by high-resolution scanning transmission electron microscopy, which reveals structural modifications at the atomic level and also can be used to introduce disorder or even controlled displacements. For example, different types of amorphous 2D systems will be compared. I will also show a new approach to image radiation-sensitive molecular species on graphene, based on distributing the dose over many identical structures, besides sandwiching and using low energies. In the second part, I will discuss a novel approach to study free-standing membranes by dual-probe scanning tunneling microscopy (STM), where two STM tips are brought into contact with the graphene membrane from opposing sides. At the closest point, the two tips are separated only by the thickness of the membrane. The interaction of the two probes across the membrane provides insights to both the membrane properties as well as to the fundamental interactions between the probe and the material.

### 10:30

### Structure and energetics of carbon double wall nanotubes

Annick Loiseau[1], Ahmed Ghedjatti[1], Frédéric Fossard[1], Guillaume Wang[2], Emmanuel Flahaut[3], Hakim Amara[1], Jean-Sébastien Lauret[4]
[1]LEM, CNRS-ONERA, Chatillon
[2]MPQ, U. Paris Diderot-Paris 7, Paris, France
[3]CIRIMAT, U. Toulouse, Toulouse, France
[4]LAC – ENS Cachan, Orsay France,

Single-walled carbon nanotubes (SWNTs) have shown oustanding capabilities in the realization of new functional devices but are extremely sensitive to any slight changes in their environment, altering their physical properties. A strategy to overcome this difficulty is to use double-walled carbon nanotubes (DWNTs), consisting of two concentric tubes. In order to better know the basic properties of this kind of tubes in linkage with their structure, we have developed a systematic and robust procedure using acHR-TEM (aberration corrected Transmitting High Resolution Electron Microscopy) to determine the atomic structure of several tens of tubes. Statistical analyses of their diameters and twist angle between inner and outer tubes show that whatever the synthesis technique, some configurations are strongly favored whereas some other are never observed. These results reveal the existence of strong coupling between the two concentric tubes in a DWNT for the smaller diameters below 2 nm. To complete this analysis, we performed Monte Carlo calculations with an empirical model in order to understand the nature of the coupling and explain the selectivity of observed configurations.

### 11:00

## Single files of dipoles aligned in carbon nanotubes

Sofie Cambré[1], Jochen Campo[1], Wouter van Werveke[1], Stein van Bezouw[1], Joeri Defillet[1], Charlie Beirnaert[1], Christof C. Verlackt[1], Pegie Cool[1], Wim Wenseleers[1]
[1]Physics Department, University of Antwerp, Antwerp

Asymmetric dye molecules, acting as electric ‘rectifiers’ with a large second-order nonlinear optical (NLO) response (hyperpolarizability $\beta$), find applications in ultrafast electro-optic switches for optical telecommunication and wavelength conversion of lasers. In 3D bulk materials, however, such dipolar molecules tend to align in a pairwise anti-parallel way, cancelling each other’s directional properties, such as the NLO response.

We show that by encapsulating such elongated dipolar molecules in the 1D internal channel of single-wall carbon nanotubes (SWNTs), Coulomb interactions naturally favor a polar head-to-tail alignment of the molecular dipoles, leading to a coherent addition of their second-order NLO responses. The encapsulation is evidenced by extensive wavelength-dependent fluorescence-excitation and resonance Raman experiments on bile-salt solubilized dye-filled SWNTs, revealing the critical diameter for filling through the effect of encapsulation on the vibrational and electronic properties of the SWNTs and the encapsulated molecules. Wavelength-dependent second-harmonic light scattering indeed shows that these organic-SWNT nanohybrids possess giant NLO responses, also allowing the domain size of head-to-tail aligned chromophores to be determined.

### 11:30

## Low-dimensional metal-organic nanostructures

Hidetsugu Shiozawa[1]
[1]Faculty of Physics, University of Vienna, Vienna

Molecular arrays and nanomagnets that are assembled in low-dimensional nanostructures can outperform their bulky counterparts. We show that encapsulated inside single-wall carbon nanotubes (SWCNTs) or carbon fibers, iron, cobalt and nickel clusters behave as stable single-domain magnets exhibiting large coercive fields as the cluster size becomes as small as the exchange length. Transition metal ions in coordination compounds arranged in one dimension are ideal systems in which we study anisotropic magnetic coupling. In metal-organic frameworks (MOFs), metal ions are coordinated to form low-dimensional metal frames and porous structures. Arrays of metal ions exposed to the interior voids react with infiltrating molecules, leading to MOF's gas-sensing abilities. Our experiments using Raman, photoemission, SQUID, X-ray magnetic circular dichroism spectroscopy, electron microscopy, and magnetotransport measurements probe electronic and magnetic interactions at molecular interfaces that are responsible for their unique physical properties. We demonstrate that the MOF's electrical conduction and magnetic ordering temperature can tuned by molecular doping.

### 18:30

### Synthesis of Single-Walled Carbon Nanotubes with Specific Structure

Yan Li[1], Feng Yang[1], Xiao Wang[1], Daqi Zhang[1], Juan Yang[1]
[1]College of Chemistry and Molecular Engineering, Peking University, Beijing

Single-walled carbon nanotubes (SWNTs) have shown great potentials in various applications attribute to their unique structure-dependent properties. Therefore the controlled preparation of chemically and structurally pristine SWNTs is a crucial issue for their advanced applications (e.g. nanoelectronics) and has been a great challenge for two decades. Inspired by the specificity of enzyme-catalyzed reactions, we realized that only catalysts with unique crystal structure and desired atomic arrangements can act as the structural templates for chirality specific growth of SWNTs, relying on the high selectivity in geometry match between catalysts and SWNTs. We developed a new family of catalysts, tungsten-based intermetallic compounds, which have high melting point and very special crystal structure, to synthesize SWNTs with designed chirality. The chirality-specific growth of SWNTs is realized by the cooperation of two factors: the structural match between SWNTs and the catalysts makes the growth of SWNTs with specific chirality thermodynamically favourable; and further manipulation of CVD conditions obtains optimized growth kinetics for SWNTs with this designed chirality.

### 19:00

### Tuning thermoelectric properties of chirality selected single wall carbon nanotubes by electric double layer carrier injections

Kazuhiro Yanagi[1]
[1]Physics, Tokyo Metropolitan University, Tokyo

Thermoelectrics are a very important technology for efficiently converting waste heat into electric power. Hicks and Dresselhaus proposed an important approach to innovate its performance, which involves using one-dimensional materials, and properly tuning their Fermi level.[1] Thus, to maximize the thermoelectric performance, understanding of the relationships between the thermoelectric performance, the electronic structure, and the position of the Fermi level is of great importance. Single wall carbon nanotubes (SWCNTs) are an ideal model for one-dimensional materials. Previously we have tuned the Fermi level of SWCNTs by electric double layer carrier injection using ionic liquids, and investigated their various physical properties.[2] Recently, we revealed the Fermi-level dependence of thermoelectric properties of semiconducting SWCNTs with diameter of 1.4 nm.[3] Here, I discuss how the chiralities of SWCNTs influence on their thermoelectric properties.

1. Hicks & Dresselhaus, PRB 47, 16631 (1993),
2. Yanagi et al., Adv. Mater. 23, 2811 (2011), PRL 110, 86801 (2013), PRL 114, 176807 (2015),
3. Yanagi et al., Nano Lett. 14, 6437 (2014)

### 19:30

## Phonons in Free-standing Silicon Membranes: an insight into heat transport in the Nano scale

Clivia M. Sotomayor Torres[1,2,3]
[1]Catalan Institute of Nanoscience and Nanotechnology, Bellaterra
[2]ICREA, Barcelona, Spain
[3]Royal Institute of Technology KTH, Kista, Sweden

The contribution of acoustic phonons to the thermal conductivity is studied in ultra-thin free-standing Si membranes. Our understanding so far is based on measured and modelled acoustic phonon dispersion relations, their lifetime, transport in the diffusive and ballistic regimes, the presence of native oxide and of 2-D phononic crystals and the direct in-plane thermal conductivity measurements based on laser-Raman thermometry.

The dispersion relations of membranes of thickness down to 8 nm are measured and simulated and found to be discretised flexural and dilatational modes. The group velocity is obtained from these measurements and shown to decrease by a factor larger than 20. The lifetimes of the experimentally accessible first order dilatational mode is observed to decrease over one order of magnitude compared to bulk values. Boundary scattering and normal processes are found to contribute to the thermal transport as well as the native oxide and surface topography.

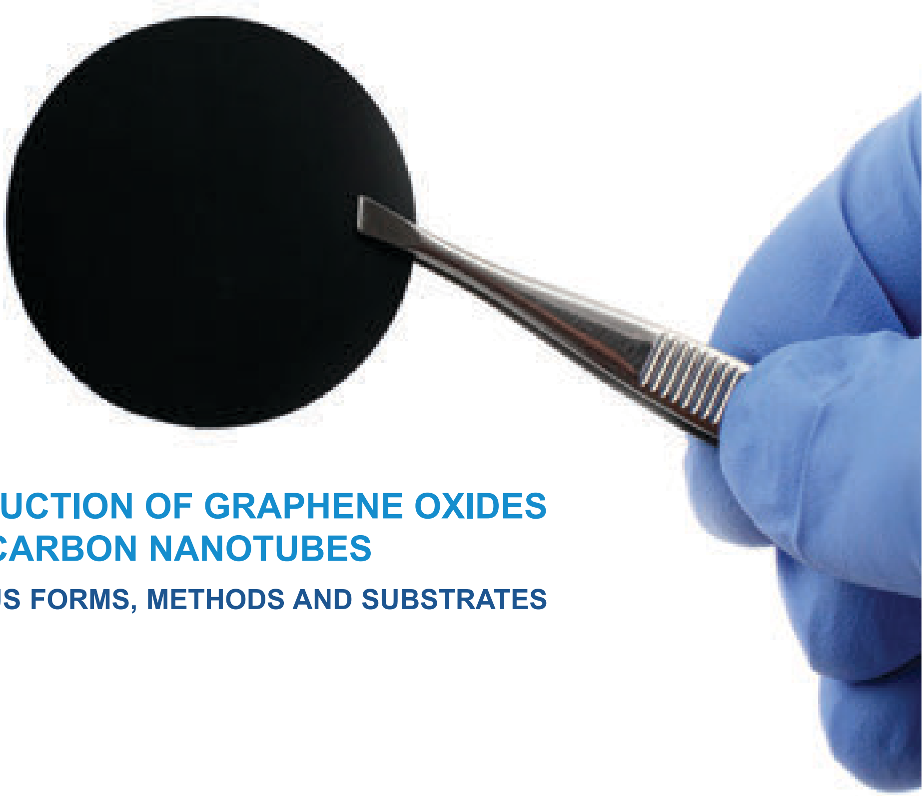
In collaboration with: E Chavez-Angel, F Alzina, J S Reparaz, B Graczykowski, A El Sachat, M R Wagner, M Sledzinka , A Shchepetov, M Prunnila and J Ahopelto, J Jaramillo-Fernandez, S Neogi and D Donadio.

### 20:00
## Nanopores in 2D materials

Aleksandra Radenovic[1]
[1]IBI, EPFL, Lausanne

Next generation sequencing methods based on nanopore technology have recently gained considerable attention, mainly because they promise affordable and fast genome sequencing by providing long read-lengths (5kbp) and do not require additional DNA amplification or enzymatic incorporation of modified nucleotides. During the DNA translocation, the ionic current is partially blocked, leading to a reduction in the current and allowing differentiation between the four different nucleotides. The amplitude and duration of these blockades depend on the length and width of the translocating polymer. Although single nucleotide identification and DNA sequencing using biological pores have already been demonstrated their fragility, difficulties related to measuring pA-range ionic currents together with their dependence on biochemical reagents, make solid state nanopores an attractive alternative.

In this talk I will address novel applications that address identification of single nucleotides but as well go beyond DNA sequencing. We use novel solid state nanopore platform based on atomically thin nanopore membranes in 2 D materials such as graphene or molybdenum disulfide.



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|---|---|
| 08:30 – 09:30 | T. Heinz, Stanford<br>*Optical properties of atomically thin semiconductors and heterostructures* |
| 09:30 – 10:00 | A. Swan, Boston<br>*Temperature-Dependent Photoluminescence Spectra of* $MoS_2$*: Trion Peak Asymmetry* |
| 10:00 – 10:30 | coffee break |
| 10:30 – 11:00 | N. Wang, Hong Kong<br>*Probing quantum transport in atomically thin transition metal dichalcogenides* |
| 11:00 – 11:30 | S. Dash, Gothenburg<br>*Spintronics with two-dimensional materials and heterostructures* |
| 11:30 – 12:00 | H. Yang, Suwon<br>*Electronic and optical properties of monoclinic MoTe2* |
| 12:00 – 17:00 | mini workshops |
| 17:00 – 18:30 | Dinner |
| 18:30 – 19:00 | V. Perebeinos, Moscow<br>*Microscopic modelling of electrical and optical properties of 2D materials* |
| 19:00 – 19:30 | K. Crozier, Melbourne<br>*Recent progress in semiconductor nanowire photodetectors for multispectral imaging and in nanoscale sensing using surface-enhanced Raman spectroscopy* |
| 19:30 – 20:00 | G. Scalia, Luxembourg<br>*Carpets of ordered organic nanowires by concerted action of molecular self assembly and solvent structure* |
| 20:00 | Poster I |

### 08:30

### Optical properties of atomically thin semiconductors and heterostructures

Tony F Heinz[1]

[1]Dept. of Applied Physics, Stanford University, Stanford

We discuss recent advances in our understanding of the electronic and optical properties of monolayers of the transition metal dichalcogenide (TMDC) materials, including $MoS_2$ $MoSe_2$, $MoTe_2$, $WS_2$, $WSe_2$. These materials share several unusual characteristics, including a transition from an indirect-gap material in the bulk to a direct-gap, emissive material at monolayer thickness. They also exhibit selectivity to excitation of the degenerate K or K' valley under circularly polarized radiation.

In this paper, we will highlight progress in understanding two types of interactions in these materials: the many-body interactions between charge carriers in one layer and interactions between carriers that arise when two monolayer sheets of materials stacked on one another to form a bilayer.

### 09:30

### Temperature-Dependent Photoluminescence Spectra of $MoS_2$: Trion Peak Asymmetry

Anna K Swan[1]
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In low dimensional materials, Coulomb interactions are weakly screened and optical excitations are dominated by excitons even at room temperature. In transition metal dichalcogenides, (TMDs), photoluminescence (PL) spectra show so called A and B excitons split by valence band spin-orbit interactions, as well as a trion peak $A^-$, an exciton with an extra bound electron. Here we focus on the trion's temperature dependent contribution to the PL spectra in monolayer $MoS_2$ from $LN_2$ to 473K. Unlike excitons, trions can radiatively decay with non-zero momentum by ejecting an electron. This causes a slight asymmetry with a low energy tail in the trion PL peak. Fitting the temperature-dependent trion PL asymmetry yields information on its Bohr radius and the ratio of the hole and electron masses. The temperature dependent variation of the trion and A exciton PL intensity yields the electron binding energy. The analysis and concepts presented here are applicable to other TMDs where trions have been observed such as $MoSe_2$ and $WSe_2$. We use spatial and spectral Raman correlations in order to identify strain, charge and temperature effects in both in $MoS_2$ and graphene.

## 10:30

## Probing quantum transport in atomically thin transition metal dichalcogenides

Ning Wang[1]

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I present effective methods for improving the quality of atomically thin transition metal dichalcogenide (TMDC) channel materials prepared by mechanical exfoliation. We have achieved high-quality TMDC field-effect devices with mobilities up to 20,000 cm2/V s at cryogenic temperatures. Interesting quantum Hall transport phenomena, Zeeman splitting effects and Landau level degeneracies have been probed electrically. For example, in some few-layer TMDC, the conduction bands along the ΓK directions shift downward energetically in the presence of interlayer interactions, forming six Q valleys related by three-fold rotational symmetry and time reversal symmetry. In even-layers the extra inversion symmetry requires all states to be Kramers degenerate, whereas in odd-layers the intrinsic inversion asymmetry dictates the Q valleys to be spin-valley coupled. We observed interesting Shubnikov-de Hass oscillations and Quantum Hall effect involving Q-valleys, such as the valley Zeeman effect in all odd-layer TMD devices and the spin Zeeman effect in all even-layer TMD devices.

### 11:00

## Spintronics with two-dimensional materials and heterostructures

Saroj Prasad Dash[1]
[1]Microtechnology and Nanoscience, Chalmers University of Technology, Gothenburg

Two-dimensional (2D) atomic crystals provide a large class of materials proposed to be important for spintronics. Graphene is considered to be an ideal material for spin transport due to the high mobility and long spin lifetime of the carriers. Recently, we demonstrated spin transport over distances of 16 $\mu$m and spin lifetimes up to 1.2 ns in large area CVD graphene on SiO2/Si substrate at room temperature [Nature Communications 6, 6766 (2015)]. Subsequently, using the 2D h-BN as a tunnel barrier on graphene, we observe an enhancement in spin polarization [2], and its negative sign for thicker h-BN layers [Scientific Reports 4, 61446 (2014)]. These signatures provide an experimental evidence of the spin filtering across the ferromagnet/hBN-graphene van der Waals heterostructures. We further aim to address the issue of spin manipulation in graphene by employing heterostructures with other 2D semiconductors, topological insulators [ACS Nano 8 (1), 476 (2014); Nano Letters 15 (12), 7976 (2015)] and materials with novel spin textures. These findings open a platform for exploring novel spin functionalities in 2D materials heterostructures and understanding the basic science that control their behavior.

## 11:30
## Electronic and optical properties of monoclinic MoTe2

Heejun Yang[1]
[1]Department of Energy Science, Sungkyunkwan University, Suwon

Transition metal dichalcogenides (TMDs), together with metallic graphene and highly insulating hexagonal boron nitride, have recently attracted renewed interests as an important two-dimensional component of next-generation devices [1,2].
In this presentation, I will discuss on structural phase transition between hexagonal and stable monoclinic (distorted octahedral or 1T') phase in bulk single-crystalline MoTe2, and an electronic phase transition between semi-metallic (bulk) and semi-conducting (few-layered) 1T'-MoTe2. Our density functional theory calculations identify strong interband spin-orbit coupling (SOC) as the origin of bandgap opening in the few-layered monoclinic MoTe2. It will be shown that the Peierls distortion is a key mechanism to stabilize the monoclinic structure.

[1] D. H. Keum, S. Cho et al. Nature Physics 11, 482 (2015)
[2] S. Cho et al. Science 349, 625 (2015)

## 18:30

## Microscopic modelling of electrical and optical properties of 2D materials

Vasili Perebeinos[1]
[1]Skoltech, Moscow, Russia

In recent years, 2D materials, such as black phosphorus and transition metal dichalcogenides, have attracted much attention due to their excellent transport and optical properties. Using a tight-binding model of the electron-phonon interaction we explore phonon limited mobility in black phosphorous monolayer as a function of temperature and doping level. Using a Bethe-Salpeter equation, we investigate optical and excitonic properties of $\mathrm{MoS}_2$ monolayers in an applied in-plane electric field. We predict a quadratic Stark shift and its scaling with the exciton binding energy, determined by the dielectric environment.

### 19:00

### Recent progress in semiconductor nanowire photodetectors for multispectral imaging and in nanoscale sensing using surface-enhanced Raman spectroscopy

Kenneth Crozier[1,2]
[1]School of Physics, University of Melbourne
[2]Department of Electrical and Electronic Engineering, University of Melbourne

We present recent studies in which engineering the interaction between light and nanoscale materials has been pursued for applications in image sensors and in spectroscopy. In the first, we present recent work by the author and colleagues on the use of silicon and germanium nanowires for multispectral imaging. We show that their ability to support waveguide modes leads to spectrally-selective absorption properties. We show that this in turn enables the nanowires to be used as filters or photodetectors for colour and multispectral imaging. In the second study, we review recent work by the author and colleagues on plasmonic structures for surface-enhanced Raman scattering (SERS). We demonstrate a micro-patterned silicon structure that enables the preparation of a SERS substrate and pre-concentration of the analyte molecules. If time permits, we will discuss recent work on the experimental demonstration that quantum mechanical tunnelling across gaps between nanoparticles limits the enhancement in SERS.

### 19:30

## Carpets of ordered organic nanowires by concerted action of molecular self assembly and solvent structure

Ji Hyun Park[1,2], Kyung Ho Kim[3], Yoichi Takanishi[4], Massimo Labardi[5], Yung Woo Park[3], Youn Sang Kim[2], Jun Yamamoto[4], Jan P. F. Lagerwall[1], Giusy Scalia[1,2]
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[4]Department of Physics, Graduate School of Science, Kyoto University, Kita-Shirakawa, Kyoto 606-8502, Japan
[5]CNR-IPCF, UOS Pisa, Italy

The controlled manipulation of nanowires presents an important challenge in the application of nanotechnology. Self-organization is a possible route, hence molecules possessing liquid crystal (LC) phases offer clear advantages. LCs from disk-like molecules (discotics) form columns, regularly positioned on a 2D lattice. In the presence of solvent, the self-assembly changes, due to contributions from e.g. changes to wetting behaviour and chemically specific interactions with solvent molecules. Aromatic solvents match the aromatic cores of discotic molecules while alkane solvents interact better with their aliphatic chains, each thus influencing the hierarchical assembly in different ways. Depositing a triphenylene based LC from toluene solution, nanostructured films composed of very long wires, uniformly aligned over macroscopic areas, can be realized. These ordered wires show drastically higher conductivity upon doping than pristine or disorganized structures of the same molecules, making them attractive for realizing, in a facile way, conductive channels. The general mechanism driving this ordering can most likely be applied also to other cases of organic molecule self-assembly.

## MON 1
## Hexagonal boron nitride films as tunnel barrier, clean substrates and gate insulator

Gulibusitan Abulizi[1], Andreas Baumgartner[1], Christian Schönenberger[1]
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We report on the fabrication and low temperature transport characteristics of several different types of carbon nanotube (CNT) nanostructures made using hexagonal boron nitride (hBN) sheets of different thicknesses either as clean substrates, gate insulators, or as tunnel barriers to the CNTs. We have manufactured CNTs of several micrometer length with 200nm wide hBN tunnel contact as source and drain with 300nm spacing. The differential conductance at low temperature as a function of the backgate voltage and the bias shows Coulomb blockade features characteristic for quantum dots (QDs) with a charging energy of 1meV and excited state energies of 0.3meV. These numbers suggest a confinement length on the order of $3\mu$m, which is significantly larger than the spacing between the tunnel contacts. This suggests these QDs are confined by the CNT ends or by very few potential fluctuations, rather than the source-drain contacts, in stark contrast to standard metallic contacts to CNTs. Our results are very promising first steps in the fabrication of substrate-bound very clean CNT devices, which should allow us to exploit the many advantageous properties of CNTs in versatile structures.

## MON 2
## Direct Synthesis of Functionalized Buckybowls

Konstantin Amsharov[1], Olena Papaianina[1], Vladimir Akhmetov[2], Alexey Gorynkov[2]
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Bowl-shaped polycyclic aromatic hydrocarbons or buckybowls which can be considered as substructures of fullerenes or nanotubes display superior characteristics which render them ideal candidates for the application in molecular electronics, material sciences, and nanotechnologies. In this respect functionalized buckybowls are of particular interest due to the possibility to tune precisely required properties. However, synthesis of functionalized buckybowls remains a challenge since the fabrication of distorted bowl systems requires harsh reaction conditions that do not tolerate functional group. Here we present efficient strategy for the direct synthesis of functional buckybowls via fluorine promoted Aryl-Aryl coupling.[1] Our methodology is based on the synthesis of polycyclic aromatic hydrocarbons which already contain all necessary carbon atoms and required functionality in appropriate positions. The following intramolecular condensation leads directly to the desired functionalized bowl-shaped molecule. The strategy presented opens the possibility for facile synthesis of extended functionalized bowls in bulk amounts with close to quantitative yield.

[1] K.Yu. Amsharov, M. Kabdulov, M. Jansen, Angew. Chem. Int. Ed. 2012, 51, 4594.

## MON 3
## Selective synthesis of single walled carbon nanotubes with W-based bimetallic catalyst

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The application of single-walled carbon nanotubes (SWNTs) in nanodevices is limited by the impurities and mixed chiralities of SWNTs assembles. Direct synthesis of single chirality of SWNTs is challenging but attracts considerable attention among researchers. CoW is reported to grow a single chirality, (12,6) with over 90% abundance through high-temperature (1030°C) reduction and growth [1]. Here, we show that a sputtered CoW catalyst can selectively grow (12,6) SWNTs by chemical vapor deposition at low temperature. Statistical Raman mapping analysis and optical absorption spectrum of the as-grown SWNTs reveal that the abundance of (12,6) is over 50%. Parametric study of this CoW bimetallic catalyst system demonstrates that the reduction temperature before growth is critical for the selectivity. Moreover, the morphology and structure of catalyst is investigated by transmission electron microscope, which discloses the complicated structure changes before and after growth. Further study is needed to optimize conditions to obtain the chirality control of SWNTs.

[1] F. Yang et al., Nature 510, 522(2014).

## MON 4
## Formation of sp carbon chains by femtosecond laser ablation of graphite

Natalia R Arutyunyan[1,2], Vitaly V. Kononenko[1,2], Viktor M. Gololobov[1], Elena D. Obraztsova[1,2]
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[2]National Research Nuclear University MEPhI

Polyynic chains of carbon atoms linked by alternating triple and single bonds are the typical example of 1D carbon material. The mechanism of their formation in liquid media is not completely investigated, and its understanding requires more profound studies. In this work the results on the formation of polyynic linear carbon chains (LCC) by method of laser ablation of micron graphite particles suspended in hexane are presented. The carbon chains of various length (6-20 carbon atoms) were formed. The efficiency of the LCC synthesis depended on the intensity of the laser irradiation and was significantly nonlinear. Three regions could be distinguished. In the first region, from 0 to 10 J/cm2, the laser fluence was below the threshold of the LCC formation, and no LCC were found. In the second region of moderate laser power the dependence of LCC content on the laser fluence was logarithmic, and typical ablation of graphite particles occurred. When laser fluence was over 50 J/cm2, the filamentation of the laser beam took place, the volume of the hot zone was increased, and the content of LCC grew nonlinearly.

Acknowledgements. The work was supported by RFBR project 15-02-08199_a.

## MON 5

## On the O 1s XPS spectra of adsorbed oxygen on metallicity-sorted carbon nanotubes

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In our recent studies, looking at the C1s photoemission line, we reported a higher binding energy signal due to the formation of carbonyl groups [C=O] as reaction byproducts during adsorption on the tube defects. Making use of metallicity separated tubes, we have performed high resolution studies on the O1s region and studied its components in detail assisted by DFT calculations. This allows one to determine the specific functional groups or bonding environments measured in x-ray photoelectron spectroscopy (XPS). We have demonstrated how computed binding energies may be used to decompose a measured spectrum into its individual components. We find the XPS O 1s signal arises mostly due to the adsorption on SWCNT defects of three O-containing functional groups: ketene (C=C=O), epoxy (C2>O), and carbonyl (C2>C=O). The peak intensity for each species on the metallic SWCNT sample is almost twice that on the semiconducting SWCNT sample. This suggests a greater abundance of O-containing defect structures on the oxidized metallic SWCNT sample. For both metallic and semiconducting SWCNTs, we find O2 does not contribute to the XPS O 1s spectra.

## MON 6
## Liquid exfoliation of layered materials beyond graphene and transition metal dichalogenides: GaS and black phosphorus

Claudia Backes[1,2], Damien Hanlon[1], Andrew Harvey[1], Nina C. Berner[3], Niall McEvoy[3], Evie Doherty[1,3], Hannah C. Nerl[1,3], Valeria Nicolosi[1,3], Georg S. Duesberg[3], Jonathan N. Coleman[1,3]
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Liquid phase exfoliation (LPE) has become an increasingly important technique for the production of two-dimensional nanomaterials such as graphene and MoS2. This method involves the exfoliation of layered crystals, e.g. by exposure to sonication, to form large quantities of nanosheets stabilized in liquids. This enables further solution processing. Possibly, the greatest strength is the applicability to a broad range of materials.

This is shown in this contribution. We have recently expanded the palette of solution processable 2D-materials by demonstrating that GaS [1] as representative III-VI semiconductor and black phosphorus [2] can be exfoliated in suitable solvents. Control over nanosheet size and thickness was achieved by liquid cascade centrifugation and size dependent optical properties were analysed. This lead for example to the measurement of mono- and few-layered photoluminescence of black phosphorus in liquids. In addition, we were able to show that a suitable solvent can protect the basal plane of black phosphorus from degradation under ambient conditions.

1. Chem. Mater., 2015, 27, 3483. 2. Nat. Commun., 2015, 6, 8563.

## MON 7
## Fabrication of One Dimensional Zig-Zag PCBM Nanoribbons from Two Dimensional Nanosheets

Hamid Reza Barzegar[1,2,3,4], Eduardo Gracia-Espino[1,5], Tiva Sharifi[1], Aiming Yan[2,3,4], Alex Zettl[2,3,4], Thomas Wågberg[1]
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We demonstrate a facile solution-based method for synthesizing molecular nanoribbons, comprising [6,6]-Phenyl-C61-butyric acid methyl ester (PCBM) molecules. Exploiting the hydrophobic nature of PCBM molecules the nanoribbons are produced by folding/cutting two-dimensional PCBM sheets in a hydrophilic environment. The synthesized nanoribbons exhibit uniform width of 3.8 ± 0.3 nm, equivalent to four PCBM molecules, and lengths of 20-400 nm. These nanoribbons show well-defined crystalline structure with a hexagonal arrangement of PCBM molecules. First principle calculations and detailed experimental characterization provides an insight into the structure and formation mechanism of the PCBM nanoribbons. Given the dimensions and the physical properties of the PCBM nanoribbons, it is plausible that they should be ideal as acceptor material in organic solar cells.

### MON 8

### High-resolution electron microscopy of h-BN growth and 2D/non-2D materials integration

Bernhard C. Bayer[1], Sabina Caneva[2], Adrianus I. Aria[2], Reinhard A. Kaindl[3], Timothy J. Pennycook[1], Jani Kotakoski[1], Clemens Mangler[1], Wolfgang Waldhauser[3], Stephan Hofmann[2], Jannik C. Meyer[1]
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The translation of two-dimensional (2D) materials such as graphene, hexagonal Boron-Nitride (h-BN) or Molybdenum Disulfide ($MoS_2$) into real world applications hinges on controlled growth of the 2D materials and on seamless integration of the 2D materials with other functional non-2D materials such as metals or metal-oxides. The understanding of the 2D growth mechanisms and the structural, chemical and electronic 2D/non-2D interfacing remains however elusive, in particular on the atomically resolved level.

Here, we show how atomically resolved scanning transmission electron microscopy (STEM), combined with bright- and dark-field transmission electron microscopy (TEM), provides critically required mechanistic insights: First, we elucidate non-equilibrium layer stacking and a controlled grain boundary structure in h-BN layers grown by scalable chemical vapour deposition (CVD). Second, we examine atomic layer deposition (ALD) of the important high-k dielectric $HfO_2$ on CVD graphene and identify $HfO_2$ nucleation modes on graphene. Finally we study - as an alternative to CVD - physical vapour deposited (PVD) $MoS_2$ layers on CVD graphene and evidence electron-beam induced $MoS_2$ crystallisation and the possibility of epitaxial $MoS_2$-graphene integration.

### MON 9

### Raman spectroscopy and nanoindentation study of C60 transformation into nanoclustered graphene phase at high pressure/high temperature

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C60 fullerene collapses/transforms at high pressure, high temperature (p,T) to a disordered carbon phase exhibiting a remarkable combination of mechanical properties–high hardness and about 90% elastic recovery after deformation[1]. The transformation mechanism to this phase which is comprised of 7-12 layer graphene clusters with lateral dimension of 2-4 nm (nanostructured graphene phase (NGP)) is still unknown. Here we report on a combined Raman and nanohardness study of a sample where an incomplete C60-NGP transformation was quenched from 8 GPa and 750 °C. In order to obtain information about the structure evolution and mechanical properties of the material on different stages of the phase transition we performed a correlated 2D spectral mapping and nanohardness cartography of selected particles which exhibit signatures of both parent (C60) and NGP phase. Remarkably, already a minor presence of the NGP in the C60 dimer-derived phase across the phase boundary resulted in hardness increase of the latter phase from 2 to 20 GPa reaching finally 35 GPa in pure NGP with an elastic modulus around 200 GPa. A detailed analysis of Raman/nanohardness data is presented and the C60 - NGP transition pathways are discussed.

[1] Chernogorova O, et al. Applied Physics Letters, 104, 043

## MON 10

## Selectively enhanced Raman scattering from molecular thin films between two graphene layers

Nina C. Berner[1], Christian Wirtz[1], Mario Marcia[2], Andreas Hirsch[2], Georg S. Duesberg[1]
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Surface enhanced Raman scattering (SERS) as well as the recently discovered graphene enhanced Raman scattering (GERS) have important implications for the detection of signals that are usually too weak to register.

In this study, we report GERS mapping of monolayer arrangements of perylene bisimide derivatives (PBIs) on CVD graphene. Moreover, we found that in some cases the enhancement is unusually strong if a second layer of graphene is placed on top of the molecular layer. Enhancement factors of the molecules' Raman signals range up to 10. A variety of PBIs were used in the molecular layers, since both their Raman signature as well as their adsorption behaviour on graphene are relatively well studied. Interestingly, only some of the different PBIs exhibit the additional signal enhancement in the graphene "sandwich", but not all of them. This effect appears to apply even if the laser excitation energy is off-resonance for the molecule, which may give some insight into the mechanism of this process.

To our knowledge, this particular type of molecule-selective Raman scattering enhancement has not been reported before, and might prove to be an important step towards the further understanding of the mechanisms behind GERS and GERS-related effects.

## MON 11
## In situ Raman spectroscopy of silica shell formation on colloidal CdSe/CdSe QDs

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The possibility to synthesize colloidal nanocrystals (NC) with a precise control over their size, stoichiometry and crystal structure enables the use in systems like LEDs, solar cells, and biological sensors and markers.
The use as biological marker is of high interest, since the NC are superior with respect to conventionally used dyes in quantum yield, lifetime, narrow PL, and high and broad absorbance. Unfortunately most of the materials used for colloidal NC are toxic and thus not ideal for in vivo applications. One solution can be the capping of the NC in a silica shell, which provides both a chemical boundary to the surrounding as well as making the NC soluble in water without decreasing the PL.
We discuss the influence of the silica shell on the encapsulated CdSe/CdS NC by in situ Raman spectroscopy. In particular, we monitor the synthesis in real time by Raman spectroscopy and compare these measurements with the TEM analysis of aliquots taken at different points of time during the synthesis in order to gather insights on the silica growth mechanism. While the Raman signal of the optically active CdSe core remains almost unchanged, the CdS shell signal shows a defined shift, occurring during the first hours of the synthesis, which is correlated with the reaction speed.

## MON 12
## Charge photogeneration in few-layer $MoS_2$

Tetiana Borzda[1], Christoph Gadermaier[1,2], Natasa Vujicic[3], Peter Topolovsek[1], Milos Borovsak[1,4], Tomaz Mertelj[1], Daniele Viola[5], Cristian Manzoni[5], Eva A. A. Pogna[5], Daniele Brida[6], Maria Rosa Antognazza[7], Francesco Scotognella[5,7], Guglielmo Lanzani[5,7], Giulio Cerullo[5], Dragan Mihailovic[1,2,8]
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Bulk $MoS_2$ is a layered transition metal dichalcogenide, indirect bandgap semiconductor with bandgap about 1.2 eV. Due to strong light-matter interaction optical spectra of $MoS_2$ show strongly bound Wannier-Mott excitons (binding energy is about 0.5 eV). On the other hand, the demonstration of a photodetector based on monolayer of $MoS_2$ with reasonable good characteristics suggests that photoexcitation creates not just strongly bound charge carriers in $MoS_2$.
I present the results of pump-probe spectroscopy on few-layer $MoS_2$. I discuss excitons dissociation to charge carriers in the time scale of 700 fs and also on the efficiency of this mechanism depending on pump energy and different fluences. Also to make exciton dissociation even more efficient we made blends of $MoS_2$ flakes obtained from liquid exfoliation and organic semiconductors. We find both an unexpectedly inefficient combination as well as a highly promising combination where an efficient charge transfer occurs in the first few picoseconds after photoexcitation.

## MON 13
## Stress and Charge Transfer in Uniaxially Strained CVD Graphene

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Mechanical properties of graphene prepared by chemical vapor deposition (CVD) are different from properties of nearly perfect graphene prepared by mechanical cleavage. In this work, we focus on CVD graphene simply supported or embedded in polymer matrix and uniaxially strained using the cantilever beam technique with simultaneous in-situ monitoring by Raman microspectroscopy. The shift rates of the G band are compared to the shift of the 2D band, and to the widths of both bands. In this way, the level of charge transfer doping and strain can be assessed. The strain distribution across the samples varies significantly, owing to the growth and transfer process, which induces wrinkles and faults in the CVD graphene. In simply supported specimens, the stress transfer efficiency is generally very low and the changes in Raman spectra are dominated by variations in the charge transfer originating from the realignment of the domains on the substrate upon the application of strain. In contrast, samples covered with an additional polymer layer reveal profoundly increased stress transfer efficiencies, and the changes of charge doping levels are negligible.

### MON 14
### Ultrafast photo-thermoelectric currents in graphene

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Fast charge carrier relaxation rates and high mobilities make graphene an excellent material for high-frequency optoelectronis. The origin of photocurrents in graphene remains a question of current research, in particular at high frequencies.[1-4] Both built-in electric fields and graphene's high thermopower can give rise to ultrafast photocurrents. In this work, we investigate the photocurrent dynamics of a graphene junction, where two gates control the Fermi-levels individually on both sides of the junction. In particular, we apply an ultrafast photocurrent spectroscopy [3-5] to analyze the photocurrent contributions with a picosecond time resolution.[6] We find that an ultrafast thermoelectric photocurrent dominates, and that the dependence of this ultrafast photocurrent on both gate voltages resembles the expected six-fold sign change of a thermoelectric current as a function of the two Fermi-levels.

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### MON 15
### Raman Radiation Patterns of Graphene

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We report the angular distribution of the G and 2D Raman scattering from graphene on glass by detecting back focal plane patterns. The G Raman emission can be described by a superposition of two incoherent orthogonal point dipoles oriented in the graphene plane. Due to double resonant Raman scattering, the 2D emission can be represented by the sum of either three incoherent dipoles oriented 120° with respect to each other, or two orthogonal incoherent ones with a 3:1 weight ratio. Parameter-free calculations of the G and 2D intensities are in excellent agreement with the experimental radiation patterns. We show that the 2D polarization ratio and the 2D/G intensity ratio depend on the numerical aperture of the microscope objective. This is due to the depolarization of the emission and excitation light when graphene is on a dielectric substrate, as well as to tight focusing. The polarization contrast decreases substantially for increasing collection angle, due to polarization mixing caused by the air-dielectric interface. This also influences the intensity ratio I(2D)/I(G), a crucial quantity for estimating the doping in graphene.

## MON 16
## N-sites for anchoring of noble metal atoms active in formic acid decomposition

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The use of N-doped instead of N-free carbon support for deposition of noble metal atoms, such as Pt, Pd, and Ru, results in an enhancement of catalytic activity of metal in the process of hydrogen production from formic acid. We consider a set of N-doped graphene models with single or two N atoms substituted from carbon atoms at zigzag or armchair graphene edge, vacancy boundary, and in the center. The interaction energies of noble metals with N-sites in graphene network were calculated within density functional theory (DFT) at the pbe/LACVP level. Independently on the type of the N-site the following trend of metal atoms Ru>Pt>Pd occurred according to the strength of the interaction. By comparing this dependence with the catalytic activity of corresponding metals, we conclude that the interaction of metal with the support should be not too strong as for Ru and not too weak as for Pd. The most active site of Pt and Pd for the formic acid decomposition is a single atom attached to a couple of pyridininc N at the graphene edge. Atomic distribution of metals over N-doped carbon support was confirmed by an aberration-corrected HAADF/STEM study.

## MON 17
## Prussian Blue and its analogs as catalyst precursors for the growth of single-walled carbon nanotubes (SWCNTs)

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The unique electronic properties of SWCNTs are directly related to their atomic structure. Achieving chiral-selective growth of SWCNTs is therefore a key element to exploit their properties to their full potential. It has been shown that the size, composition, and structure of the catalyst is of crucial importance in this process. In particular, using bimetallic catalysts is often invoked as an efficient way for gaining selectivity although the role played by a bimetallicity remains rather obscure.

In order to get insight on a bimetallicity driven selectivity, we are studying in this work a nanoalloying effect on the growth by comparing pure Fe and NiFe catalysts. These catalysts are prepared from Prussian Blue analog precursors using a multistep fabrication process based on coordination chemistry and surface chemistry that allows us to control the surface density of the catalyst particles on the catalyst support, as well as their size and composition. Before the chemical vapor deposition growth of the SWCNTs using methane, the catalyst precursor undergoes a pre-treatment at growth temperature to be transformed into the effective metallic catalyst. Particle and tube structure are studied by coupling Raman spectroscopy and transmission electronic microscopy.

## MON 18
## Vibrational response of graphene in the highly-doped regime

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Graphene, an exceptional 2D-material, is expected to superconduct when alkali-metal intercalation is achieved. Alkali-metal intercalation is known to induce high $e^-$ doping levels in graphene, and the influence of doping can be resolved by Raman spectroscopy. However, the complexity and instability of this system have made the study of highly-doped graphene particularly challenging. Here we induced ultra-high doping levels in graphene (up to 1.3eV) by K intercalation. We measured the intrinsic vibrational Raman response of mono- and multi-layer graphene $in-situ$ as a function of doping. We observed a frequency change of the graphene G line that turns into a highly asymmetric Fano line in the highly-doped regime. We found meta-stable and reversible doping stages in graphene where the 2D-line intensity is reduced as a function of doping until it vanishes. We extracted the Fermi energy level from the highly doped graphene obtaining a 1.3eV shift in agreement to ARPES studies. This work is an outstanding approach as a non destructive, versatile, and accurate technique in the study of intercalated graphene. Acknowledgements to the Marie-Curie Point-2014 DRS Fellowship of FU-Berlin.

## MON 19

## Synthesis and characterization of single-walled carbon nanotube silica aerogels

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Aerogels are widely used in scientific and industrial applications due to their large surface areas, ultrafine pore sizes, low densities and extremely low thermal conductivity. We describe the synthesis and characterization of monolithic, ultralow density, optical-grade single and multi-walled carbon nanotube silica aerogels. Materials were characterized with Raman, absorption and photoluminescence spectroscopies and transmission electron microscopy. We investigate optical properties of arc-discharge and larger diameter single-walled carbon nanotubes aerogels. Solution and surfactant-free silica aerogels demonstrate reduced environmental interaction of embedded nanotubes. Optical-grade aerogels are promising for photonics applications.

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## MON 20

## Structural phase transition and superconductivity in MoTe2

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Recently, distorted transition metal ditelluride systems, MoTe2, WTe2 and IrTe2, show fascinating behaviors with high mobility, large magnetoresistance(MR) and Shubnikov-de Haas oscillation having strong spin-orbit coupling. Those distorted transition metal ditelluride series have rather enhanced inter-layer interaction while planar hexagonal TMDs have weak van der Waals interaction. The competition between inter-layer and intra-layer interaction could lead to the phase transition in distorted transition metal ditelluride system. We synthesized 1T'-MoTe2 single crystal using flux method. We conducted high resolution powder x-ray diffraction varying measurement temperature from 10 K to 300 K. We found that the structural phase transition from 1T' to Td structure is occurred around 250 K accompanying the sign change of Hall coefficient. We also observed the superconducting behavior with critical temperature around 2 K. Electrical resistivity shows clear anomalies which might be related with phase transition in MoTe2.

### MON 21

### Probing and Controlling Electronic and Vibrational Coherences in Individual Carbon Nanotubes using Femtosecond Laser Pulse-Shaping

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We report on the coherent control of the electronic and vibrational states of single-walled carbon nanotubes (SWCNTs) at room temperature. In our experiments, we probe and coherently manipulate the electronic level population of individual semiconducting SWCNTs at room temperature using femtosecond laser pulse shaping microscopy [1,2]. The exciton state $E_{11}$ of defect-doped (5,4)-SWCNTs is resonantly excited by a pair of phase-locked 20 fs laser pulses with tunable delay and carrier envelope phase. Here, the photoluminescence (PL) emission of the defect state $E_{11}^{D}$ serves as reporter for the $E_{11}$-population. We show, that light absorption of individual SWCNTs can be controlled within their electronic dephasing time, ranging from 20 to 66 fs for different nanotubes. We find, that this process can be described very accurately by a quantum mechanical two-level system. On a longer time scale of several hundreds of fs, coherent phonon wavepacket oscillations of the radial breathing mode are visible.

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### MON 22

### Reversible functionalization of chemical vapour deposition grown two-dimensional 2H-MoS$_2$ by copper carboxylates

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While transition metal dichalcogenides (TMDs) have received much scientific attention in terms of optimizing their growth and for potential future applications, there has been surprisingly little effort towards their chemical functionalization. Functionalizing these materials makes their already notable properties more tuneable and adaptable towards specific applications. Inspired by previous work on liquid-exfoliated $MoS_2$ [1], we have achieved reversible functionalization of both CVD-grown monolayers and vapor-grown $MoS_2$ thin films using organic copper carboxylates and acidic solutions.

After functionalization, X-ray Photoelectron Spectroscopy (XPS) shows a distinct component in the S 2p spectrum, in agreement with [1]. After treatment with acidic solutions, the $MoS_2$ was found to be defunctionalized. Notably, this entire process was achieved on the semiconducting, thermodynamically stable 2H-polytype of $MoS_2$ where almost all previously reported functionalisation of CVD $MoS_2$ has been possible on the metallic and unstable

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## MON 23
## 1D SiC/graphene nanomaterials –promising scaffolds for bioengineering

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Combustion synthesis (SHS) is the well-known method for nanomaterials production. Among its advantages one may point out the remarkable number of materials possible to design. It starts from the mixture of strong reducer and oxidant and leads to the variety of materials (also metastable). The process is carried out under high pressure (up to 5 MPa) in the reaction chamber and, in average, after initiation by ohmic heating, takes less than few seconds. As nowadays the growing interest in bioengineering materials is observed, the aim of this paper is to present the preliminary results on SHS usefulness in biocompatible nanomaterials production. The following reactants systems have been tested: Si/PTFE/NaCl and Si/CFx in order to obtain graphene flakes and SiC nanowires. The compositions of both materials, after characterization, may be promised for neurons and tissues supports. The process mechanism (thermodynamics, kinetics of wave propagation) and its in situ diagnostics, optimization and control will be also discussed. Ackonwledgement: This research has been supported by NCN grant No. 2012/05/B/ST5/00709.

## MON 24
## Synthesis of Covalently Porphyrin-Functionalized Graphene Nanohybrids Materials

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The modification of the properties of graphene for applications has been a challenging task since the last years. For this purpose, we present a covalent wet chemical functionalization method for graphene layers by reacting them with different porphyrin diazonium salts. Pristine graphite was therefore intercalated with potassium in order to yield charged graphene sheets, which are now chemically activated and very reactive for follow-up reactions. Thereafter, the graphene sheets were covalently functionalized with porphyrins via a diazonium strategy, due to the fact that diazonium compounds are one of the most effective and facile methods for covalent functionalization of carbon materials. For the first time, porphyrin systems could be directly attached to the graphene lattice without any linking group. Thus, it is ensured that the pi-system of the porphyrin is perpendicular to the one of graphene. The successful functionalization of graphene could be proved by scanning Raman spectroscopy, thermogravimetric analysis coupled with mass spectrometry UV-vis and fluorescence spectroscopy. These new graphene-porphyrin nanohybrids materials are promising candidates for photovoltaic devices.

## MON 25

## Finite element simulation of scattering near-field optical microscopy (s-SNOM) measurement of carbon nanotubes

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Finite element simulation is a useful technique in the understanding of the possibilities of s-SNOM measurement method. To gain full insight into the technical and theoretical features, the implementation of the entire measurement setup and numerical data processing steps is important.

Initial validation of the simulation technique was done by comparing simulated and measured data with known analytical calculations [1] on simple spherical gold nanoparticles on SiO2 substrate. Data acquired from the different sources mentioned above showed good agreement indicating the validity of our simulation method. Moving beyond simple configurations we have investigated the more complex carbon nanotube system, for which analytical models are still unknown, making simulation techniques the only way of real exploration. Using the dimensions of actual nanotube bundles, and optical properties of metallic and semiconducting nanotubes, qualitative agreement was found between the computed and measured phase and amplitude values.

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## MON 26
## High visibility Aharonov-Bohm oscillations in graphene rings

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The van der Waals assembly of two-dimensional materials enables the fabrication of graphene encapsulated in hexagonal boron nitride (hBN) in micrometer sized samples with unique electronic properties. The pattering of these samples in the sub-micron scale provides the basis for the observation of a large variety of mesoscopic transport phenomena in graphene-hBN devices. Here, we present low-temperature magneto-transport measurements and tight binding calculations on a high mobility graphene ring. In particular, we discuss phase-coherent transport near or in the quantum Hall regime. We show the presence of Aharonov-Bohm (AB) oscillations over the full range 0-9T of magnetic field. For intermediate magnetic fields, we observe magnetic focusing effects of charge carriers. These resonances are analyzed and reproduced by tight binding simulations and they can be related with the cyclotron radius matching relevant sample dimensions. Finally, we report on the observation of the AB effect in the quantum Hall regime at reasonable high magnetic fields, where we find in some regions strongly enhanced visibility of AB oscillations, and investigate this effect with supporting tight binding calculations.

## MON 27
## 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 [1]. 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 [2]. We propose to use this excellent sensitivity capability to detect and manipulate the nuclear spins of the 13C atoms naturally present in the carbon nanotube. For this,

we use the specific nuclear magnetic resonance protocol developed by Nichol et al. [3] and 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.

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## MON 28

## Electronic properties modulation in 13C/12C twisted bilayer graphene via direct compression

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In the last years, bilayer graphene samples, in which the two graphene layers are not conventionally stacked but relatively rotated, have attracted a wide interest due to their peculiar electronic and optical properties, strongly dependent of the rotation angle [1]. In this work we present the so far unexplored effect of the interlayer distance between graphene sheets (d) on the electronic and optical properties of this new material. In order to modulate d a gem anvil cell is used, coupled to a Raman spectrometer for in-situ characterization [2]. The phenomenon is also theoretically analyzed based on the extended tight binding method [3]. Our combined results prove that the electronic density of states in twisted bilayer graphene can be modulated by changing d, which strongly affects both the intensity and the energy separation of the van Hove singularities.

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## MON 29

## Thermodynamics of pi-stacking functionalization of carbon nanotubes and graphene

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The $sp^2$ configuration of carbon in SWNTs and graphene brings an invaluable handle for pi stacking functionalization[1]. Here, we report on the noncovalent functionalization of both SWNTs and graphene flakes with porphyrin molecules in micellar aqueous suspensions. An efficient energy transfer from the porphyrins molecules to SNWTs was demonstrated through photoluminescence experiments. We carried the kinetic and thermodynamical study of the reaction to extract time constants and Gibbs energies. We show that the reaction can be described by a cooperative adsorption Hill model. The evolution of the Gibbs energy as a function of the nanotube diameter is studied for 16 nanotube chiral species[2], and compared with DFT calculations[3]. The fine control of the reaction allows to reach a monolayer molecular coverage for each nanotube species and for graphene nanosheets.

Finally, by using different surfactant mixtures, we report preliminary results that highlight the role of micelles in the functionalization process.

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## MON 30
## 1D molecular magnets arranged in single-wall carbon nanotubes

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Metal-organic molecular magnets are of great interest because of their unique magnetic properties which arise from interactions between the molecular compounds. The confined nanospace of single-wall carbon nanotubes (SWCNT) allow molecules to be arranged in one-dimensional structures. We study the magnetic, electronic and structural properties of such molecular chains by means of X-ray/UV Photoemission Spectroscopy (XPS, UPS), X-ray Absorbtion Spectroscopy (XAS), X-ray magnetic circular dichroism (XMCD), XRD and SQUID. XRD data analyzed with the Rietveld method suggests that the intermolecular spacing of the chains is dependent on the nanotube diameter. We discuss magnetic ground states, superparamagnetism and possible bulk magnetic ordering of this system as well as the effect of electron doping by potassium intercalation. Our work provides interesting insight into the properties of 1D molecule chains that would pave the way towards advanced molecule-based magnets.

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## MON 31
## Non-equilibrium spin-crossover in copper phthalocyanine

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We demonstrate the non-equilibrium tip induced control of the spin state of copper phthalocyanine on an insulator coated substrate. We find that, under the condition of energetic proximity of many-body neutral excited states to the anionic ground state, the system can undergo a population inversion towards these excited states. The resulting state of the system is accompanied by a change in the total spin quantum number. Experimental signatures of the crossover are the appearance of additional nodal planes in the topographical STM images as well as a strong suppression of the current near the center of the molecule. The robustness of the effect against moderate charge conserving relaxation processes has also been tested.

## MON 32
## Spin lifetimes exceeding 12 nanoseconds in graphene non-local spin valve devices

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We present spin transport measurements on graphene non-local spin valve devices where the electrodes are patterned first and the graphene is subsequently transfered on top using hexagonal boron nitride (hBN). We achieve spin lifetimes of 12.6 ns, spin diffusion length of 30 $\mu$m and charge carrier mobilites of more than $20,000$ cm$^2$/(Vs) at room temperature. Furthermore, we will investigate our contact properties by scanning force microscopy (SFM) and conductive SFM and we will discuss the importance of using large area hBN for the transfer process.
This improvement in the spin transport properties exceeds all current models for contact induced spin dephasing which is one of the main sources of spin dephasing in graphene. Therefore these results pave the way towards probing the intrinsic spin properties of graphene.

## MON 33
## Novel Insights in the Reductive Exfoliation/Funtionalization of Synthetic Carbon Allotropes

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The tuning and optimization of the material properties of synthetic carbon allotropes (SCAs) - like fullerenes, carbon nanotubes, and graphene - for their implementation into applications is an important aspect of current research. For this purpose, the covalent derivatization of SCAs with functional entities has become a frequently used technique. The wet-chemical approach of functionalization relies on alkali metal intercalation as initial activation step in order to generate the negatively charged SCA-ide intermediates. A problem arising from the activation via alkali metal intercalation is that after the addition of the electrophilic trapping reagent, remaining charges on the respective SCA framework lead to undesired side-functionalization reactions. Therefore, we developed a new method to oxidize and to spectroscopically characterize these remaining charges in an inert way.

### MON 34
### High efficiency graded band gap perovskite solar cells

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We report high efficiency graded band gap perovskite solar cells with very large current output and high power conversion efficiencies (PCE) by using simultaneously mixed halides (CH3NH3SnI3 and CH3NH3PbI3-xBrx) perovskite absorber layers. An analysis of the experimental data yields a high fill factor (FF) of $\sim$75% and high short circuit current density (Jsc) of up to 46.2 mA/cm2. These devices provide the highest current output aiming above 20% PCE.

### MON 35
### Controlling the interaction of filled SWCNTs with reactive NO2

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Controlling the interaction between gases and Single-Wall Carbon Nanotubes (SWCNTs) is a key point for sensors made with nano-carbons [1]. Here we present the

latest progress on the understanding of the interaction between nitrogen dioxide and metallicity-sorted ultrapure SWCNTs filled with Ni and Fe [2]. The effect of the different gas dosing on the SWCNTs was measured using UPS, XPS and XAS carried out at SUPERESCA beamline in ELETTRA. The interaction with gas is recognized in the core levels, valence bands and transport measurements. Gas desorption at room temperature was observed, followed by major change in the density of states at the Fermi level. The innovative results help us to get highest selectivity and sensitivity for gas sensing at room temperature.
We acknowledge the financial support by the FWF, EU.

[1] G. Ruiz et al., ACSNano 8, 1375 (2014)

[2] M. Kharlamova et al., Nanoscale 7.4 1383-1391 (2015)

## MON 36

## THz-Time Domain Spectroscopy and IR on MoS2

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In the increasing research field of 2D materials such graphene, Molybdenum disulfide MoS2 attracted a great interest due to potential applications [1] as thin film transistors, light-emitting diodes [2] or photodetectors [3]. Differently than graphene, the existence of a direct bandgap in monolayer MoS2, gives the possibility of performing MoS2 field-effect transistors or optoelectronic devices. We analyzed by THz-Time Domain Spectroscopy (THz-TDS) up to 3THz and infrared (IR) spectroscopy in the range from 350 to 4000 cm-1, CVD obtained MoS2 deposited on a sapphire substrate. From THz-TDS we obtained the transmittance, conductivity and attenuation. From IR spectroscopy on the same samples we deduced the transmittance at IR frequency range. We observed the coherence of both spectroscopic methods. The advantage of THz-TDS method is that we can get significant parameters related to the sample quality without the need of depositing any electrical contacts or sample preparation.

[1] W. J. Zhu, T. Low, Y.H. Lee, H. Wang, et al. Nat. Commun. 2014, 5, 3087.

[2] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, A. Kis, Nat. Nanotechnol. 2011, 6, 146.

[3] O. Lopez-Sanchez, D. Lembke, M. Kayci, A. Radenovic, A. Kis, Nat. Nanotechnol. 2013, 8, 497.

## MON 37

## Growth of SWNTs from alloy catalyst nanoparticles

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Single wall carbon nanotubes are seen as excellent candidates for application in nanoelectronic devices because of their remarkable electronic and mechanical properties. These unique properties highly depend on their structure. Therefore, structure controlled growth of SWNTs are highly desired for the fabrication of SWNT-based electronics.

In this work, we present a new approach based on coordination chemistry and HF-CVD to control the diameter of SWNTs and eventually their chirality. Because of their potential to control the SWNT's chirality, alloy nanoclusters (Fe-Ru, Ni-Ru, Co-Ru) with controlled structure are used as catalyst. Those nanoclusters are prepared by pyrolysis of bimetallic coordination network nanoparticles with a well-defined stoechiometry and narrow size distribution.

The microscopy and spectroscopy analysis demonstrate the high quality of SWNTs. By changing CVD condition, we modulate the semi-conductor percentage from 47% up to 85% according to Raman spectroscopy using three excitation wavelengths. The nanotube were furthermore integrated into high-quality SWCNTs-FET with a $10^6$ Ion/Ioff average ratio.

## MON 38
## Excitons in $MoS_2$ coupled to a Microcavity

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Two-dimensional atomic crystals of transition metal dichalcogenides exhibit attractive optoelectronic properties in the limit of direct band-gap monolayers [1]. In the scope of this work we investigate excitons in monolayer molybdenum disulphide ($MoS_2$) coupled to an optical microcavity. Due to sizeable exciton binding energy and oscillator strength collective strong coupling of monolayer excitons and cavity photons is stable up to room temperature [2]. In our experiments we use a tunable open-access cavity with one curved fiber-based mirror and one planar mirror which supports extended monoalyer $MoS_2$ flakes. This configuration allows us to control the spacing between the cavity mirrors and thereby to explore the coupling strength as a function of the cavity length. We present first evidence for the strong coupling regime and compare the experimental results with simulations. Moreover, lateral scanning enables two-dimensional cavity imaging of extended monolayer flakes to probe variations in the local crystal quality and the dielectric environment.

[1] Xu et al., Spin and pseudospins in layered transition metal dichalcogenides, Nat. Phys. 10, 343 (2014).

[2] Liu et al., Strong light–matter coupling in two-dimensional atomic crystals, Nat. Photon. 9, 30 (2015).

## MON 39

## Quantification of uniaxial strain in monolayer graphene via the Raman 2D' mode

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Accurate and simple local strain assessment in graphene is one of the crucial tasks in device characterization. Raman spectroscopy is often used for that purpose through monitoring of the G and 2D modes. However, the shifts of those two bands might be biased, especially under uniaxial strain, by the effects of charge-transfer doping. Therefore, it is extremely desirable to use another Raman band, less affected by doping, but with a defined and measurable behavior under strain. The Raman 2D' mode [1] is in this sense the ideal feature for the evaluation of strain levels in stretched graphene monolayers, suitable for this task even under different experimental conditions. The sensitivity and accuracy of the approach through 2D' mode [2] is on the same level as through the G mode, however, the clear advantage of the 2D' arises when doping effects are present in the sample.

[1] Narula R. and Reich S. Phys.Rev.B 87, 115424 (2013).

[2] del Corro E., Kavan L., Kalbac M., Frank O. J.Phys.Chem.C 119, 25651 (2015).

## MON 40

## Magnetically confined quantum dots in graphene revealed by scanning tunneling spectroscopy

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Confining graphene's chiral massless charge carriers by carving out nano-structures to circumvent Klein-tunneling suffers from disordered edges, impeding the control of the quasi-relativistic particles. Here, we use the electrostatic potential of an STM tip in combination with an homogeneous magnetic field to confine electrons in graphene without edges[1].

The confinement becomes visible as a fourfold charging sequence at $B > 2$T, as expected from valley and spin degeneracy. Up to 40 charging peaks are observed in the hole and electron sector. The deduced charging energy range is $5 - 10$meV. Characteristic spatial charging patterns, created by potential modulations of the commensurate G on BN[2], are found.

[1] G. Giavaras and F. Nori, PRB 85, 165446 (2012)

[2] C. R. Woods et al., Nat. Phys. 10(6), 451-456 (2014)

## MON 41

## Scanning x-ray microscopy and HRTEM measurements of carbon nanotubes filled with $Er_3N@C_{80}$ fullerenes

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High resolution transmission electron microscopy (HRTEM) is often used to study the structure of nanomaterials. Scanning transmission x-ray microscopy (STXM) is a synchrotron based nano-spectroscopy technique for recording nano-scaled images with chemical and magnetic contrast.

Here we present a combined HRTEM and STXM study of carbon nanotube (CNT) bundles filled with $Er_3N@C_{80}$ fullerenes. The measurements demonstrate that unique CNT bundles can be located and studied with the two techniques. We also obtained erbium M5 edge x-ray absorption spectra from a single bundle. Images recorded on and off resonance provide an erbium map of the sample.

We correlate HRTEM and STXM images of the same nanometer scaled object and discuss the combination of the two techniques.

## MON 42

## Liquid phase exfoliated two-dimensional transition-metal dichalcogenides for electrocatalysis hydrogen evolution application

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[2]CRANN and AMBER

Hydrogen energy is a clean source of energy and is a promising candidates for replacing fossil fuel in the future. Recently two dimensional transition metal dichalcogenides (TMDs) such as MoS2 and WS2 have drawn great attention especially in electrocatalysis and photocatalysis owing to their interesting electronic and optical properties besides their stability and low cost as Pt replacement.

Herein we employed liquid phase exfoliation (LPE) to prepare single and multi-layer nano-sheets for a number of TMDs such as MoS2, MoSe2, MoTe2, WS2, WSe2, WTe2, TaSe2, TaS2, ReS2 and GaS for HER study. Knowing that some of these TMDs suffer from low electrical conductivity, we have designed hybrid electrodes of TMDs nano-flakes mixed with conductive carbon nanotube (SWCNTs). The composite films with certain mass and thicknesses were transferred onto the desire electrodes and their HER activity and other behaviors were studies by various electrochemical techniques in a three-electrode electrochemical cell. The relationship between the flake size, chemical structure and conductivity of nanosheets with their HER activity were studied by comparing different parameter extracted from electrochemical impedance spectroscopic data modelling and Tafel plots.

### MON 43

### Dominant Excitonic Transitions in Molybdenum Dichalcogenides

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Novel two-dimensional materials from the group of layered transition metal dichalcogenides (TMD) have recently attracted scientific interest for their unusual physical properties. An interesting quality is their strong optical response that stems from the quantum confinement of electrons and holes in the quasi-2D geometry. The modified screening strongly enhances the binding of electron-hole pairs leading to binding energies of the lowest-lying excitonic transition of magnitude 0.5 eV in Mo and W based TMDs [1]. Despite this, a closer analysis of the nature of the excitonic transitions contributing to observed absorption peaks is still lacking so far.

We have thus performed ab initio calculations of the theoretical dielectric functions including electron-hole interaction of $MoS_2$, $MoSe_2$, and $MoTe_2$ in both their mono- and bilayer forms and analyzed the k-space representation and spatial extend of the dominant excitons for excitation energies up to 3 eV. Our results suggest that the changes of electronic structure from variation of the chalcogen atoms and interlayer interactions lead to a noticeable change of the fundamental transitions and can be explained by band nesting between valence and conduction bands.

[1] Umeda et al., Nature Materials 13, 1091 (2014)

### MON 44

### Molecular switches on plasmonically active surfaces: Turning off the plasmon resonance

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The electron oscillation in plasmonic particles generates strong localized fields in their close proximity. This phenomenon has been widely exploited for enhanced Raman spectroscopy or plasmon enhanced fluorescence. An emerging plasmonic application is the manipulation of the isomerization behavior of photochromic molecular switches. Here we present an approach to functionalize metal nanoparticles with diarylethene molecular switches via thiol groups. By attaching the photoswitch to the nanoparticle surface we observed a 50% faster forward switching (ring-closure) and a 50% slower backward switching (ring-opening). Interestingly, absorption and scattering by the plasmon resonance disappears after ring closing of the molecule and re-appears after ring-opening.

## MON 45

## Tuning graphene mechanical resonators by linear actuators

Matthias Goldsche[1,2], Gerard Verbiest[1], Shabir Barzanjeh[3], Tymofiy Khodkov[1,2], Jens Sonntag[1,2], Nils von den Driesch[2], Dan Buca[2], Stefan Trellenkamp[2], Christoph Stampfer[1,2]
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Graphene possesses many material properties, such as a low mass density, high Young's modulus and high electron mobility that are well suited for its use in nanoelectromechanical systems. The highly gate tunable conductance enables a full electrical readout of the mechanical motion. However, due to the low bending stiffness of graphene, the transport properties are highly susceptible to strain effects. Here, we present a method to systematically study these strain effects by integrating a suspended graphene flake into a micro actuator that is operational at cryogenic temperatures and compatible with radio frequency measurements. In addition to the usual tuning of doping and strain with a local gate, the micro actuator allows for sole mechanical strain via a capacitive force between a suspended and a fixed part. We measure 3 resonance frequencies using the amplitude modulated down-mixing technique. The quality factors are >2000. Surprisingly, the mechanical coupling between the graphene and the actuator is so strong that 2 of the 3 resonances (around approx. 11 MHz) are only separated by 700 kHz. The third resonance is at approximately 22 MHz. Moreover, we can tune the resonance frequency of the graphene sheet with a local gate and, simultaneously, with the micro actuator.

## MON 46

## Experimental Investigation of Exciton Dispersion Relation in Carbon Nanotubes Determined by Resonant Raman Scattering

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In carbon nanotubes (CNTs) optical properties are dominated by excitons (electron-hole pairs). In CNTs the excitonic binding energy is higher than the thermal energy at room temperatures due to the one-dimensional crystal structure, which leads to strongly pronounced excitonic properties. Though energy levels of CNT excitonic states were experimentally established, the mechanisms of photon-exciton and exciton-phonon coupling remain disputed. In previous works it was reported that the 2D mode in carbon nanotubes is due to double-resonant Raman process. The Excitation-energy dependence was modeled assuming band to band transitions, analogously to other carbon materials but electron-hole coupling was not taken into account. We performed wavelength dependent Raman experiments on chirality-enriched semiconducting CNT species in solution. We studied the position and the intensity of 2D mode with excitation wavelengths from 488 to 730 nm (1.69 to 2.5 eV). The nonlinear dispersion is assigned to a double resonant Raman process, where the exciton is scattered by the phonon between $E_{22}$ and $E_{11}$ states. The saddle like dispersion line shape around the $E_{22}$ transition can be explained by exciton-polariton formation, the strongly coupled state of a photon and an exciton.

## MON 47
## Molecular dynamics simulation of hydrocarbon formation from ferrocene molecules in carbon nanotubes

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Recent Raman studies showed that an appropriate heat treatment of small diameter carbon nanotubes filled with ferrocene molecules results in the formation of hydrocarbon molecules [1, 2]. In order to have deeper insight into possible processes, molecular dynamics simulations were performed. In our study, two different approximations were used. One was the open source code LAMMPS, where all the interatomic interactions – including carbon, hydrogen and iron atoms - were calculated with an appropriate bond order based force field. In the other method – using a self-made code - the carbon-carbon interactions inside the hydrocarbon molecule were calculated with a tight binding method, whereas the interaction between the molecule and the nanotube was taken into account with a Girifalco-potential. In both methods the temperature inside the nanotube was controlled by a Nosé-Hoover thermostat. The three main parameters influencing the reaction products are the diameter of the nanotube, the density of the ferrocene molecules and the temperature.

[1] Kuzmany et al., Phys. Status Solidi B 252, 2530 (2015)
[2] Kürti et al., Phys. Status Solidi B 252, 2541 (2015)

## MON 48
## The dependence of electrical characteristics of CNFETs on Cr adhesion layer thickness

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Electrical characteristics of individual single-walled carbon nanotube (SWCNT) based field-effect transistors (CNFETs) are significantly affected by the electrical contacts. To ensure that the electrodes adhere well to dielectric substrates, an adhesion metal layer in addition to the electrode noble metal is often used [1]. In this work we present the effect of the Cr adhesion layer thickness on the transfer characteristics of Cr/Au-contacted devices. 76 individual SWCNT-based CNFETs were fabricated by photolithography on four chips with different Cr thicknesses. We show that 0.4 nm Cr deposit already has an impact on the charge carrier transport in Schottky-barrier-modulated CNFETs. The ratio of the p- and n-branch on-resistances increased by 8 times when the Cr thickness increased from 0 to 8 nm. We observed long lifetime of devices (longer as 90 days) even for non-passivated CNFETs using Cr layer thinner than 2 nm in Cr/Au contacts. Our results show a direct relationship between the Cr adhesion metal thickness and CNFET type and lifetime, suggesting that it must be carefully considered in CNFET device fabrication.
[1] W. Liu et al., Beilstein J. Nanotech. 5 (2014) 2202

## MON 49
## Point contacts in encapsulated graphene

Clevin Handschin[1,2], Bálint Fülöp[1,3], Péter Makk[1], Sofya Blanter[1], Markus Weiss[1], Kenji Watanabe[4], Takashi Taniguchi[4], Szabolcs Csonka[3], Christian Schönenberger[1,2]
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We present a method to establish inner point contacts on hexagonal boron nitride (hBN) encapsulated graphene heterostructures with dimensions as small as 100 nm by pre-patterning the top-hBN in a separate step prior to dry-stacking [1,2]. 2 and 4-terminal field effect measurements between different lead combinations were performed and are in qualitative agreement with an electrostatic model assuming point-like contacts. The measured contact resistances are 0.5-1.5 k$\Omega$ per contact, which is quite low for such small contacts. By applying a perpendicular magnetic fields, an insulating behavior in the quantum Hall regime was observed, as expected for inner contacts. The fabrication procedure is compatible with high mobility graphene structures and contacts which have dimensions on the order of 30 nm or even smaller. Consequently, this technique opens up the possibility to realize several electron optics analogues, in particular lensing experiments.

[1] C. Handschin et al. Appl. Phys. Lett. 103 18318 (2015)

[2] L.Wang et al. Science 313 614 (2013)

## MON 50
## Carbon nanotube encapsulated dye molecules probe surface-enhanced Raman scattering

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Surface-enhanced Raman scattering (SERS) is the giant increase in the Raman signal of molecules by surface plasmons of metal nanostructures. Even after 40 years of SERS, quantifying enhancement and refining our understanding of the underlying mechanism is challenging: the exact location of a molecule in a SERS hotspot, the orientation of its transition dipole and chemical interactions with the metal remain impossible to control experimentally. Here we overcome these limitations by probing SERS with aligned $\alpha$-sexithiophene (6T) molecules encapsulated inside carbon nanotubes. The tubes (i) carry the 6T into SERS hotspots by directed dielectrophoretic deposition, (ii) render them chemically inert and (iii) simultaneously define and reveal their location and orientation. We access SERS enhancement with unprecedented accuracy, both experimentally and by simulations according to the electromagnetic theory (EM) of SERS. The experimental enhancement exceeds the calculated value by two orders of magnitude and – in the absence of chemical enhancement - calls for treating SERS beyond the EM approach, e.g. within perturbation theory, where the plasmon forms an integral part of the Raman process.

## MON 51
## Self-propagating high-temperature fast reduction of magnesium oxalate to novel nanocarbons

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Combustion synthesis, which does not require vacuum facilities, has been reported as a cost-effective technique to produce many novel ceramic nanostructures such as nitrides, carbides and intermetallic compounds. Herein, we report such extremely fast chemical transformation of magnesium-magnesium oxalate mixtures into solid products containing MgO and different nanocarbons. Despite a wide range of molar ratios of reactants all combustions, carried out in Ar at 10 bar, were successful. The solid products were chemically purified (leaching of MgO) and characterized using XRD, SEM/EDS, TEM, TGA, and Raman spectroscopy. The residue contained mostly layered (ca several nm thick), petal-like carbon nanostructures and some carbon-coated MgO nanocrystallites.

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## MON 52
## Imaging ellipsometry of individual graphene oxide flakes

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Graphene oxide (GO) is considered a promising material for some optoelectronic applications, e.g. solar cells. However, there are contradictory results in the literature regarding basic optical characteristics of GO like the magnitude of the optical band gap and its direct vs. indirect nature. Measurement of transmittance and reflectance of a thin film is a standard technique for determining material´s optical properties. But in the case of GO, such a thin film is made of a huge amount of individual GO flakes making essentially each GO sample unique. The problem could be overcome by measuring a single GO flake.

Here we show that this goal can be indeed achieved by combination of a proper preparation technique and imaging ellipsometry. We have deposited single GO flakes with a lateral size of tens of micrometres on a substrate by a Langmuir-Blodgett technique. Lateral resolution of our imaging ellipsometer down to 2 $\mu$m enables us to determine the optical constants of the individual flakes. We have focused on a dependence of indices of refraction on the GO thickness and oxidation/reduction level. From that, general implications for the optical properties of GO are drawn.

## MON 53
## Study of Local Deformation of 2D-Materials by Dual-Probe AFM/STM

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Strain engineering is a very promising tool for changing the physical properties of 2D materials. In recent years, different experimental and theoretical studies have shown that graphene and other 2D materials (e.g. $MoS_2$) are very sensitive to strain regarding charge transport, electrical and phononic band structure, etc. Up to now, most experimental methods for the investigation of strain induced effects on 2D materials are based on either employing MEMS devices or applying uniaxial strain by using a flexible substrate. In these experiments, one is either limited in sample size due to the MEMS structure or has to account for the underlying substrate. In this work, I will show recent results of a novel type of strain measurement based on a Dual-Probe AFM/STM setup, where the two probes approach a suspended membrane from opposite sides. With this setup, we can explore local deformations of 2D materials caused by an approaching STM tip, while performing AFM measurements on the same site. By inverting this method, i.e. pushing or pulling with AFM during STM imaging, we can explore the effect of local strain on the electronic properties of the 2D materials.

| | |
|---|---|
| 08:30 – 09:00 | N. McEvoy, Dublin<br>*Growth of Transition Metal Dichalcogenides by Thermally Assisted Conversion* |
| 09:00 – 09:30 | S. Hofmann, Cambridge<br>*Towards integrated manufacturing of 2D materials* |
| 09:30 – 10:00 | G. Abellán, Erlangen<br>*Chemical Functionalization of 2D Materials* |
| 10:00 – 10:30 | coffee break |
| 10:30 – 11:00 | H. Cheng, Shenyang<br>*CVD Growth of High-Quality 2D Transitional Metal Sulfides and Carbides* |
| 11:00 – 11:30 | G. Bepete, Pessac<br>*Single layer graphene in water* |
| 11:30 – 12:00 | E. Vázquez, Ciudad Real<br>*Graphene in water: Preparation and Applications* |
| 12:00 – 17:00 | mini workshops |
| 17:00 – 18:30 | Dinner |
| 18:30 – 19:00 | N. Martín, Madrid<br>*New Organic Compounds for Photovoltaic Devices* |
| 19:00 – 19:30 | M. Halik, Erlangen<br>*Self-assembled carbon electronics* |
| 19:30 – 20:00 | M. Loi, Groningen<br>*Polymer-SWNT hybrids: toward high performance field effect transistors* |
| 20:00 | Poster II |

### 08:30

## Growth of Transition Metal Dichalcogenides by Thermally Assisted Conversion

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Two-dimensional transition metal dichalcogenides (TMDs) have moved to the foreground of the research community owing to their fascinating properties which make them of great interest for both fundamental studies and emerging applications. Thermally assisted conversion (TAC) of predeposited transition metal films is a method which shows great promise for the scalable and industry-compatible synthesis of these materials. Here we outline the production of an assortment of TMDs by TAC, including $MoS_2$ and $WSe_2$. The potential of TAC derived TMDs for various applications in the realm of electronics and energy will be discussed. The fabrication of high-performance gas sensors, consisting of $MoS_2$ channels, will be described. The fabrication of large-scale heterojunction diodes, formed by transferring $MoS_2$ onto Si, will be outlined. Additionally, the low-temperature synthesis of $PtSe_2$, its characterisation by Raman spectroscopy and its use in heterojunction diodes, will be discussed.

## 09:00

## Towards integrated manufacturing of 2D materials

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The commercial potential of 2D materials hinges on the development of growth and integration techniques that are scalable and allow an adequate level of structural control. Chemical vapor deposition (CVD) now dominates the carbon nanotube market and rapid progress is being made to develop it also for the manufacture of graphene and other 2D materials. A key challenge thereby is to increase the level of structural growth selectivity and control. With a focus on diverse applications in the electronics and display industry, we are developing integrated process rationales for these nanomaterials that are informed by a fundamental understanding of the catalytic growth process.

This talk will focus on the scalable CVD of monolayer hexagonal boron nitride (h-BN) single crystals and our current understanding of the formation mechanisms of such compound 2D material on various catalyst systems [1,2]. Strategies for controlling the number of layers, stoichiometry, and crystal structure, i.e. domain size, connectivity, and orientation, will be compared to graphene CVD [3-5], and the potential of the direct CVD of various 2D heterostructures discussed. The talk thereby will also outline current challenges for integrated manufacturing and industrial device integration of these 2D materials [6].

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7. Kidambi et al., Appl. Phys. Lett. 106, 063304 (2015).

## 09:30

## Chemical Functionalization of 2D Materials

Gonzalo Abellán[1,2], Frank Hauke[1,2], Andreas Hirsch[1,2]
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Chemical functionalization of graphene (G) and related 2D materials is of fundamental interest and opens the door to unprecedented materials applications. Although the chemistry of G has just begun to start, several pathways towards covalent and non-covalent functionalization have been developed. Moreover, other 2D materials like layered double hydroxides (LDH), transition metal dichalcogenides (TMDC) or black phosphorus (BP) have emerged in the last years attracting a considerable level of attention. Herein, we will present a rational approach towards the exfoliation and functionalization of G, LDH, molybdenum disulphide (MoS2) and BP, involving different approaches. With respect to G, we will discuss its exfoliation, functionalization and processing using tailor-made perylenes and metal graphenides. Concerning LDH, we will show the last efforts we made towards their exfoliation and applications. Among TMDCs, we will explore the basal-plane functionalization of chemically exfoliated MoS2. Finally, in the case of BP –the newest member of the 2D family– we will present a series of novel results about its chemical exfoliation, stability and functionalization via molecular doping.

### 10:30

## CVD Growth of High-Quality 2D Transitional Metal Sulfides and Carbides

Chuan Xu[1], Yang Gao[1], Libin Wang[2], Zhibo Liu[1], Xiu-Liang Ma[1], Dong-Ming Sun[1], Zhi-Yong Zhang[2], Lian-Mao Peng[2], Ning Kang[2], Wencai Ren[1], Hui-Ming Cheng[1]
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Like graphene, large-size high-quality two-dimensional (2D) crystals are essentially important for investigating new physics and properties in the 2D limit, and for many fascinating applications in particular electronics and optoelectronics. 2D transition metal sulfides (TMSs) and carbides (TMCs) are a large family of materials with many intriguing properties and applications. Here we report the growth of large-size high-quality single-crystal monolayer $WS_2$ domains and ultrathin $\alpha$-$Mo_2C$ crystals by ambient-pressure CVD. We found that, similar to the CVD growth of graphene on copper, the catalytic activity of gold together with its low solubility for tungsten allows the self-limited catalytic surface growth of a uniform monolayer of $WS_2$. On the other hand, the CVD process is versatile for the fabrication of high-quality 2D TMC crystals and, for example, ultrathin $\alpha$-$Mo_2C$, WC and TaC crystals have been fabricated. These ultrathin TMC crystals have some interesting physical properties such as superconductivity.

### 11:00

### Single layer graphene in water

George Bepete[1,2], Eric Anglaret[3], Carlos Drummond[1,2], Alain Penicaud[1,2]
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[2]Universite de Bordeaux 1
[3]Univ. Montpellier-II, Laboratoire Charles Coulomb (L2C)

Graphite intercalation compounds can be readily exfoliated down to single layers in aprotic solvents due to the favorable entropic contribution of dissociating counterions, yielding graphenide solutions. The resulting graphenide solutions are prone to re-aggregation after oxidation and must be handled in a dry, oxygen-free environment. In this study we show that homogeneous air-stable dispersions of single layer graphene in water with no surfactant added can be obtained by mixing air-exposed graphenide solutions in tetrahydrofuran (THF) with water under certain conditions and evaporating the organic solvent.

In situ Raman spectroscopy of this single layer graphene in water show bands at 1343, 1586, 1620 and 2681 cm-1 corresponding to the D, G, D' and 2D bands of graphene respectively. The 2D band at 2681 cm-1 is well fitted with a sharp lorentzian line ($\sim$28 cm-1) which is a hallmark of single layer graphene. Coatings on glass substrates from these graphene dispersions have conductivities of up to 30 kS/m.

### 11:30

## Graphene in water: Preparation and Applications

Ester Vázquez[1]
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Graphene is considered the ultimate material for applications in many fields, from electronics to composites and biosensors. Biological studies on graphene and graphene oxide are also currently underway in many laboratories. Large amounts of exfoliated graphene are therefore necessary for solution studies and applications in water and organic solvents.

Graphene is usually prepared by the well known scotch tape technique or by CVD. As such, graphene cannot be dispersed in water or biological media, owing to its complete insolubility. Novel ways to prepare dispersible graphene in water are very much needed. Ball milling of graphite in the presence of melamine, developed in our labs, has proven a method of choice to exfoliate graphite and generate dispersions of few-layer graphene in many solvents, including water.

During this talk, we will discuss (i) optimized ways to generate graphene in solvents using ball milling; (ii) the use of graphene dispersions in water for the preparation of hybrid hydrogels as new electroactive scaffolds with self-healing capacity.

## 18:30

## New Organic Compounds for Photovoltaic Devices

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Energy is currently the most important problem facing mankind. Photovoltaic (PV) solar cells are currently a hot topic in science, and different semiconducting materials (inorganic, organic, molecular, polymeric, hybrids, quantum dots, etc.) have been used for transforming sun light into chemical energy. Photo- and electro-active organic materials are promising due to the possibility of processing from solution, affording lighter, cheaper and flexible all-organic PV devices. The design of new organic functional molecules able to harvest sun light and efficiently undergo photon to current energy conversion processes is at the forefront of chemical challenges. In this presentation, the recent advances on fullerene derivatives as n-type materials as well as on hole transport materials in perovskites solar cells is presented in a systematic way through the variety of organic compounds synthesized in our research group.

## 19:00

## Self-assembled carbon electronics

Marcus Halik[1]
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Selective self-assembly of electronically active materials provides an enabling technique in low-cost electronics [1]. Thereby region-selectivity (right in place in device structures) as well as defined stacking capability can be realized by applying directing functionality of substituents.

Concepts have been developed and validated for 0D-fullerenes, 1D-carbon nanotubes and 2D-graphene in order to self-assembly them with precise region-selectivity and integrate them in devices [2]. The package density and the orientation of the carbon materials strongly correlate to their electrical performance and can be tuned by varying the self-assembly driving forces [3-5].

Additionally first results on defined inter-carbon architectures will be discussed based on selective reactions of particular designed materials adapted from nanoparticle assembly [6].

References:

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[6] S. H. Etschel et al. Angew. Chem. Int. Ed. 54 (2015) 9235

### 19:30

### Polymer-SWNT hybrids: toward high performance field effect transistors

Maria Antonietta Loi[1]

[1]Zernike Institute for Advanced Materials, University of Groningen, Groningen

Although many techniques have been developed in the past years to select semiconducting single-walled carbon nanotubes (SWNTs), the so-called conjugated polymer wrapping is one of the most promising and powerful selection strategies. The procedure involves de-bundling and dispersion of SWNTs by wrapping semi-flexible conjugated polymers, around the SWNTs, and results in the SWNT selection by diameter and helicity. Hereby, the conjugated backbone of the polymers interacts with the two-dimensional, graphene-like surface of the nanotubes, the solubilizing alkyl side chains of optimal length support de-bundling and dispersion in organic solvents.

In my presentation I will discuss as the careful structural design of the conjugated polymers allows for a selective and preferential dispersion of SWNTs of different diameters, and of specific helicity. Furthermore I will show that the efficiency of this polymer-assisted selection is confirmed by the performance of field-effect transistors fabricated with the hybrid ink.

## TUE 1

## Secondary interference from trigonal warping in clean carbon nanotubes

A. Dirnaichner[1,2], M. del Valle[2], K. Götz[1], F. Schupp[1], N. Paradiso[1], M. Grifoni[2], A. K. Hüttel[1], Ch. Strunk[1]
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[2]Institute for Theoretical Physics, Universität Regensburg, Regensburg

We investigate experimentally and theoretically a Fabry-Perot resonator based on a clean carbon nanotube. The trigonal warping of the Dirac cones away from the charge degeneracy point leads to a superstructure in the interference pattern. This secondary interference results from the presence of the valley degree of freedom. Single wall carbon nanotubes can be classified to be either zigzag, armchair, zigzag-like, or armchair-like. In any armchair case two interferometer channels with different wave vectors exist; specifically in the armchair-like (chiral with finite-$k_{||}$ Dirac point) nanotube case these two channels additionally mix on reflection at the interferometer ends. The wave vector difference depends on the chiral angle; this way we can use the resulting slow modulation of the average conductance to estimate the chiral angle of the measured nanotube. Measurements on an ultraclean, long and suspended carbon nanotube device at millikelvin temperatures are complemented with tight binding calculations of the transmission for specific chiralities and analytic modelling.

## TUE 2

## Light emission from all $MoS_2$ p-n devices

Achint Jain[1], Palash Bharadwaj[1], Markus Parzefall[1], Lukas Novotny[1]
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Semiconducting 2D TMDCs such as $MoS_2$, $WSe_2$, etc. exhibit a direct bandgap in the visible region which makes them an attractive candidate for optoelectronic applications like photodetection and LEDs [1]. Here we report light emission from an all $MoS_2$ p-n device. P- and n-doped $MoS_2$ flakes obtained by mechanical exfoliation from bulk crystals are stacked together on a Si-$SiO_2$ substrate to form a gate controlled p-n homojunction [2]. The device behaves as a forward rectifying diode and exhibits electroluminescence under high forward bias. The light emission originates from the A ($\sim$ 673 nm) and B ($\sim$ 628 nm) direct excitonic transitions of $MoS_2$ in good agreement with the PL spectrum. We also studied fully 2D $MoS_2$ p-n devices on glass substrates using multi-layer graphene and h-BN as the back gate electrode and dielectric respectively [3] and observed backward diode behavior.

[1] D. Lembke, S. Bertolazzi, and A. Kis. *Acc. Chem. Res.* **48**, 100-10 (2015).

[2] J. Suh, *et al. Nano Lett.* **14**, 6976-82 (2014).

[3] N. Flöry, *et al. Appl. Phys. Lett.* **107**, 123106 (2015).

## TUE 3
## In situ Study of Metal Induced Crystallization Processes for Low-Dimensional Materials Synthesis

Robert Wenisch[1,2], Daniel Janke[1], Irene Heras[3], René Heller[1], Daniel Hanf[1], René Hübner[1], Frans Munnik[1], Sibylle Gemming[1,2], Matthias Krause[1]
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Metal induced crystallization (MIC) is a promising technique for low-temperature thin film transistor fabrication and graphene synthesis. In MIC, a transition metal catalyzes the crystallization of the amorphous phase of a group IV element by bond screening near the interface and facilitation of nucleation. So far, in situ studies have been performed using X-ray diffraction, which is sensitive to the degree of crystallinity. In situ Rutherford backscattering spectrometry has the advantage of elemental depth resolution and time resolved tracking of diffusion and layer exchange processes. Graphene formation through MIC has been demonstrated with an a-C/Ni layer stack [1].

As a model system for MIC, the Si/Ag bilayer system is studied here. The Si/Ag layer stacks are annealed at temperatures of 380 to 700 °C. Depth profiles of the elements are investigated by in situ RBS. Their analysis reveals the diffusion kinetics of the elements. The changes in the phase structure are explored by in situ Raman spectroscopy. Both the quick initial nucleation and ensuing growth processes are investigated.

[1] Weatherup et al., Nano Letters 13, pp. 4624 (2013)

## TUE 4
## Active hydrogen evolution reaction over MoTe2 and WTe2

ByungDo Ji[1], Jinbong Seok[1,2], Jun-Ho Lee[3], Suyeon Cho[2], Hyo Won Kim[4], Young Hee Lee[1,2], Young-Woo Son[3], Heejun Yang[1]
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Efficient hydrogen evolution reaction (HER) is a solution for next generation clean energy source without carbon emission by using fossil fuels. For industrial applications, active electrochemical catalysts are strongly demanded for the HER. Noble metals such as platinum are excellent catalysts for HER; however, there have been many researches to replace the platinum due to its high cost. Recently, transition metal dichalcogenides (TMDs) with diverse physical and electrical properties are rising as a promising catalyst. But engineering surface atoms, structuring optimized catalysts of TMDs, to improve electrochemical performances remains as an issue. Here, we report active HER performances by semi-metallic 1T'-MoTe2 and 1T'-WTe2 single crystals with naturally given surface structuring, Peierls-type lattice distortions. Our MoTe2 and WTe2 studies demonstrate 1) turnover frequency of 0.14 s-1, similar to platinum, 2) Tafel slope of 22 mV per decade and 3) exchange current density 1.0 mA/cm2. First-principles calculations and STM studies explain the result by a lattice distortion and local charge density distribution at Te sites.

## TUE 5

## Nanoscale measurements of unoccupied band dispersion in Van der Waals materials

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The properties of any material are fundamentally determined by its electronic band structure. The occupied bands, that is, the filled electron states below the Fermi level, can be routinely measured. However, it is remarkably difficult to characterize the empty part of the band structure experimentally. Here, we present direct measurements of unoccupied bands of monolayer, bilayer and trilayer graphene. To obtain these, we introduce a technique based on low-energy electron microscopy (J. Jobst et al. Nature Communications 6, 8926 (2015)). It relies on the dependence of the electron reflectivity on incidence angle and energy and has a spatial resolution $\sim$10 nm, which is five orders of magnitude better than other techniques. The method can be easily applied to other nanomaterials such as van der Waals structures that are available in small crystals only. We demonstrate this for exfoliated few-layer hexagonal boron nitride.

## TUE 6

## Formation mechanism of s-SWCNTs and m-SWCNTs synthesized by a pulsed arc-discharge process

Oliver Jost[1]
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The pulsed arc-discharge synthesis of Single Walled Carbon Nanotubes (SWCNTs), as developed by Fraunhofer, is able to synthesize kg quantities of SWCNTs per day, with the only by-products being small graphene flakes and passivated metal catalyst particles. Evaporation-grown SWCNTs like those synthesized by the pulsed arc-discharge process are well known to feature a comparatively low number of structural defects including point defects. In particular interesting is a proper control of the type of SWCNTs i.e. the preferred or even exclusive growth of either semiconducting SWCNTs (s-SWCNTs) or metallic SWCNTs (m-SWCNTs) with a narrow diameter distribution and dozens of grams of them per day. To synthesize 100% s-SWCNTs and roughly 90% m-SWCNTs, a number of experimental conditions need to be in place. Experiment shows a clear picture for the impact of different synthesis parameters which is not surprising as evaporation-based SWCNT growth proceeds in near-equilibrium. This allows to draw an extensive set of conclusions regarding the formation mechanism leading to such a large-scale synthesis of s-SWCNTs or m-SWCNTs.

## TUE 7

## Towards biomedical sensing with chemically functionalized graphene FETs

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Graphene field-effect transistor (GFET) biosensors can intrinsically possess a very high sensitivity up to the fM level. However, this sensitivity is difficult to achieve in combination with high selectivity and specificity of the biomolecular binding events. Thus, covalent functionalization of GFETs results in impairing the electronic structure of graphene, which significantly reduces the device mobility. The functionalization of graphene via physisorption typically causes larger distances between the analyte and graphene plane, which reduces the number of charge carriers induced in graphene per binding event. Both effects reduce sensitivity of GFET biosensors. To overcome these problems, we employ ultrathin ($\sim 1$ nm) dielectric carbon nanomembranes (CNMs) to chemically functionalize GFETs without impairing the electronic performance. A CNM is placed on top of graphene in the manner of all-carbon van der Waals heterostructures and acts as an analyte-specific electrochemical transducer [1]. We present and analyze the electronic characteristics of the fabricated hybrid CNM/graphene FET arrays.

[1] M. Woszczyna et al. Adv. Mater. 26, 4831 (2014)

## TUE 8

## Raman spectroscopy 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 $MX\text{-}TX_2$ 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 $CrS_2$ [1]. 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 [2]. We investigate the vibrational properties of MLC nanotubes via Raman spectroscopy and discuss the results regarding previously published TEM methods.

[1] L. S. Pancharkarla et al., J. Phys. Chem. Lett. 5, 3724-3736 (2014)
[2] L. S. Pancharkarla et al., Angew. Chem. 126, 7040-7044 (2014)

## TUE 9

## Picosecond photocurrents in single-walled carbon nanotubes

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The exciton dynamics in carbon nanotubes are typically detected in a time-resolved way by optical techniques such as the transient absorption technique and the time-resolved photoluminescence spectroscopy. Both methods focus mainly on the dynamics of localized charge carriers within the carbon nanotubes. Many questions remain concerning the separation and the transport of photogenerated charge carriers to source and drain leads in an optoelectronic device structure. We address these questions by an ultrafast photocurrent spectroscopy, which is based on an on-chip THz time domain spectroscopy [1]. We find a combination of an optically induced ultrafast displacement current and interband charge-carrier recombination processes to dominate the ultrafast photocurrent of the single-walled carbon nanotubes [2]. We further discuss inter-subband relaxation processes after the optical excitation [3].

We acknowledge financial support from the ERC-grant “NanoREAL” and the DFG excellence cluster “Nanosystems Initiative Munich” (NIM).

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[2] L. Prechtel et al., Nano Letters, 10, 1021, (2011).
[3] C. Karnetzky et al. (2016).

## TUE 10

## Room temperature proximity induced ferromagnetism in graphene-YIG devices

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Several methods for introducing ferromagnetism in graphene have been reported such as functionalization with adatoms, introduction of defects and shaping with

zigzag edge formation. In practice all these approaches imply the modification of the graphene surface and leads to a substantial degradation of its transport properties. A less invasive and more robust method is to transfer graphene onto an insulating ferrimagnetic substrate [1].
In this work we study the spin transport in graphene monolayer transferred on top of Yttrium Iron Garnet (YIG) [2]. Being in the vicinity of YIG, graphene adopts the exchange interaction and becomes ferromagnetic even at room temperature. The resulting exchange field influences directly the spin transport in the channel by causing an additional spin precession. We model the observed spin transport with modified Bloch diffusion equation and extract a value of 200 mT for the exchange field. Our results show that the exchange field can be used to control spin currents in graphene which is of practical interest for novel spintronics devices.

[1] Z.Wang et.al., PRL 114, 016603 (2015)
[2] J.C. Leutenantsmeyer et. al., submitted.

### TUE 11

## Hall measurements in metallic single walled carbon nanotube networks with ionic liquid gating

Hideki Kawai[1], Kai Hasegawa[1], Kazuhiro Yanagi[1]
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Single walled carbon nanotubes (SWCNTs) significantly change their electrical, optical, and thermoelectric properties depending on their Fermi level [1][2]. Electrical transport mechanisms in their networks significantly changes as results of high-density carrier injections. In such a case, carrier mobility should also be significantly changed by carrier injections. A lot of studies have reported the temperature dependence of electrical conductivity of SWCNT networks. However, relationships between the carrier mobility, temperature and the amount of injected carrier have not been clarified yet. In our research, to reveal how the carrier mobility changes as a function of carrier injections, we performed Hall measurement of metallic single-wall carbon nanotube networks in a situation where the amount of injected carriers was well controlled by ionic liquid gating. Detaille will be discussed in the poster.

Reference:
[1] Yanagi et al., Adv. Mater. 23, p2811(2011),
[2] Yanagi et al., Nano Lett. 14, p6437(2014)

### TUE 12

## Inner tube growth properties and electronic structure of metallocene-filled single-walled carbon nanotubes

Marianna V. Kharlamova[1], Christian Kramberger[1], Markus Sauer[1], Kazuhiro Yanagi[2], Takeshi Saito[3], Hidetsugu Shiozawa[1], Thomas Pichler[1]
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The filling of single-walled carbon nanotubes (SWCNTs) with metallocene molecules opens a way of fine tuning their electronic properties and formation of double-walled carbon nanotubes (DWCNTs) [1]. In the present work, we carried out the synthesis of nickelocene- and cobaltocene-filled SWCNTs [2] *via* the gas phase method and transformed them to DWCNTs *via* thermal annealing in vacuum. We studied the time- and temperature-dependent inner tube growth by *in situ* Raman spectroscopy. The rates and activation energies of the growth of individual-chirality inner tubes were calculated and their dependence on the tube diameter and metal type was revealed. We performed the investigation of the electronic properties of the nickelocene-filled semiconducting and metallic SWCNTs by photoemission spectroscopy. It was shown that the doping level of nanotubes can be tailored precisely and switched from *n*- to *p*-type by annealing. The changes in the doping level were found to depend on the metallicity type of SWCNTs.

The work is supported by FWF.

[1] M.V. Kharlamova, Prog. Mater. Sci. (2015), DOI: 10.1016/j.pmatsci.2015.09.001

[2] M.V. Kharlamova et al., Nanoscale 7, 1383 (2015)

## TUE 13
## Electron diffusion-driven structural phase transition in MoTe2

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Two-dimensional layered transition metal dichalcogenides (TMDs) have attracted academic interests by their diverse lattice structures producing novel electrical, physical and mechanical properties. In particular, MoTe2, a group 6 TMD, has semiconducting 2H and semimetallic 1T' phases. The structural phase transition between 2H and 1T' phases in MoTe2 has been studied by various methods since the small energy difference between 2H- and 1T'- MoTe2 ($\sim$30 meV) easy.

Here, we report a phase transition of MoTe2, with a characteristic length of $\sim$100 nm, by contacting the MoTe2 to Ca2N which is a two-dimensional electride with low work function of 2.6 eV. When we exfoliated 2H-MoTe2 flakes on the Ca2N, the structural phase transition occurred from 2H to 1T' phases. The phase transition was confirmed by Raman spectroscopy, X-ray photoemission spectroscopy and frictional force microscopy. Electrons in Ca2N were diffused into the MoTe2 due to their large work function difference ($\sim$1.8 eV) and the diffused electrons generated the phase transition.

## TUE 14
## Field emission from single-wall carbon nanotubes filled with CuCl

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[2]A.M. Prokhorov General Physics Institute, Moscow, Russia
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A substantial shift of Fermi level down into the valence band has been demonstrated recently for single-wall carbon nanotubes (SWCNTs) filled with CuCl by gas-phase technique (Fedotov et al., PSS B, 2014). The energy level shift may be assigned to variation of work function (WF) at nanotubes surface. Comparative field emission studies were performed in this work for the films of doped and pristine SWCNTs to identify the difference of their WFs. The FE measurements were performed using a flat phosphor screen technique and scanning anode FE microscopy. It was found that emission threshold field does not change with CuCl doping. At the same time other FE parameters such as the slope of Fowler-Nordheim plot demonstrated significant variations. The results of FE measurements and other characteristics of SWCNT films obtained with SEM, TEM, optical absorption and Raman are discussed to reveal a possible mechanism of electronic properties variation for SWCNT after their filling with CuCl. The work was supported by Russian Science Foundation grant 15-02-30041.

## TUE 15
## Electrochemical charging of the suspended single-layer graphene membrane

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In-situ Raman spectroelectrochemistry has been applied to study chemical vapor-deposition-grown single-layer graphene suspended on a patterned SiO2/Si substrate. The SiO2/Si substrate is known to dope graphene, thus the substrate can significantly influence the properties of graphene during electrochemical charging. Raman spectroscopy is a versatile and efficient tool to study the electronic properties of graphene. In this study we focused on the behavior of the Raman bands of the suspended graphene during applying of electrode potential. Generally, the doping of graphene leads to a shift of the Fermi level, which is reflected in a change of Raman spectra. We analyzed the change of the Raman intensity of the G and G' modes as a function of electrode potential for suspended graphene and we compared the results to those obtained for the same graphene sample on substrate. Because of elimination of the influence of supporting substrate we have been able to achieve more efficient doping of graphene by applied electrode potentials.

## TUE 16

## Electrochemical performance of MoS2 based composite materials

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Electrochemical performance of 2D TDMs (two dimensional transitional metal dichalcogenides) is intensively studied during the last years, because of combination of it's capacity and working current density promising new generation of high performance batteries and supercapacitors. Resent research is focused on preparation of restacked materials with high conductivity or enhancing conductivity making composites with different forms of carbon nanomaterials. $MoS_2$ is considered one of the most promising among TDMs, since it is composed of relatively light elements and has large interlayer distance ($MoS_2$ – 6.15Å vs $NbS_2$ – 5.98Å).

We have used hydrothermal synthesis technique to obtain materials based on $MoS_2$ deposited on wide range of carbon materials, such as multiwall nanotubes arrays, single walled nanotubes or few layer graphene.

Electrochemical performance of the materials was evaluated using 3-electrode cell capacitance measurements and Li intercalation. The materials obtained have enhanced capacity and cyclability in comparison to initial carbon materials and pristine $MoS_2$. The work is supported by Russian foundation of basic research grant #14-29-04062.

## TUE 17

## Toward Two-Dimensional All-Carbon Heterostructures via Ion Beam Patterning of Single-Layer Graphene

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Graphene is the thinnest possible membrane, it has unique electronic and excellent mechanical properties, and it provides the perfect model structure for studying materials science at the atomic level. However, for many practical studies and applications the ordered hexagon arrangement of carbon atoms in graphene is not directly suitable. Here, we show that the atoms can be locally either removed or rearranged into a random pattern of polygons using a focused ion beam (FIB). The atomic structure of the disordered regions is confirmed with atomic-resolution scanning transmission electron microscopy images. These structural modifications can be made on macroscopic scales with a spatial resolution determined only by the size of the ion beam. With just one processing step, three types of structures can be defined within a graphene layer: chemically inert graphene, chemically active amorphous 2D carbon, and empty areas. This, along with the changes in properties, gives promise that FIB patterning of graphene will open the way for creating all-carbon heterostructures to be used in fields ranging from nanoelectronics and chemical sensing to composite materials.

References

[1] Kotakoski et al., Nano Lett. 15, 5944–5949 (2015)

### TUE 18
### Confining supercurrent in graphene bilayer weak links

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Designing nanostructures based on electrostatic gating has been at the heart of the research in mesoscopic physics for the last thirty years. While graphene undergoes Klein tunneling, making it inappropriate for charge carrier confinement, it is possible to create nanostructure based electrostatic confinement in graphene bilayer. Based on edge connected hBN-graphene-hBN heterostructures, we have induced displacement fields between an overall back-gate and a top split-gate to confine the electrons and holes within a one-dimensional constriction.

By using superconducting leads we are able to measure supercurrent amplitudes in this ballistic system. We have studied the confinement of the supercurrent by observing the variations of the periodicity of the Fraunhofer pattern while the constriction is formed. A detailed analysis of the complex Fourier transform allows us to directly assess the supercurrent desity profile and therefore the geometry of the induced constriction. Here we demonstrate that it is possible to fully gate-control both amplitude and density profile of an induced supercurrent.

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### TUE 19
### Identification of organic molecules on graphene support from low-dose STEM data

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Direct imaging of individual organic molecules in transmission electron microscopy (TEM) is severely challenged by their notoriously low radiation damage thresholds. We propose to use graphene as a supporting membrane for sub-mono layers of organic molecules and demonstrate an algorithm that can retrieve molecular entities at atomic resolution from many individual low-dose scanning TEM micrographs. These are automatically acquired with ultra quick scans (0.2 $\mu$s per pixel) and without any prior on-site exposure for adjustment or tuning. Our likelihood maximization approach [1] takes advantage of the full symmetry of the supporting graphene sheet and can compile atomic views of the deposited molecules from reoccurring correlations in the bulk of all noisy micrographs. Numerical benchmarks suggest that even as elusive molecules as sparsely deposited (0.015 $\mathrm{nm}^{-2}$) isolated nucleobases can be retrieved from mapping a sample area of $\sim 0.1\,\mu\mathrm{m}^2$.

[1] Ultramicroscopy, Vol. 145, pp. 13-21, 2014

## TUE 20
## Nickel-Enhanced Graphitic Ordering of Carbon Ad-Atoms during Physical Vapor Deposition

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Compatibility with commonly used substrate materials is of crucial importance for graphene device production. Low-temperature synthesis approaches are needed to cope with this challenge. Therefore it has to be clarified, to which extend physical vapor deposition can be used to produce ordered graphene structures.

In this contribution, the mechanism of graphitic ordering of atomic C on Ni was investigated at temperatures ranging from room temperature to 550 °C. The C/Ni films were prepared by ion beam sputtering. A temperature-induced and a Ni-induced enhancement of graphitic ordering is demonstrated. The Ni-effect is responsible for the formation of a bi-layer structure of the C films at higher deposition temperatures. In the bi-layers, C forms graphenic planes parallel to the Ni surface within a thickness range of 1-2 nm. Further deposited C grows preferentially perpendicular to the surface. The results are discussed on the basis of hyperthermal atom deposition, surface diffusion, metal-induced crystallization and dissolution-precipitation. Our findings point to a dominating role of surface diffusion-assisted crystallization in the carbon ordering process.

## TUE 21
## Reductive Functionalization of SWCNTs via the Modified Birch Reduction

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The reductive pathway has become a versatile tool for the functionalization of single walled carbon nanotubes (SWCNTs). However, the mechanism of this type of reaction is influenced by many factors that are not fully understood until now. Here we applied Modified Birch conditions to obtain charged CNTs - so called nanotubides - which were trapped with 4-tert-butyl phenyldiazoniumtetrafluoroborat as electrophile. A variation of the concentration of the diazonium salt as well as the comparison to the non-reductive pathway carried out in CHP at different reaction times give first insights into the electronic-type selectivity, the degree of functionalization as well as the kinetic behavior of this complex reaction. Furthermore, the reversibility of the reaction was tested by applying Raman spectroscopy before and after thermal annealing of the sample.

### TUE 22
### Bacterial response to diamond nanoparticles and graphene sheets

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Nanodiamond (NDs) and graphene (G) have attracted an attention of researchers for biomedical applications due their tailorable surface properties. Here we report on antibacterial activity of NDs/G evaluated by the colony number and area. NDs and G were either oxidized (O-ND, GO) or reduced (H-ND, rGO). Firstly, NDs or G were diluted in Mueller-Hinton (MH) broth with Escherichia coli at concentration 1 mg/ml. The E. coli suspension was cultivated on MH agar for 24 h at 37 °C at relative concentrations $10^{-8}$ to $10^{-6}$ (i.e. 10 and 1000 CFU/ml). For the relative concentration $10^{-6}$ we observed a reduction of colony area by 39–51 % for NDs and GO samples compared to the reference. Low dispersion of the rGO sample limited its evaluation. In the second set of experiments, NDs or G were diluted in MH broth at 1 mg/ml together with E. coli at relative concentration $10^{-3}$ ($10^{6}$ CFU/ml). After 24 h cultivation the broth was diluted to the relative concentrations of E. coli ranging from $10^{-9}$ to $10^{-6}$ (1 and 1000 CFU/ml) and dispersed on MH agar and once again cultivated for 24 h. We observed a significant colony number reduction by 60–78 % for the rGO sample depending on E. coli concentrations.

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### TUE 23
### High-pressure Optical Study of Small-Diameter Single-Chirality Single-Walled Carbon Nanotubes

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Due to common synthesis techniques, single-walled carbon nanotubes (SWCNTs) are usually produced in a mix of many chiralities. Their slightly different electronic properties broaden their optical spectra and thus the interpretation is difficult. Huge effort has been put in the development of procedures to obtain pure single-chirality SWCNT samples and it led to better understanding of their properties.

Here we report on the mechanical stability of small-diameter SWCNTs (d=0.75 nm). Optical absorption measurements in the near-infrared/visible frequency range were carried out on a thin film of single-chirality (6,5) SWCNTs up to high pressure (22 GPa). The small-diameter SWCNTs show a more sensitive behavior in terms of the pressure-induced red-shift of the optical transitions compared to larger-diameter, mixed-chirality SWCNTs (d≈1.4 nm). Furthermore, the relative shift shows no abrupt anomalies and saturates at intermediate pressure.

## TUE 24

## Near infrared electroluminescence and photocurrent spectroscopy with polymer-wrapped SWCNTs

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We have measured near infrared electroluminescence and photocurrent spectra of polymer-wrapped semiconducting SWCNTs. We observe emission lines in the telecommunication band which are surprisingly narrow and comparable to photoluminescence spectra even though the devices are of a short channel type and operated at high bias. The results have to be considered in the context of hot carrier relaxation and exciton-phonon coupling. Photocurrent spectra on the other hand show a strong sensitivity to substrate induced interference effects amplifying the photocurrent in certain wavelength ranges and enabling detection of intrinsically weak phonon-assisted photocurrents. The data will be discussed in the context of modelling the light field intensity at the position of the SWCNT. Furthermore we have measured an unexpected reduction of the photocurrent efficiency with increasing illumination which we believe is due to excition-excition annihilation.

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## TUE 25

## Optical Microspectroscopy Study of Single-Chirality SWCNTs and $C_{60}$-Peapods under Pressure

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According to recent optical absorption measurements [1] bundled single-walled carbon nanotubes (SWCNTs) with average tube diameter of 1.4 nm show a sequence of structural transformations under external pressure: a phase transition at $P_{c1}\sim 3$ GPa, where the tubes' cross section is deformed from a circular to an oval shape, at $P_{c2}\sim 7$ GPa a more drastic change in the cross section from oval to racetrack or peanut-type shape, and a collapse of the tubes at $P_{c3}\sim 13$ GPa. When filled with $C_{60}$-molecules ($C_{60}$-peapods) the first anomaly is shifted to a higher critical pressure ($P_{c1}\sim 6.5$ GPa).

Here, we compare the mechanical stability of single-chirality (11,10) SWCNTs (diameter: 1.44 nm) with that of mixed-chirality SWCNTs (d$\approx$ 1.4 nm). To this end, we carried out pressure-dependent absorption measurements in the near-infrared/visible frequency range on an (11,10) SWCNT film. Furthermore, we encapsulated $C_{60}$ molecules in the (11,10) SWCNTs and carried out corresponding pressure-dependent optical measurements on such single-chirality peapods. The obtained results will be compared with the pressure effects on $C_{60}$-peapods with mixed chiralities.

[1] B. Anis et al., J. Phys. Chem. C 118, 27048 (2014).

## TUE 26

## Hydrocarbon chains and rings: bond length alternation in finite molecules

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We present a theoretical study of bond length alternation (BLA) in carbon rings. We demonstrate using the Longuet-Higgins–Salem model that the appearance of BLA in conjugated carbon polymers is independent of the boundary conditions and does in fact appear in carbon rings as in carbon chains. We use the Hartree–Fock approximation and density functional theory to show that this behaviour is retained at the first principles level. The results are based on our recent paper [1].

[1] J.Kürti, J.Koltai, B.Gyimesi, V.Zólyomi, Theor. Chem. Acc. (2015) 134:114

## TUE 27

## The coupling mechanism of plasmons: A wavelength dependent Raman study on asymmetric dimers

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Surface-enhanced Raman scattering (SERS) is a key technique to study the vibrational and electronic properties of single molecules. Plasmons, the collective excitation of free electron in a metal, lead to the giant enhancement of the inelastic scattered light in the SERS process. In the last years SERS has been very successfully used in fundamental research, forensics, biology, chemistry or medicine. Despite the great achievements, the coupling mechanism between the localized surface plasmon and the Raman scatterer has not been fully explained. We performed wavelength-dependent Raman experiments to study the coupling mechanism between a localized surface plasmon and a sample. The plasmons were excited between two gold nanoparticles (dimer). We used graphene, a non-resonant Raman scatterer, as probe and varied the size of one of the gold particle to investigate asymmetric dimers. Small asymmetries lead to a broad gaussian-like enhancement profile with very sharp resonances on top. Increasing the asymmetry resulted in a broadening and finally vanishing of the sharp resonances. This behaviour is explained by the activation of dark plasmons, that were excited by electromagnetic fields in asymmetric dimers.

## TUE 28

## New Raman lines in small-diameter endohedrally functionalized DIPS carbon nanotubes

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If molecules are small enough and carbon rich, they are expected to enter into the tubes and undergo chemical reactions inside. In several recently performed experiments new Raman lines appear after transformation of the reacted material at elevated temperatures. In such experiments ferrocene was appropriate and new Raman lines were observed. These so called $C_n$-lines are in resonance with red lasers around 2 eV and were assigned to extended carbon rich oligomers. In a set of new experiments using small diameter DIPS tubes (D $\sim$ 1.3 nm) we found that the reactions definitely perform inside the tubes. This was concluded from a comparison between tubes which were opened or not opened before the reaction process, respectively. Only the opened tubes revealed the $C_n$-lines after transformation. In addition, performing detailed studies with other laser lines in the spectral range of 2.17 to 2.34 eV new Raman lines were observed at e.g. 1226, 1265, and 1345 $\mathrm{cm}^{-1}$ with a blue shifted resonance as compared to the $\mathrm{C}_n$-lines. It is concluded that during the transformation process several new compounds grow inside the tubes after transformation.

## TUE 29
## Quantum Hall states in bilayer graphene probed by transconductance fluctuations

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The charge localization behaviour in quantum Hall regime can be captured by a simple measurement of transconductance. Unlike normal transport measurements these fluctuations reflect processes of charge localization and allows observing fragile quantum Hall states such as high order fractional quantum Hall states and broken symmetry states. We have investigated fractional quantum Hall states in Bernal-stacked bilayer graphene using the indirect measurements. Various odd-denominator fractional quantum Hall states $\nu \to \nu + 2$ symmetry and the even-denominator fractional QH state at filling $-1/2$ is observed, as previously reported. However, the particle-hole symmetric state at filling $1/2$ is detected as well in contrast with the previous studies. These observations suggest that the stability of both odd and even denominator fractional quantum Hall states is very sensitive to local transverse electric fields in bilayer graphene.

## TUE 30
## Electron optics in graphene nanostructures

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We simulate electron transport through large-scale graphene nanostructures featuring spatially varying potentials, such as p-n junctions patterned by electrostatic gates. While for a sharp interface the p-n junction acts as a focusing lens for an incident divergent electron beam (Veselago lens), for a smooth transition region the p-n junction acts as a shaper of a narrow beam with near-zero divergence, providing the basis for electron-optics in graphene nanostructures. We quantitatively show that these

effects are robust in presence of interface roughness and disorder, and provide upper bounds for their experimental realizations.
Eigenstates of the Wigner-Eisenbud-Smith time delay operator yield a measure for the electron dwell time inside the structure, and associated particle-like eigenstates corresponding to classical paths through the sample. Comparing linear (graphene-like) and parabolic dispersion relations yields valuable insights into the properties of bandstructure and resonances. We propose a protocol to extract information on classical paths from conductance measurements, using transport through a wide graphene ribbon gated by an STM tip.

### TUE 31

### Two-Dimensional Raman Mapping of $MoS_2$ Crystals at Cryogenic Temperatures

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Molybdenum disulfide ($MoS_2$) exhibits fascinating optical properties when thinned down to a two-dimensional monolayer [1]. Complementary to photoluminescence, Raman spectroscopy provides versatile and powerful means for the inspection of material quality being sensitive to the number of layers [2] or the degrees of charge doping [3] and strain [4] in crystalline layered $MoS_2$. In our studies we implement cryogenic two-dimensional Raman mapping of individual $MoS_2$ monolayer crystals grown by chemical vapor deposition and transferred onto silicon oxide substrates. By raster-scanning the sample with respect to the focal spot of $\sim 0.7\ \mu$m in diameter we acquired spatial maps of single- and poly-crystalline flakes at the cryogenic temperature of 3.1 K. We observe significant inhomogeneities in the characteristics of vibrational Raman modes over the $MoS_2$ flake and interpret our findings on the basis of spatial variations in the crystal quality, charge doping level, and local environment.

[1] X. Xu et al., Nat. Phys. 10, 343 (2014)
[2] C. Lee et al., ACS Nano 4, 2695 (2010)
[3] B. Chakraborty et al., Phys. Rev. B 85, 161403(R) (2012)
[4] C. Rice et al., Phys. Rev. B 87, 081307(R) (2013)

### TUE 32

### Atomic resolution structure of defects in graphene and $MoS_2$

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Graphene and $MoS_2$ epitomize the family of two-dimensional materials. While they are both interesting for applications, they also serve as a great playground for atomic-scale structural manipulation. For this study we created defects in graphene in a controlled manner, using the electron beam of a transmission electron microscope operated at 150 and 200 kV. To hinder the destructive effects of chemical etching during the process, these experiments were carried out at 150°C. The rate of amorphization due to increasing defect density was monitored via the changes observed in the diffraction pattern. The atomic structure of the created defects was imaged with a Nion UltraSTEM scanning transmission electron microscope operated at 60 kV later. The structure analysis was then carried out through automatic atom detection and ring analysis. In the case of $MoS_2$, the samples were irradiated with Xe 30+ and Xe 40+ ions. This resulted in the creation of nanopores with a well-controlled size and concentration, as confirmed via atomic-resolution imaging. Detailed analysis of both of the structural defects in graphene as well as the pore size distribution in $MoS_2$ will be presented.

## TUE 33

## STM investigation of point defects in various transition-metal dichalcogenide single layers

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In the last few years more and more two dimensional (2D) materials have been isolated [1], and the possibility to design 2D heterostructures is becoming more and more appealing. However to exploit the potential of such complex structures it requires the detailed understanding of the realistic properties of their 2D building blocks. One of the limiting factors is the relatively high concentration of the native structural defects occurring in these materials. Usually the higher the defect concentration, the lower the electronic device performance one can achieve. In the case of transition-metal dichalcogenide (TMDC) single layers, Scanning Tunneling Microscopy (STM) is a versatile and non-invasive tool for investigating the native point defect concentration and distributions without modifying the material. Furthermore, their atomic and electronic structure of these defects can also be studied. We have performed detailed STM investigations of single layers of four fairly common members of the TMDC family ($MoS_2$, $MoSe_2$, $WS_2$ and $WSe_2$) and compared the measured native point defect concentration to predict their performance in realistic electronic device applications.

[1] G. Zs. Magda, et al., Sci. Rep. 5(2015) 14714

## TUE 34
## Ultrafast Coulomb-induced intervalley coupling in atomically thin WS$_2$

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Monolayers of semiconducting transition metal dichalcogenides hold the promise for a new paradigm in optoelectronics by exploiting the valley degree of freedom in addition to charge and spin. For these materials, valley polarization can be conveniently initialized and read out by circularly polarized light. However, the underlying microscopic processes governing the valley dynamics in these atomically thin equivalents of graphene are still not fully understood. Here, we present a joint theory-experiment study on the ultrafast time-resolved intervalley dynamics in monolayer WS$_2$.

Based on a microscopic theory, we reveal the many-particle mechanisms behind the spectral features observed in polarization-resolved pump-probe experiments. We show that Coulomb-induced intervalley coupling explains the immediate and prominent pump-probe signal in the unpumped valley and the seemingly low valley polarization typically observed in pump-probe measurements compared to photoluminescence studies. The gained insights are also applicable to other light-emitting monolayer transition metal dichalcogenides, where the Coulomb-induced intervalley coupling also determines the initial carrier dynamics.

## TUE 35
## Carbon nanotubes in high magnetic field

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A parallel magnetic field affects strongly the electronic transport through a carbon nanotube (CNT) via its coupling to the orbital degree of freedom. Although such a wire-like system can host neither the fully developed Hofstadter butterflies nor Landau levels, the magnetic field has nevertheless a deep influence on the CNT's spectrum and wave functions. We report here on the results of both theoretical calculations and experimental measurements of a CNT quantum dot. The two experimental results on which we focus are a strong suppression of the conductance by the parallel magnetic field and an unusual evolution of the spectral lines. The unique boundary conditions, which couple the transverse and longitudinal momentum, are responsible both for decreased transmission through the CNT and for the remarkable dependence of the longitudinal momentum on the magnetic field.

## TUE 36

## Anisotropic Spin Relaxation in Graphite Intercalated Compounds

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The phenomena of spin relaxation in nano carbon materials is really interesting. These efforts were highlighted by the possibility of using graphene for spintronics. It is generally accepted that in graphene the spin lifetime should be of the order of 100 ns, which seems to be long enough for applications. However, this theoretical finding has not yet been proven by any experimental results, mainly due to extrinsic scattering effects. Because of this technical difficulty, the graphite intercalated compounds (GIC) are investigated as a model system of graphene, due to many similarities. We prepared Li, K, Rb, Cs doped stage-I, II compounds. The most used method to measure spin relaxation is with electron spin resonance (ESR) spectroscopy. We determined the spin lifetime for the mentioned materials using angular dependent ESR and we found that surprisingly the relaxation is anisotropic. Usual spin relaxation phenomena to describe the relaxation of conducting electrons, the Elliott-Yafet theory does not predict anisotropy. We present a model Hamiltonian, which includes the anisotropic spin relaxation, thus agrees with the phenomena found in GICs. We believe that the result is relevant for the spin relaxation properties of chemically doped or biased graphene.

## TUE 37

## Films of single-walled carbon nanotubes as stable and efficient electron - blocking layers and transparent electrodes for solar cells

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Films of single-walled carbon nanotubes (SWNTs) network are promising flexible transparent-conductive layer for various solar cells. In addition, we found that SWNT film or doped graphene can be a stable conductive electron blocking layer (EBL). We have demonstrated these characteristics in honeycomb-structured SWNTs-Si solar cells [1], dry-deposited SWNTs-Si solar cells [2], graphene-Si solar cells, organic solar

cell (OSC) [3], and perovskite-type solar cells [4]. Using millimeter-scale single-crystal graphene [5] and honeycomb-structured SWNT network can enhance the performance of these solar cells.

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[5] X. Chen et al., Carbon, 94 (2015) 810.

## TUE 38
## Silver nanoparticles for applications in osteogenesis and bone infection treatment

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In the case of post-traumatic or post-implant bone regeneration the most dreaded complications are infections localized at the regeneration site. We aimed to develop a novel silver based bio-nanostructure with a dual role in bone regeneration and infection treatment. Silver nanoparticles (AgNP) were obtained by reducing Ag ions in the presence of citrate and then functionalized with a biological active protein fragment. The characteristic surface plasmon resonance band for silver nanoparticles was observed by UV-Vis spectroscopy. Size and polydispersity index was assessed by means of dynamic light scattering. While functionalization success was confirmed by registering the IR spectra of the nanostructures before and after functionalization. The bio-nanostructure was subjected to atomic force microscopy investigations in order to investigate size and shape. Biocompatibility was assessed using MTT assay and the annexin V staining for apoptosis detection. The obtained bio-nanostructure presents a high potential for bone infection treatment and bone regeneration.

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## TUE 39
## Edge reconstruction and spontaneous time-reversal symmetry breaking in two- dimensional topological insulators

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Topological insulators (TIs) are electronic materials whose bulk band gap gives rise to protected conducting states on their edge or surface. In two dimensions these are one-dimensional helical edge modes that, due to time reversal symmetry (TRS), come in counter-propogating pairs. The TRS protection of these modes has led to a plethora of proposed applications, ranging from spintronics to quantum computation. Here we show, employing standard frameworks, that, unlike the infinitely sharp edge utilized in traditional calculations, employing an experimentally realistic smooth edge may lead 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 all proposed applications of TIs.

## TUE 40

## Electro-optical properties of individual CdS nanowires

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Individual CdS nanowires (NWs) grown by hydrothermal methods with diameters in the range of 50 nm are investigated by confocal photo luminescence (PL-) spectroscopy, Kelvin Probe Force Microscopy (KPFM), and electrical transport measurements.

We will show how charges distribute along free standing NWs upon local illumination with a confocal microscope. We demonstrate that photo generated electrons spread much wider along the nanowires than the holes, which leads to a charge imbalance that can be measured by KPFM. PL measurements of CdS-NWs, where charges are injected through patterned gold contacts show a reversible Pl-quenching of the NWs upon hole injection such that the PL can be modulated in a frequency range up to 10 kHz. Also we investigated the process of local photo conductivity of contacted individual CdS-NWs by applying a combination of confocal microscopy and KPFM. We measure the potential profiles along the contacted NWs with and without local illumination and compare the data with theoretical simulations.

## TUE 41

## States of antiferromagnetic molecules detected with a carbon nanotube quantum dot

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Carbon nanotubes (CNTs) have some outstanding properties like their high sensitiveness towards changes in the environment and spin-dependent conductance. Thus, they are ideal devices to investigate the states of antiferromagnetic molecules via electronic transport experiments on functionalized CNTs.

In this work, we present experimental data on quantum transport through CNTs covalently functionalized with antiferromagnetic tetramanganese coordination complexes. The experiments reveal a random telegraph signal (RTS), which is presumably caused by interactions between electron spin and the antiferromagnetic spin system. Furthermore, the statistics of the RTS indicate the relevant time and energy scales for transitions in this regime.

## TUE 42
## Theory of flexoelectricity and piezoelectricity in 2D crystals

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Piezo-and flexoelectricity are manifestations of electro- mechanical coupling in solids. The former is the electric polarization response to strain in non-centrosymmetric dielectrics, the latter is the polarization response to a strain gradient. Potential technological use of flexoelectricity will depend on progress in nanoscale materials. Exploiting analogies with curvature induced polarization in BN nanotubes, Naumov et al. PRL 102(2009) have shown by first principles calculations that a monolayer BN sheet becomes macroscopically polarized in a corrugated state. The direction of polarization is in-plane and depends on the corrugation wave vector. We have investigated the interplay of layer corrugation and in-plane polarization by lattice dynamics theory. The coupling between flexural modes and in-plane atomic displacements is an anharmonic effect.The theory is applied to 2D h-BN and transition metal dichalcogenides and dioxides.

## TUE 43
## Resonant Raman spectroscopy on $MoS_2$

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Transition metal dichalcogenides (TMDCs) such as $MoS_2$ have attracted attention due to their extraordinary properties such as a transition from indirect to direct band gap in the monolayer limit, large exciton binding energies and spin/valley polarization

[1]. The phonon spectrum of TMDCs provides access to a variety of properties such as the number of layers, strain and charge carrier density [2].

Moreover, resonance phenomena in Raman scattering have been used in different material systems to gain information about the electronic structure and electron phonon interaction. We perform resonant Raman measurements in dependence of temperature, polarization, carrier density and number of layers in order to gain further insight to the electron phonon interaction in $MoS_2$.

[1] Wang et al., Nature Nanotech. 7, 699 (2012)

[2] Miller et al., Appl. Phys. Lett. 106, 122103 (2015)

### TUE 44

### Raman excitation profiles and electronic properties of deformed carbon nanotubes

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Deformations produce a number of interesting observable effects important in designing electromechanical devices. Systematic analysis of Raman excitation profiles (REPs) for deformed configurations of carbon nanotubes (CNTs) is given. A number of interference effects appear when two resonant transitions come close together. The type of interference and its influence on the REPs is shown to be determined by electron−phonon coupling. Collapse of Raman intensity in resonant scattering experiments and the change in the G-mode profile are explained.

Measurements by Cullinan and Culpepper (Carbon 51, 2013) show significant quantitative mismatch with the existing theory. In order to resolve this issue, we study effects of strain induced deformations onto electronic properties of CNTs and show that if the deformation coupling is fully taken into account, alteration of electronic band structure is significantly lower than predicted by Yang and Han (PRL 85, 2000). Our results match the observation of reduced gauge factor in CNT-based piezoresistive sensors. We find that interaction of electrons with longitudinal high-energy Raman mode is crucial for the attenuated modifications of the electro-optical properties.

### TUE 45

### Topological phase diagram of superconducting carbon nanotubes

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The topological superconducting phase diagram of pure zigzag carbon nanotubes is discussed. Under the assumption of a short-ranged pairing potential, there are two spin-singlet states: an $s$-wave and an exotic $p + ip$-wave that are possible because of the special structure of the honeycomb lattice. The consequences for the possible presence of Majorana edge states in carbon nanotubes are addressed. In particular, regions in the magnetic field-chemical potential plane possibly hosting localized Majorana modes are discussed.

## TUE 46
## A New Raman Metric for the Characterisation of Graphene oxide and its Derivatives

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Raman spectroscopy is among the primary techniques for the characterisation of graphene materials, as it provides insights into the quality of measured graphenes including their structure and conductivity as well as the presence of dopants. However, our ability to draw conclusions based on such spectra is limited by a lack of understanding regarding the origins of the peaks. Consequently, traditional characterisation techniques, which estimate the quality of the graphene material using the intensity ratio between the D and the G peaks, are unreliable for both GO and rGO. Herein we reanalyse the Raman spectra of graphenes and show that traditional methods rely upon an apparent G peak which is in fact a superposition of the G and D' peaks. We use this understanding to develop a new Raman characterisation method for graphenes that considers the D' peak by using its overtone the 2D'. We demonstrate the superiority and consistency of this method for calculating the oxygen content of graphenes, and use the relationship between the D' peak and graphene quality to define three regimes. This has important implications for purification techniques because, once GO is reduced beyond a critical threshold, further reduction offers limited gain in conductivity.

## TUE 47
## Chirality in van der Waals heterostructures

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Dirac fermions in graphene are chiral - that is, the amplitude of their two-component wavefunctions is coupled to the direction of motion. Crucially, their chiral nature plays role in various relativistic experiments, including Klein tunnelling and Zitterbewegung. At the same time, it is extremely difficult to visualise their chirality directly. Here we demonstrate a direct observation of chirality in tunnelling experiments between two graphene layers in parallel magnetic field. To this end we

fabricated resonant tunnelling transistor devices using an atomically thin hexagonal boron nitride sandwiched by the two graphene layers with aligned crystallographic axes. By changing the angle between in-plane magnetic field and graphene crystal axis, we separated the tunnelling contributions from all six corners of graphene Brillouin zone. As graphene chirality modulates the tunnelling current in the presence of strong in-plane magnetic field, we were able to detect chirality of graphene via angular dependence of magnetic field on tunnelling conductivity. Therefore, our experiments demonstrate a mechanism which allows preparing quasi-relativistic electrons in a particular quantum state.

## TUE 48
## Rayleigh Scattering Spectroscopy of Single-Walled Carbon Nanotubes in Various Environments

Takeshi Okochi[1], Toru Osawa[1], Yoritaka Furukawa[1], Rong Xiang[1], Taiki Inoue[1], Shohei Chiashi[1], Shigeo Maruyama[1,2]
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Because the electronic structure of single-walled carbon nanotubes (SWNTs) can be readily modified by surrounding environments due to the one-dimensional nature, accurate and in-situ evaluation of electronic structure is crucial for high-performance electronic devices. In this study, we measured Rayleigh scattering spectra [1,2] to investigate the electronic structure of SWNT samples in various environments. We constructed the optical system to obtain Rayleigh scattering spectra and Rayleigh scattering images. The attenuated continuum laser (400 - 2500 nm in wavelength) was focused on SWNTs and scattered light was detected with several acquisition systems. We compare Rayleigh scattering spectra of dispersed SWNTs in the surfactant solutions [3], dry-deposited SWNT films [4], suspended SWNTs over a trench, horizontally aligned SWNTs [5], and vertically aligned SWNTs on substrates. Based on experimental results, we will discuss the influence on the electronic structure of SWNTs caused by surrounding environments.

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[2] K. Liu et al., Nat. Nanotechnol. 8, 917 (2013).
[3] H. Liu et al., Nat. Commun. 2, 309 (2011).
[4] A. Kaskela et al., Nano Lett. 10, 4349 (2010).
[5] T. Inoue et al., J. Mater. Chem. A, 3, 15119 (2015).

## TUE 49
## Fabrication and optical properties of transition metal dichalcogenide heterostructures

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Semiconductor transition metal dichalcogenides (TMD) have been subject of increasing interest over the last years. In particular single layers of $MoS_2$ show strong photoluminescence associated with a direct-gap transition, in contrast to bulk. Heterostructures of TMDs will lead to modifications of their individual optical properties. Calculations predict that the band alignment of different monolayer TMDs is, for many combinations, of type II, leading to spatially indirect excitons. Nevertheless, clear experimental evidence is still missing.

Here we present our results on the influence of heterostructure fabrication on their optical properties. We used a dry transfer method, using a polymer stamp as an intermediate substrate, as proposed in Ref. [1], as well as a wet transfer method following Ref. [2]. The optical properties are investigated by Raman and photoluminescence spectroscopy. We studied few-layer $MoS_2$ obtained by stacking individual layers, and heterostructures of $MoSe_2$ and $WS_2$. The cleanness of the layers, the influence of the transfer method as well as the influence of the substrate are analyzed.

We thank Ute Kaiser, Tibor Lehnert and Gerardo Algara-Siller for helpful discussions on the transfer method. This work was supported by the European Research C

## TUE 50

## Selection rules and carrier-concentration dependence of the enhancement factor in tip-enhanced Raman scattering

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We present an experimental study and a quantum mechanical model of the intrinsic mechanism of tip-enhanced Raman scattering (TERS). The near-field light-matter interaction strongly differs from the usual far-field case mainly because of the many-body nature of the process. In a conical metallic tip, photons can excite localized surface plasmons (LSPs) or can couple with plasmons into surface plasmon polaritons (SPPs). LSPs and SPPs can decay one into the other. This plasmonic and polaritonic mediation, which takes place at the tip apex, becomes an integral part of the scattering process preventing a purely classical description. The coupled photon of the evanescent field, which is an intrinsic property of SPPs, can contribute to the scattering process only by photon tunneling into the sample. Experimental data on graphene, carbon nanotubes, and highly doped gallium nitride epilayers show that the tunneling photons do not preserve the incoming light polarization with a consequent change of selection rules. In our experiments, the enhancement factor is independent of the incoming light polarization and reflects only the plasmonic contribution as a function of carrier concentration of the material.

## TUE 51
## Helical Raman spectroscopy of transition metal dichalcogenides

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Transition metal dichacogenides (TMDs) have attracted a lot of interest due to their unique properties. Especially the strong photoluminescence from the direct gap in few layered samples has been repeatedly investigated. Furthermore, TMDs have recently become promising materials for spin- and valleytronics as circular polarized excitation leads to the generation of electron-hole-pairs with distinct spin at either K or K'. However, questions remain unanswered about the mechanisms of the scaterring proccesses, especially on phonons.
In our work we investigate the scattering processes in TMDs by measuring circular polarization resolved Raman spectra. We observe that the scattering of specific phonons is only allowed under specific helical excitation.

## TUE 52
## UV Raman Spectroscopy of diamondoid dimers

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We analyze the electronic and vibronic properties of double-bond coupled diamondoids[1,2] via resonant (ultra-violet) Raman spectroscopy.
In contrast to the equivalent parent diamondoids, we find the optical gap to be reduced from the deep-UV down to approximately 4.7 eV. Furthermore, we observe three additional characteristic vibrations in the Raman spectra. We assign them to a C=C stretching mode around 1660 $\mathrm{cm}^{-1}$, a localized torsion-like mode (760 $\mathrm{cm}^{-1}$) of the double-bond carbon atoms, and in case of the dimers that have an additional carbon atom between the double bond and the diamondoid, we observe a hindered rotation of the entire ethylene-like centers of the dimers around 200 $\mathrm{cm}^{-1}$.
A strong enhancement of the C=C stretching mode occurs under UV excitation. This is associated with a localization of the $\pi$-HOMO and LUMO and an elongation of the carbon bond during the vibration[3]. We support our experimental findings with density functional theory computations of both the vibrational modes and the electronic states.
[1] New J. Chem. 38 (1), 28 (2014)

[2] Angew. Chem. Int. Ed. 47, 1022 (2008)
[3] J. Chem. Phys., 140, 034309 (2014)

### TUE 53

### Double-resonant Raman processes in individual SWCNTs from theory and experiment

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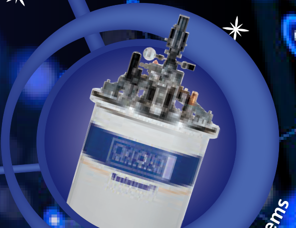
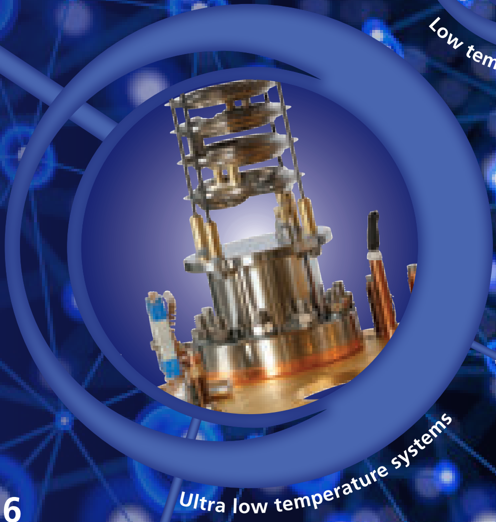
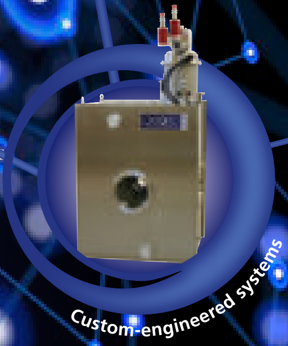
Raman spectroscopy on single-walled carbon nanotubes (SWCNTs) is often performed on dispersions, i.e., ensembles of individual tubes, or on interacting nanotubes or small bundles, deposited on a substrate. In this case however, less intense, strongly dispersive Raman modes can be obscured. By studying perfectly aligned, individual SWCNTs across a wide range of excitation wavelengths, we observe several well-defined double-resonant Raman modes in the range of the intermediate frequency modes (IFM) and of the G mode. We attribute them to overtones and Stokes-/anti-Stokes combinations of phonons from the $ZA$–, $ZO$–, and $TO$–branches, activated by a DR process close to $K$. This assignment is validated by calculations of the DR Raman intensities from these phonon branches for a large number of SWCNTs. By comparing these theoretical results to our experimental data, we gain deeper insight into which DR processes give dominant contributions to the observed signal.


Optical systems


Low temperature magnet systems


Ultra low temperature systems


Custom-engineered systems

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|---|---|
| 08:30 – 09:00 | K. Bolotin, Berlin<br>*Bending, pulling, and cutting wrinkled two-dimensional materials* |
| 09:00 – 09:30 | N. Bendiab, Grenoble<br>*Phonons in low dimensional sp2 carbon systems* |
| 09:30 – 10:00 | C. Neumann, Aachen<br>*Raman spectroscopy as probe of nanometer-scale strain variations in graphene* |
| 10:00 – 10:30 | coffee break |
| 10:30 – 11:00 | D. Roy, London<br>*Nanospectroscopy for Functional Nanomaterials* |
| 11:00 – 11:30 | Y. Kim, New York<br>*Bright Visible Light Emission from Graphene* |
| 11:30 – 12:00 | L. Ju, Ithaca<br>*Topological valley transport at bilayer graphene domain walls* |
| 12:00 – 17:00 | mini workshops |
| 17:00 – 18:30 | Dinner |
| 18:30 – 19:00 | I. Grigorieva, Manchester<br>*Superconductivity in alkali-metal doped graphene* |
| 19:00 – 19:30 | F. Mauri, Paris<br>*Anharmonic matter: charge-density-waves in dichalcogenides and hydrogen sulfide superconductor* |
| 19:30 – 20:00 | S. Adam, Singapore<br>*Theory of disorder induced magnetotransport in 2D materials* |
| 20:00 – 20:30 | E. Rossi, Williamsburg<br>*Two-dimensional heterostructures with spin-orbit coupling* |

### 08:30

## Bending, pulling, and cutting wrinkled two-dimensional materials

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Two-dimensional materials (2DMs) are inevitably crumpled in the out-of-plane direction. This crumpling originates both from static wrinkling associated with uneven stresses and dynamic wrinkling resulting from the “flexural” phonon branch of these materials. While this crumpling has been predicted to dominate electronic, mechanical, and thermal properties of 2D materials, its effects are hard to probe experimentally.

Here, we investigate the effects of the out-of-plane crumpling on thermal expansion, mechanical stiffness, and bending rigidity of a prototypical two-dimensional material, graphene. We show that the out-of-plane crumpling renders the thermal expansion coefficient negative and substrate-dependent, decreases the Young’s modulus, and greatly increases the bending rigidity of graphene. To carry out these measurements, we developed approaches to sensitively probe mechanics of supported and suspended single- and doubly-clamped graphene cantilevers at room and cryogenic temperatures.

### 09:00
### Phonons in low dimensional sp2 carbon systems

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Optical phonons, in low dimensional sp2 carbon systems, couple easily with different elementary excitations (electron, acoustic phonon, photon), allowing us to be sensitive to various physical phenomena: strain field, mechanical resonances, but also charge transfer and/or energy transfer. To illustrate the mechanical coupling, I will show how optical phonons can be used to reveal the nature of strain transfer between compressively strained graphene and various substrates. The monolayer geometry, the interfacial properties, and the presence of wrinkles lead to highly non-uniform strain in the graphene, varying from uniaxial to biaxial. To illustrate electron-phonon and phonon-photon coupling, an optical gating of photo-active molecules grafted on an isolated DWNT (graphene) based transistor will be shown. A huge modification of optical phonons is measured. This photo-induced phenomenon will be elucidated in terms of photo-induced excitation transfer between the grafted molecules and the DWNT component whereas in graphene this effect is different. Finally, by optical gating, this DWNT-hybrid FETs can be used as an optically controlled memory.

## 09:30

## Raman spectroscopy as probe of nanometer-scale strain variations in graphene

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Raman spectroscopy is widely used for the characterization of graphene, as important material parameters e.g. doping, strain, and defect density can be accessed quickly and noninvasively. With confocal Raman setups these quantities can be extracted on length scales below a micron, limited by the size of the laser spot. By employing a magnetic field, we investigate the broadening mechanisms of the prominent Raman lines of graphene, the G and 2D lines. We deduce that both Raman lines, most prominently the 2D line, are strongly broadened by strain variations within the laser spot, i.e. on length scales of nanometers to several tenth of nanometers. Such strain variations are naturally pronounced in graphene due to its mono-atomic thickness. Importantly, such nanometer-scale strain variations have been shown to be detrimental for the charge carrier mobility of graphene. As a consequence, the 2D line yields important information on the strain homogeneity of graphene on short length scales as well as the possible electronic quality of a device, which highlights the great potential of Raman spectroscopy for monitoring fabrication and synthesis processes of graphene samples.

### 10:30

### Nanospectroscopy for Functional Nanomaterials

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Novel functional devices use complex nanomaterials systems, where nanoscale morphology and chemistry can crucially affect performance. However, currently the lack of analytical techniques that can directly correlate morphology with functions or chemical composition at nanometre length-scales presents a major gap. We have utilised nanospectroscopy that allows non-destructive simultaneous measurement of topographical, chemical, optical and electrical properties with nanoscale resolution ($<$ 20 nm) by combining plasmonic optical signal enhancement with electrical mode scanning probe microscopy and novel data analysis. As a proof of concept we apply this method to operating organic solar cells and demonstrate the direct identification of nanomorphology, and its direct impact in photocurrent generation and collection. We have applied this approach in 2D materials such as graphene and MoS2 as a step towards comprehensive understanding of electronic and structural properties. This new approach should prove relevant in other fields such as optoelectronics, sensors and nanoelectronics, where the ability to directly correlate structure and function is highly sought-after.

### 11:00

## Bright Visible Light Emission from Graphene

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Bright and broadband light emission in two-dimensional materials such as graphene and related heterostructures are essential for the realization of unprecedented atomically thin, flexible and transparent optoelectronics. However, electrically driven bright visible-light emission from gapless graphene has remained elusive. Here, we report bright visible light emission from electrically biased suspended graphene. In suspended graphene, the dissipation of heat through the substrate and extrinsic scattering of charge carriers are greatly reduced; thus allowing for hot electrons (2800 K) to be spatially localised under modest electric fields. This results in a 1000-fold enhancement in the thermal radiated power compared with the case of graphene on a substrate. Moreover, strong optical interference between the suspended graphene and substrate can be used to tune the emission spectrum. We also demonstrate the scalability of this technique by realizing arrays of chemical-vapour-deposited graphene light emitters.

### 11:30

### Topological valley transport at bilayer graphene domain walls

Long Ju[1,2], Zhiwen Shi[2], Nityan Nair[2], Yinchuan Lv[2], Chenhao Jin[2], Jairo Velasco Jr.[2], Claudia Ojeda-Aristizabal[2], Hans A Bechtel[3], Michael C Martin[3], Alex Zettl[2,3], James Analytis[2,3], Feng Wang[2,3]
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Electron valley, a degree of freedom that is analogous to spin, can lead to novel topological phases in bilayer graphene. An external electric field can induce a tunable bandgap in bilayer graphene, and domain walls between AB- and BA-stacked bilayer graphene can support protected chiral edge states of quantum valley Hall insulators. In this talk, I will present our efforts on revealing the topologically protected edge states at AB-BA domain walls by combining near field infrared nanoscopy with electrical transport measurement. These one-dimensional valley-polarized conducting channels feature a ballistic length of about 400 nanometres at 4 kelvin. With further engineering, such domain walls can provide a platform for novel electronic devices based on the electron valleys.

### 18:30

### Superconductivity in alkali-metal doped graphene

Irina Grigorieva[1], James Chapman[1], Yang Su[1], Dmitro Kundys[1], Alexander Grigorienko[1], Francisco Guinea[1], Andre K. Geim[1], Rahul Raveendran Nair[1]
[1]University of Manchester, Manchester, UK

I will review our recent findings of superconductivity in alkali-metal-coated graphene. Graphene, a zero-gap semimetal, can be transformed into a metallic, semiconducting or insulating state using physical or chemical means. Superconductivity was conspicuously absent among these states despite considerable experimental effort, as well as many theoretical proposals. We were able to achieve superconductivity in Ca-coated graphene by intercalation of graphene laminates that consist of well separated and electronically decoupled graphene crystals. Having tried several different intercalants (calcium, potassium, caesium and lithium) we found that Ca is the only dopant that induces superconductivity in graphene laminates above 1.8 K. Ca-coated graphene becomes superconducting at ~6 K and the transition temperature is strongly dependent on the confinement of the Ca layer and the induced charge carrier concentration. In addition to the first evidence for superconducting graphene, our work shows a possibility of inducing and studying superconductivity in other 2D materials using their laminates.

## 19:00

## Anharmonic matter: charge-density-waves in dichalcogenides and hydrogen sulfide superconductor

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Anharmonic effect can generally be treated within perturbation theory. Such an approach breaks down when the harmonic solution is dynamically unstable or the anharmonic correction of the phonon energies is larger than the harmonic frequencies themselves. This is the case near second order phase transitions such as charge-density-wave (CDW) instabilities or in H-containg materials, where the large zero-point motion of the proton can result in a violation of the harmonic approximation. We developed a stochastic implementation of the self-consistent harmonic approximation valid to treat anharmonicity in the nonperturbative regime and to obtain from-first principles the structural and vibrational properties of strongly anharmonic systems. I will present applications to the description of CWDs and phonons in NbS2 and NbSe2 in the bulk and in the monolayer case, where we are able to predict the CDW transition temperature and the evolution of phonons with temperature. I will also discuss the large impact of anharmonic zero-point motion on the phase diagram and superconducting properties of the newly discovered record superconductor, H3S, with a Tc of 203 K at 150 Gpa.

### 19:30

## Theory of disorder induced magnetotransport in 2D materials

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In this talk, I will discuss two recent works concerning disorder-induced magnetoresistance in two-dimensional materials. In the first, we predict theoretically and demonstrate experimentally that a disorder-induced carrier density inhomogeneity induces a classical magnetoresistance that is quadratic at low magnetic fields and linear at larger fields [1]. Using both effective medium and random resistor network models, we demonstrate that the magnetoresitance is a function only of the ratio of carrier density to fluctuations in the carrier density, a power law when this ratio is large, and in excellent agreement with experiments on graphene. In the second part, I discuss the low temperature quantum transport, where the crossover from weak antilocalization at low magnetic fields to weak localization at larger fields reveals information about the dominant scattering mechanism in these materials. Our studies on highly n-doped monolayers of $MoS_2$ reveal that this crossover is set by the electron spin lifetime of the system. The spin lifetime is inversely proportional to momentum relaxation time indicating that spin relaxation in these monoloayer dichalcogenides occurs via the Dyakonov-Perel mechanism [2].

This work is supported by the National Research Foundation Singapore under its Fellowship program (NRF-NRFF2012-01) and by the National University of Singapore through its Young Investigator Award (R-607-000-094-133).

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## 20:00

## Two-dimensional heterostructures with spin-orbit coupling

Enrico Rossi[1]
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In this talk I will present some of our work on two-dimensional heterostructures in which one of the layers has strong spin-orbit coupling. I will first discuss the case of heterostructures formed by one sheet of graphene, or bilayer graphene, and a topological insulator. I will show how the twist angle between the graphene layer and the TI can be used to tune the electronic properties of such heterostructures and I will discuss their spin-dependent transport properties. In the second part of the talk I will present our results for heterostructures in which one of the layers has strong spin-orbit coupling and one layer is superconducting. I will show that in some of these heterostructures a odd-frequency pairing term can be induced due to the interplay of spin-orbit coupling and superconductivity. Finally, I will briefly discuss how the presence of spin-orbit coupling affects the bound states induced by impurities in superconductors.

| | |
|---|---|
| 08:30 – 09:30 | P. Brouwer, Berlin<br>*Strong, weak, and weak-and-strong topological insulators* |
| 09:30 – 10:00 | B. Dora, Budapest<br>*From Floquet to Dicke: quantum spin-Hall insulator in quantum light* |
| 10:00 – 10:30 | coffee break |
| 10:30 – 11:00 | S. Hart, Cambridge<br>*Induced Superconductivity and Unconventional Pairing in HgTe/HgCdTe Quantum Wells* |
| 11:00 – 11:30 | K. Nowack, Ithaca<br>*Imaging currents in 2D quantum materials* |
| 11:30 – 12:00 | P. Nemes-Incze, Aachen<br>*Tunable Pseudo-Zeeman field in graphene* |
| 12:00 – 17:00 | mini workshops |
| 17:00 – 18:30 | Dinner |
| 18:30 – 19:00 | L. Novotny, Zurich<br>*Photon Emission from hBN Tunnel Junctions* |
| 19:00 – 19:30 | D. Neumaier, Aachen<br>*The enabling role of graphene for on-chip photonic systems* |
| 19:30 – 20:00 | F. Bonaccorso, Genova<br>*Energy conversion and storage devices based on graphene and other 2D crystals* |
| 20:00 | Poster III |

### 08:30

### Strong, weak, and weak-and-strong topological insulators

Piet W. Brouwer[1]

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I'll start with an introduction to the physics of topological insulators in two and three dimensions. In two dimensions topological insulators are classified using a "Z2" index, which distinguishes topologically trivial from topologically nontrivial insulators. In three dimensions band insulators are classified using four such "Z2" indices. One of these is called the "strong index", because a nontrivial value indicates a robustness of the topological phase to essentially all time-reversal-symmetry preserving perturbations. The three remaining indices are called "weak", because they are not protected against perturbations that break the lattice translation symmetry. In the second part of my talk I'll discuss a few unique properties of topological insulators that have nontrivial weak as well as strong indices.

### 09:30

### From Floquet to Dicke: quantum spin-Hall insulator in quantum light

Balázs Dóra[1], Balázs Gulácsi[1]
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Time-periodic perturbations due to classical electromagnetic fields are useful to engineer the topological properties of matter using the Floquet theory. Here we investigate the effect of quantized electromagnetic fields by focusing on the quantized light-matter interaction on the edge state of a quantum spin-Hall insulator. A Dicke-type superradiant phase transition occurs at arbitrary weak coupling, the electronic spectrum acquires a finite gap and the resulting ground state manifold is topological with Chern number $\pm 1$. When the total number of excitations is conserved, a photocurrent is generated along the edge, being pseudo-quantized in the low frequency limit, and decaying as $1/\omega$ for high frequencies with $\omega$ the photon frequency. The photon spectral function exhibits a clean Goldstone mode, a Higgs like collective mode at the optical gap and the polariton continuum.

### 10:30

### Induced Superconductivity and Unconventional Pairing in HgTe/HgCdTe Quantum Wells

Sean Hart[1], Hechen Ren[1], Michael Kosowsky[1], Gilad Ben-Shach[1], Timo Wagner[1], Philipp Leubner[2], Mathias Mühlbauer[2], Christoph Brüne[2], Hartmut Buhmann[2], Laurens W. Molenkamp[2], Bertrand I. Halperin[1], Amir Yacoby[1]
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[2]Universität Würzburg, Würzburg, Germany

Topological insulators are a newly discovered phase of matter characterized by a gapped bulk surrounded by novel conducting boundary states. Since the theoretical discovery of these materials, it has been proposed to engineer a new variety of superconductor at their surfaces. Such topological superconductors are predicted to host localized Majorana fermions, particles whose non-Abelian braiding properties could be used for robust quantum information processing. Despite the clear theoretical motivation, a conclusive realization of topological superconductivity remains an outstanding experimental goal. In this talk we present measurements of superconductivity induced in two-dimensional HgTe/HgCdTe quantum wells, a material which becomes a quantum spin Hall insulator when the well width exceeds $d_C = 6.3$ nm. In wells that are 7.5 nm wide, we find that supercurrents are confined to the one-dimensional sample edges as the bulk density is depleted, confirming the topological nature of the system. Furthermore, when the chemical potential is tuned into the conduction band, application of an in-plane magnetic field results in unconventional superconductivity with triplet pairing.

### 11:00

### Imaging currents in 2D quantum materials

Katja Nowack[1]
[1]Physics, Cornell University, Ithaca

Magnetic imaging is uniquely suited to the non-invasive imaging of current densities, particularly in 2D devices. In this talk, I will showcase this approach by discussing our measurements on HgTe quantum well devices in the quantum spin Hall (QSH) regime. In a nutshell, we scan a superconducting quantum interference device (SQUID) to obtain maps of the magnetic field produced by the current flowing in a device. From the magnetic image we reconstruct a 2D current distribution with a spatial resolution of several microns. This allowed us to directly visualize that the edges of the devices carry most of the current when tuned into their insulating gaps - a key feature of the QSH state. In addition, from the images we disentangle conduction through the edges and the interior of a device, allowing us to study the resistance of only the edges even when the interior becomes conductive through either gating or raising the temperature. If time permits, I will both discuss strategies to improve the spatial resolution of our measurements to sub-micron length scales through a combination of improved image reconstruction and smaller sensor sizes and outline interesting opportunities for current imaging.

### 11:30

## Tunable Pseudo-Zeeman field in graphene

Peter Nemes-Incze[1], Markus Morgenstern[1]
[1]II. Institute of Physics B, RWTH Aachen, Aachen

Using the tip of a scanning tunneling microscope, we exploit the differences in van-der Waals forces between W and $SiO_2$ in order to locally lift graphene on small length scales. Molecular dynamics simulations in agreement with the experimental data reveal a sub-nm wide Gaussian bump below the scanning tip with a three-fold symmetric pseudomagnetic field in the 1000 T range. The large field polarizes the pseudospin (sublattice degree of freedom), which gets directly visible as a difference in the local density of states of the sublattices up to 30 %, if the tunneling tip is offset from the force center. Since the van-der Waals forces are tunable by the distance between tip and graphene, the pseudospin polarization can be continuously changed. This can be regarded as a manifestation of a tunable parity breaking in graphene.

### 18:30

### Photon Emission from hBN Tunnel Junctions

Markus Parzefall[1], Palash Bharadwaj[1], Achint Jain[1], Lukas Novotny[1]
[1]ETH Zurich, Photonics Laboratory, 8093 Zurich, Switzerland.

The ultrafast conversion of electrical signals to optical signals at the nanoscale is of fundamental interest for data processing, telecommunication and optical interconnects. However, the modulation bandwidths of semiconductor light-emitting diodes are limited by the spontaneous recombination rate of electron-hole pairs, and the footprint of electrically driven ultrafast lasers is too large for practical on-chip integration. A metal-insulator-metal tunnel junction approaches the ultimate size limit of electronic devices and its operating speed is fundamentally limited only by the tunneling time. We study the conversion of electrons (localized in vertical Au-hBN-Au tunnel junctions) to free-space photons, mediated by resonant slot antennas. Optical antennas efficiently bridge the size mismatch between nanoscale volumes and far-field radiation and strongly enhance the electron-photon conversion efficiency. We achieve polarized, directional and resonantly enhanced light emission from inelastic electron tunneling and establish a novel platform for studying the interaction of electrons with strongly localized electromagnetic fields.

### 19:00

### The enabling role of graphene for on-chip photonic systems

Daniel Neumaier[1]
[1]AMO GmbH, Aachen

The hetero-integration of different photonic components is the major route to further increase the performance and functionality of silicon based microelectronic devices. For guiding and routing infrared light silicon and silicon nitride are perfect materials because of their low light interaction and high refractive indices. However, because of this low light interaction the hetero-integration of different materials is needed to realize competitive key active components like modulators and photodetectors. Graphene offers high carrier mobility, broadband and electrically tunable light interaction in combination with the possibility to integrate graphene onto nearly any substrate. By adding major photonic functionalities to the silicon based platform graphene emerged as a key enabling material for integrated photonic devices.

In this talk our latest results on graphene based electro-optical devices on silicon and silicon nitride waveguides will be presented and discussed. This includes graphene based transparent heaters for efficient tuning of the refractive index of the waveguides, ultra-fast photodetectors with a bandwidth larger 70 GHz and electro-absorption as well as electro-refractive modulators.

## 19:30

## Energy conversion and storage devices based on graphene and other 2D crystals

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Energy conversion and storage applications are currently driving the development of new materials and processes,[1] able to improve the performance of existing devices or enable new ones[2,3,4,5] that are also environmentally benign. In this context, graphene and other two-dimensional (2D) crystals are emerging as promising materials.[1−5] A key requirement for applications such as flexible electronics and energy storage and conversion is the development of industrial-scale, reliable, inexpensive production processes,[2] while providing a balance between ease of fabrication and final material quality with on-demand properties.

Here, I will briefly show the potentiality of solution-processing[2] that can offer a simple and cost-effective pathway to fabricate various 2D crystal-based flexible and energy devices, presenting huge integration flexibility compared to conventional methods. I will present an overview of graphene and other 2D crystals for flexible and printed energy devices, starting from solution processing of the raw bulk layered materials,[2] the fabrication of large area electrodes[3] and their integration in the final devices.[6,7,8,9]

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## THU 1
## Analysis of radiation sensitive defects, structures and molecules on graphene

Andreas Mittelberger[1], Christian Kramberger[1], Clemens Mangler[1], Jannik C. Meyer[1]
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With today's aberration corrected machines, atomically resolved (scanning) transmission electron microscopy (TEM/STEM) has become a standard characterization technique for nanoscaled materials, especially in the evolving field of 2D-materials. However, a big limitation is beam damage because of the high required dose of energetic electrons. While reducing the acceleration voltage to 80 kV or below can prevent beam damage in pristine graphene, defects, functional groups or molecules on the surface are still strongly affected by energetic electrons. Our recently published algorithm[1] makes it possible to reconstruct defects or single molecules on graphene from simulated STEM and TEM low-dose data. In this approach, the electron dose is distributed over many copies of the same structure which makes it possible to directly image the atomic configuration of highly beam-sensitive materials in the TEM. Depending on the dose, areas up to a few square micrometer have to be imaged with atomic resolution which corresponds to up to several thousand single images. Acquiring such amounts of data efficiently is only possible via automated methods. We present such an approach implemented on our Nion UltraSTEM 100.

[1] Ultramicroscopy, Vol. 145, pp. 13-21, 2014

## THU 2
## Silver based nanostructure for applications of chemotherapeutic delivery

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Silver nanoparticles have the potential to be used as vectors for chemotherapeutics due to their capability to enter cells. It is also known that chemotherapeutics alone can induce a risk of severe infections through immunosuppression. We have developed a silver based nanocarrier for chemotherapeutics delivery. Silver nanoparticles were obtained via reduction method and covalently functionalized with a chemotherapeutic agent. UV-Vis spectroscopy analysis was used to register the surface plasmon band for the silver nanoparticles. The dynamic light scattering technique provided data regarding size and polydispersity of the final nanostructure. For the confirmation regarding the success of the functionalization step FT-IR spectra were recorded before and after this step. In order to elucidate the shape and size of the nanostructures obtained atomic force microscopy was employed. The functionalized nanostructure presents a high potential for chemotherapeutic delivery applications.

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## THU 3
## Surface-enhanced Raman scattering within perturbation theory

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Surface-enhanced Raman scattering (SERS) is the giant enhancement of the Raman scattering cross section for a molecule on a rough metal surface. The major underlying enhancement mechanism is the coupling of the Raman scatterer with the localized surface plasmon of metallic nanostructures. The widely used theory of electromagnetic enhancement treats the plasmonic nanostructure as an external antenna that enhances incoming and scattered light. Instead, we include the plasmonic excitation into the microscopic description of the Raman process and describe SERS as higher-order Raman scattering. To obtain analytic expressions for all coupling matrix elements, we employ a formalism that is based on the second quantization of the localized surface plasmon. We calculate the plasmonic enhancement of a molecule in the hot spot of a plasmonic gold nanodimer. Independent of the type of molecule, it is several orders of magnitude stronger than predicted by the current electromagnetic enhancement theory, in excellent agreement with recent experiments. To demonstrate the fundamental validity of our approach, we also apply our theory to graphene as a solid-state SERS probe.

## THU 4
## The ultimate performance of single-walled carbon nanotubes as transparent conductors?

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The ultimate performance—ratio of electrical conductivity to optical absorbance—of single-walled carbon nanotube (SWCNT) transparent conductive films (TCFs) is an issue of considerable application relevance. We have in our recent report presented the first unambiguous experimental evidence that SWCNT bundling is detrimental for TCF electro-optical performance [1]. We provide an explanation of the loss in performance as an effect of gratuitous absorbance related to a greater carbon content in large diameter bundles, which is not compensated by the simultaneous

gains achieved in bundle conductivity. As an outcome we present a semi-empirical absorbance-conductance model, suggesting an ultimate limit for pristine SWCNT TCF performance at 80 ohms per square at 90% transparency.

[1] Mustonen et al., Uncovering the ultimate performance of single-walled carbon nanotube films as transparent conductors, APL 107 (2015).

### THU 5

### Scattering near-field optical microscopy on metallic and semiconducting nanotube bundles in the infrared

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We demonstrate that scattering-type near-field optical microscopy (s-SNOM) at infrared frequencies can be effectively used to distinguish between carbon nanotube (CNT) bundles based on their electrical properties. Samples from separated metallic and semiconductor nanotubes and their mixtures were investigated using infrared lasers under near-field conditions [1]. In this frequency range, the difference in the free-carrier concentration between metallic and semiconducting tubes is expected to influence the properties of the scattered light. The obvious difference in the optical phase images proves that this is indeed the case: the metallic and semiconducting bundles are unambigously identifiable in the sample, even in case of 4 nm diameter bundles. The measurements match qualitatively with our calculations based on the extended finite dipole model using the known optical functions of the constituting nanotubes [2].

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### THU 6

### Opto-valleytronic imaging of layered semiconductors

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Monolayer transition metal dichalcogenides such as molybdenum disulfide ($MoS_2$) exhibit a direct bandgap and provide a unique optical interface to explore and control the valley pseudospin degree of freedom [1, 2]. We use cryogenic microphotoluminescence spectroscopy to study extended $MoS_2$ crystals grown by chemical vapor deposition and transferred onto silicon oxide substrates. By performing confocal raster-scan photoluminescence imaging of individual single- and poly-crystalline

flakes, we map out variations in the crystal quality and identify disorder such as point or line defects. Two-dimensional polarimetry complements our studies by identifying spatial profiles of the valley degree of freedom in single- and poly-crystalline $MoS_2$ monolayers for scalable opto-valleytronic devices [3]. Furthermore, by means of opto-valleytronic imaging of the valley polarization in a perpendicular magnetic field [4], we find regimes of thermal and non-thermal exciton valley populations that are sensitive to disorder.

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## THU 7

## Emerging Kondo screening and many-body Kramers entanglement in a carbon nanotube

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The entanglement of quantum states is at the heart of the Kondo effect. In its simplest realization, interactions between a localized spin and itinerant electrons give rise to an entangled singlet ground state with no net spin. Carbon nanotubes offer the possibility to study the emergence of this entanglement in a system with orbital and spin degrees of freedom by simply tuning a gate voltage. Here we investigate the magnetospectrum of a carbon nanotube and find the disappearance of some inelastic excitation lines when sweeping the gate voltage from the weak to the strong coupling regime where Kondo behavior is observed. We consider the global $SU(2) \otimes SU(2)$ symmetry associated to the two Kramers channels of a carbon nanotube and find that only excitations involving flips of the Kramers pseudospins are observed in the Kondo regime, revealing that are those pseudospins to be fully screened by the conduction electrons.

## THU 8

## Local optical absorption spectra of monolayer $MoS_2$ crystals revealed by scanning near-field optical microscopy measurements

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Transition metal dichalcogenide (TMDCs) and their van der Waals (vdW) heterostructures are attracting a lot of interests due to their unprecedented optical properties. Their optical properties significantly are influenced by local structures such as defects, grain boundaries. Thus, it is of great importance to reveal the relationships between local structures and corresponding optical properties. Here, we revealed local optical absorption spectra of single layer $MoS_2$ and h-BN-$MoS_2$ vdW heterostructures with a maximum spatial resolution of 100 nm using scanning near field optical microscopy (SNOM) combined with a supercontinuum laser light-source. Optical absorption spectra did not shown regional difference such as the edge or center, however, significant site-dependence, which would be mainly caused by the presence of vacancies or strains, was observed.

### THU 9

### Synthesis of Magnetic Molecular Complexes with Fullerene Anchor Groups for Single-Molecule Junctions with Epitaxial Graphene Nanoelectrodes

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In molecular electronics, the main objective is to fabricate electronic devices in which the active moieties (e.g. transistors, diodes or switches) are built from individual molecules. Along this front, a series of tailor-made paramagnetic bis-fullerene derivatives capable of bridging two adjacent graphene (G) sheets for performing magnetic single-molecule junctions (SMJ) have been developed. Specifically, magnetic molecular wires of Fe(II) and Co(II) in an octahedral environment endowed with C60 end groups have been synthetized. The use of C60 units as anchoring groups improves the contact between the G electrodes in comparison with the conventional Au-selective anchoring groups. This will result in a more electronically transparent contact, moving the principle transport barrier deeper into the molecule. Our first results show that the C60/G combination is excellently suited for improving experiments on SMJ. In addition, we identified that the external applied magnetic field has a measurable influence on the transport characteristics. These experiments will allow studying the Kondo physics, and more concretely the "Kondo in a box" phenomena through single-molecule experiments.

### THU 10

### Low-Frequency Raman Spectroscopy of Transition Metal Dichalcogenides: Layer Number and Stacking Configuration

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Layered transition metal dichalcogenides (TMDs), have attracted much attention recently due to their exceptional properties. Raman spectroscopy can be used to reveal a wealth of information about 2D materials in a fast and non-destructive manner. In particular, investigation of the low-frequency shear (SM) and layer-breathing modes (LBM) has been suggested as a universal method of layer number determination and characterisation of 2D materials.
Here we present low-frequency Raman analysis of $MoS_2$ and $MoSe_2$ grown by chemical vapor deposition[1]. Spectra are acquired over large areas allowing changes in the position and intensity of the SM and LBMs to be visualised in maps[2]. This allows detailed characterisation of mono and few-layer TMDs which is complementary to well-established (high-frequency) Raman and photoluminescence spectroscopy. This study also allows the identification of stacking configuration in these materials which we demonstrate for various 2H and 3R stacking orders up to 4 layers[3].

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## THU 11

## Structural, optical and electrophysical properties of films formed from single-wall carbon nanotubes filled with CuCl

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Conductive electrodes for optoelectronics are produced from materials with a high optical transparency and a low electrical resistance. Today the most popular material is indium tin oxide (ITO). In this work we propose and investigate a new material being able to replace ITO. This is a thin film of single-wall carbon nanotubes filled with different acceptor molecules.The filling of aerosol-grown SWNTs was performed from a gas-phase. From HRTEM images the formation of one-dimensional crystals inside nanotubes has been seen. The optical spectroscopy has shown a Fermi level shift into a valence band and a complete metallization of the nanotubes. We have measured the electrical resistance of filled SWNT films and registered a big drop of electrical resistance (of one order of magnitude). The best values were 50 Ohm/square at 90% transparency. The temperature dependence of resistance (R(T)) demonstrated two contributions – from inter-tube interactions and from filled nanotubes by themselves. For the stronger acceptor (CuCl instead of iodine) the minimum value of R(T) shifted toward low temperatures. This approach opens a new way to form the electrodes for optoelectronics.

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## THU 12

## UV laser patterning of $C_2F$ films for electrochemical microelectrodes

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The fluorinated graphite with composition $C_2F$ was synthesized using low temperature fluorination by $BrF_3$ from natural graphite. Suspension of fluorinated graphene in toluene was used to produce films having a thickness of 0.1 - 1 micron. The $C_2F$ films were prepared on polymeric substrates and in free standing forms. These films were characterized by XPS and NEXAFS. They had a high resistance and became conductive after UV irradiation. The changes in the microstructure and conductivity were found to depend on the radiation dose. Pattern of microelectrodes was drawing by UV laser and supercapacitors properties of these elements were measured.

## THU 13

## Magnetic Field Studies Near Superconducting Transition in MBE Grown Monolayer $NbSe_2$ on Bilayer Graphene

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$NbSe_2$ has been shown to be superconducting at reduced thicknesses down to the monolayer limit by works from Frindt[1], Staley et. al.[2], Tsen et. al.[3], Cao et. al.[4] and Xi et. al.[5]. Most of the studies used $NbSe_2$ from mechanical exfoliation and encapsulation with another layered material to protect from air. In this work, we have investigated the superconductivity in monolayer $NbSe_2$ prepared by molecular beam epitaxy growth (MBE) on bilayer graphene (BLG)[6]. The superconducting transition has an onset temperature of 1.9K, midpoint temperature of 0.65K and reaches zero resistance at 0.46K. The upper critical field perpendicular to the $NbSe_2$ monolayer is 0.5T at 100mK. We have observed unusual behavior in magnetoresistance near $T_c$ in this material and will compare with existing theories.

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## THU 14

## The effects of encapsulation on the opto-electronic properties of $MoS_2$

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$MoS_2$ is a semiconductor with a direct band-gap of 1.9 eV in single layer form[1]. Transistors and photodetectors made with $MoS_2$ as the conducting channel, show high on-off ratio, moderate mobilities and ultra-high responsivities[2,3]. Nevertheless, like in the case of graphene, the device performance is strongly dependent from the environment and the substrate as well as from the quality of the contacts. Encapsulated $MoS_2$ devices with graphene contacts exhibit superior characteristics, but the fabrication of these devices is more complicated[4]. In our work we explore the encapsulation of single layer $MoS_2$ with boron nitride in addition to 1T-$MoS_2$ side contacts. With this method we plan to improve the carrier transport and the contact resistance of the devices without the use of graphene to side contact the $MoS_2$ channel. Moreover by choosing the right thickness of the top boron nitride layer the photocurrent and the performance of a photodetector can be enhanced.

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3. Lopez-Sanch

## THU 15

## Ultrafast photocurrent dynamics in monolayer $MoS_2$

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Atomically thin semiconducting transition metal dichalcogenides such as $MoS_2$ are emergent materials for optical and electronic circuits. For possible high-frequency applications, we investigate the ultrafast photocurrents in monolayer $MoS_2$ on a picosecond time scale utilizing a recently developed pump-probe spectroscopy [1-3]. The observed photocurrent contains three major contributions [4]. An initial ultrafast response of $\leq 5$ ps is followed by an exponential decay within a few hundreds of picoseconds. The third very slow contribution peaks at around 1.5 ns. This slow part dominates the overall time-integrated photocurrent intensity. We discuss the impact of laser-induced heating, the one of built-in fields at metal contacts, and the role of trap states.

We acknowledge the financial support by the ERC-grant "NanoREAL", the DFG excellence cluster "Nanosystems Initiative Munich" (NIM), and BaCaTec.

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## THU 16
## Cloaking by pi-electrons in the infrared

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Hybrid materials composed of single walled carbon nanotubes (SWNT's) as hollow containers and small molecules as fillers possess intriguing physical and chemical properties. The usual method of choice to characterize hybrid systems is infrared spectroscopy. However, in this case the experiments showed a surprising negative result: regardless of the type of small molecule filled in the SWNT the IR spectrum of the hybrid system remains silent [1,2]. The possible explanation involves the highly polarizable $\pi$-electron system of the SWNT's. Image charges induced in the SWNT walls cancel out the transition dipole moment of the molecular vibrations resulting in the cloaking of the material inside the nanotube. To confirm the role of the $\pi$-electron system in this process, insulating boron nitride nanotubes filled with $C_{60}$ were also investigated. We have also demonstrated the effect in two dimensions using a thin film of $C_{60}$ covered by single layer graphene. The significance of our results lies in the fact that the cloaking layer is a real material, not a metamaterial.

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### THU 17
### Progress in disentangling charge transfer and hybridization of functionalized nanotubes

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In this contribution we will present recent progress on unraveling the influence of charge transfer, local strain and hybridization on the electronic transport properties of SWCNT and DWCNT with special emphasis on the influence of basic correlation effects on the two particle excitation and the nature of the metallic ground state. In order to tailor their properties we will compare different functionalization routes (sidewall functionalization, intercalation and advanced filling reactions e.g. with metallocenes and metalacetylacetonates followed by nanochemical reactions) and use resonance Raman, photoemission and x-ray absorption spectroscopy as probes.
Work supported by FWF and the EU.

### THU 18
### The European Graphene Flagship

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Being "the EU's biggest research initiative ever", the Graphene Flagship aims at taking graphene and related layered materials from a state of potential use to industrial revolution, creating new opportunities of economic growth in Europe. The Graphene Flagship brings together academic and industrial research in a consortium, which has the aim of realizing breakthroughs in scientific and technological innovation.
The Flagship will focus on selected topics where Europe can make a difference, both in terms of the underlying science and the possibility to exploit the research results commercially. These areas include printable and flexible electronics, high-frequency electronics, spintronics, photonic and plasmonic components, and integrated opto-electronic systems taking advantage of the specificities of graphene. Together, the scientific and technological objectives and operative targets will allow the Flagship to contribute to a sustainable development by introducing new energy efficient and environmentally friendly products based on carbon and other abundant, safe and recyclable natural resources.
This ten-year-long, 1000 million Euro research and innovation initiative has involved in an initial "ramp up" phase the activities of 142 academic and industrial partners i

### THU 19
### Picosecond light pulse generation from waveguide-coupled CNTs

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CNTs have recently been integrated into optical waveguides and operated as electrically-driven light emitters (1). Such devices could be of interest for conversion of fast electrical signals into optical within a nanophotonic circuit. Using time correlated single photon counting method we demonstrate that individual waveguide-integrated CNTs can be operated as high-speed transducers by probing picosecond light pulse generation in the GHz frequency range. These results show the potential of CNTs as high-speed light source for on-chip data communication.

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### THU 20

### Theoretical study of the Raman G peak intensity of graphene

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We present a detailed theoretical study of the Raman G peak intensity in graphene. Going beyond and improving on an earlier theoretical study by Basko [1], which relied on an analytical calculation in certain limits, we implemented a numerical calculation of the G peak intensity via a diagrammatic approach. We investigate the dependence of the G peak intensity on both the excitation energy and Fermi level. Furthermore, we demonstrate the relative importance of the different subprocesses, identify the dominant electronic transitions, and investigate the contribution of quantum interference terms.

References:

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### THU 21

### Encapsulated transition metal nanowires by cross sectional scanning transmission electron microscopy

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By vertically stacking different two dimensional crystals, Van der Waals heterostructure devices with bespoke bandstructure and enhanced functionality can be fabricated. The main advantages of these structures are the fine control of carrier injection across hexagonal boron nitride (hBN) tunnelling barriers and the atomically flat interfaces which arise from the self cleaning phenomenon.[1]
Using cross sectional high resolution scanning transmission electron microscope (STEM) imaging we show it is possible to preferentially sputter monolayer transition metal dichalcogenides to form metallic nanowires[2] whilst maintaining hBN encapsulation. This arises from the relatively high displacement cross sections of the chalcogen species and could lead to hybrid vertical-lateral heterostructures with lithographically patterned metallic domains.

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[2] Lin et al., Nature Nanotech 8, 436-442 (2014)

### THU 22
### Anomalous thermo-piezo-electric behavior of nanocomposites based on topologic-insulator platelets

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Thermo/Piezo -electric materials integrate a thermoelectrically active, heterogeneous, nanophase into a piezoactive host matrix. In such materials, stress induced internal fields of the host modify the thermoelectric properties of the conducting components in a way which is strongly dependent on the electronic structure of the nanophase. This leads to significant, stress-induced increases in the thermopower for carbon nanotube (CNT) based composites. Further, the increase in thermopower, for the CNT case, grows when the CNTs are doped by using charge donating or charge extracting moieties on the outside of the tube (contact doping). For CNTs the stress-induced change in thermopower is linear with this dopant level, however this is not the case for nanocomposites based on doped, nanoplatelets of topologic insulators (TIs) such as BiSe and (Bi,Sb)Te. In this work we demonstrate an extreme sensitivity in the thermoelectric response for TI nanoplatelets as the nanoplatelets are analogously doped. Further we compare these results to a newly synthesized organic 2D topological insulator: Nickel Bis(dithiolene) (Ni3C12S12). The composite topological systems can achieve a ZT = 0.75 and power factors exceeding 1000 $\mu$W/mK2 with these numbers increasing under applied stress.

### THU 23
### Luminescence properties of hexagonal boron nitride layers

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Hexagonal boron nitride is a wide band gap semiconductor (6.4 eV), which can be synthesized, as graphite, its carbon analog, as bulk crystallites, nanotubes and layers. These structures meet a growing interest for deep UV LED and graphene engineering [1]. We attempt to have a better comprehension of the optical and electronic properties of thin BN layers, in correlation with their structural properties and to better know how electronic properties of graphene can be impacted by underlying BN layers.

In this work, we first investigate by cathodoluminescence (CL) the optical properties of different hBN sources (HPHT, PDCs and commercial samples) in the 5-6eV energy range. Then, thin h-BN layers have been obtained by mechanical exfoliation from a commercial powder and a single crystal. We focused first on the D series, emitted at lower energy (5.2-5.7 eV) on folded flakes and measured a strong enhancement of these defects lines along the fold. Finally, we analyzed defect free hBN flakes with various thicknesses from 100L to 6L and observed a significant effect of the confinement on the luminescence, especially in the energy range 5.7-6 eV.

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### THU 24

## Mass Sensing with Graphene and Carbon Nanotube Resonators

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In recent years nanoelectromechanical resonators made out of carbon nanotubes and graphene have attracted much attention thanks to their great potential for high resolution mass sensing as well as for the study of diffusion effects [1] and phase transitions [2]. A nanoelectromechanical resonator allows to extract the mass of molecules by measuring the shift in the resonance frequency when molecules get adsorbed onto the resonator. In this work we aim to achieve single molecule mass resolution with graphene nanomechanical resonator. The record of mass resolution achieved with a Carbon nanotube resonator is 1.7 yg [3]. Up to know we managed to observe the adsorption of fullerene molecules onto a graphene resonator and we estimated its mass resolution with frequency stability measurements to be around 15.4 zg. With a single molecule on our resonator we expect to contribute to the understanding of the sources of frequency fluctuations of mechanical resonators.

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### THU 25
### Quantized one-dimensional edge channels with strong spin-orbit coupling in 3D topological insulators

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For thin films of bismuth chalcogenides, we report on millimeter-scale edge channels with a conductance quantized at a single quantum 1 $e^2/h$ at zero magnetic field. The quantum transport is found at the lateral edges of micro-fabricated circuits. The data are consistent with a lateral, one-dimensional quantum confinement of non-topological surface states with a strong Rashba spin-orbit coupling. This edge transport can be switched on and off by an electrostatic field-effect. Our results are fundamentally different from an edge transport in quantum spin Hall insulators and quantum anomalous Hall insulators.

### THU 26
### Alkali metal doped one-dimensional graphene nanoribbons: a combined ARPES and UHV Raman study

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We perform charge transfer doping of massively parallel N=7 armchair graphene nanoribbons grown along the step edges of Au(788) surface. The samples were characterized by STM, LEED, polarized Raman and ARPES. Using ARPES and in-situ Li deposition we indeed observe the appearance of the conduction band below the Fermi level which is proof that we induced a semiconductor to metal transition in a 1D ribbon. The enhanced screening caused by the extra electrons strongly renormalizes the effective electron mass yielding an almost free electron energy parabola in 1D. ARPES data of the Li-doped ribbons provide information about the quasiparticle band gap, which is estimated to be equal to 2.1 eV. We then perform the bubble transfer procedure of nanoribbons from the Au to a quartz substrate in order to measure photoluminescence, which give an excitonic band-gap equal to 1.95 eV. To monitor the changes in the Raman spectrum upon Li doping we have purpose built a unique ultrahigh vacuum (UHV) Raman spectrometer. This allows us to observe drastic changes in the Raman spectrum, in particular near the G-mode, and the shifting of the resonant Raman energy.

## THU 27
## Josephson scanning tunneling microscopy and Josephson switching current

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Employing the I(V)-characteristics of a scanning tunneling microscope (STM) Josephson junction to directly determine the local order parameter of a superconductor would give a powerful tool to understand superconductivity on the atomic scale. To realize this technique the fundamental physical aspects of the junction and the defining phenomena have to be understood (1,2). For example the energy scales of Josephson coupling, capacitive coupling and temperature define the character of the tunneling particles. Performing not only voltage but also current biased measurements of the same junction gives us a new approach to study the physics involved in the Josephson effect. Comparing the switching current in both approaches indicates which regime the junction is operated in. Opposing conventional planar tunneling geometries, STM allows for precise control of the tunneling resistance and makes it possible to tune the Josephson coupling energy. Using this ability we find the switching current to be proportional to the square of the Josephson coupling energy.

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(2) C.R. Ast, et al., arXiv:1510.08449, 2015.

## THU 28
## Extended Spiropyran-SWNTs conjugated complexes: A new class of photochromic materials

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Here we report about a nondestructive, controlled synthesis of covalently functionalized single walled carbon nanotubes. The covalent decoration of the tubes' sidewall, even at high density of functional groups, does not disrupt their extended sigma network and preserves their unique quantum optoelectronic properties. Our scheme provides a strong platform to immobilize desired functional species on the nanotubes sidewall.

By conjugating the photochromic molecular switching spiropyran/merocyanine moiety to the tubes, we create novel heterostructures exhibiting phenomenology not observable in standard functionalization approaches. Changes in the physical and chemical properties of the two isomeric configuration of the photochrome result in different interactions with the tubes. In this way, we are able to to quench the emission of our complexes by exposing them to radiation of the proper wavelength.

## THU 29
## Revealing the band gap of long linear carbon chains

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The band gap of short linear carbon chains (LCCs) with less than 44 carbon atoms has been well studied in ether gas phase [1] or in solvent [2]. However, the band gap for long LCCs (LLCCs) still keeps unknown due to the lack of proper stable samples. Recently, we successfully synthesized extremely long LCCs composed of thousands of carbon atoms inside double walled carbon nanotubes (DWCNTs) [3]. Unlike the normal method tested by absorption spectroscopy, here the band gaps of those LLCCs were revealed by resonance Raman spectroscopy under various temperatures, because of the indistinguishable absorption of LLCCs compared to the absorption of their host nanotubes. The results show that the band gaps of LLCCs in the range of 1.8 - 2.3 eV inversely proportional to their lengths, which is also perfectly consistent with our DFT calculations.

We thank the FWF (NanoBlends I 943–N19) and the EU.

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## THU 30
## Synthesis and characterization of unconventional fullerene peapods

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We present evidence pointing to the possible synthesis of unconventional $C_{66}$ and $C_{68}$ fullerenes in the interior of single walled carbon nanotubes. The production proceeds from $C_{60}$-toluene/benzene clathrates encapsulated inside the nanotubes using heat-driven nanotesttube chemistry. All isomers violate the so-called isolated pentagon rule and are stabilized solely by the proximity of the wall of the host nanotube. We present detailed characterization of the unconventional fullerenes using Raman spectroscopy, $^{13}C$ isotope labeling of the benzene molecules, transmission electron microscopy, X-ray diffractometry, and first-principles calculations. Multiple isomers of both $C_{66}$ and $C_{68}$ are identified in the sample. We argue that our method opens the way to high-yield synthesis of unconventional fullerenes [1].
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## THU 31
## Kinetics of oxidation of graphite and reduction of graphene oxide

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Oxidation process of graphite leads to exfoliation of graphene oxide (GO) single layers turning to electrical insulator. In order to restore the graphene properties, oxide groups must be removed. At the process of reduction, the atomic structure degrades together with material properties expected for graphene. In this work we study kinetics of the oxidation process of graphite in order to find the lowest oxidation stage when the exfoliation of graphite to single layers is possible. The goal is to minimize the degradation of the atomic structure and, consequently, of the graphene electronic properties. We study evolution of intercalation of oxygen between graphitic layers correlating the content of oxygen with the interlayer distance in graphite crystal, using XPS and XRD analyses along different steps of oxidation process. Atomic structure of the exfoliated GO layers is further characterized by STEM down to atomic level. Removal of the oxide groups from GO was achieved by heating and the reduction process was recorded by DSC and TGA. The effect of reduction temperature on electronic transport, optical absorption and Raman spectra will be also presented.

## THU 32
## Double walled carbon nanotubes shock-compressed to 0.5 MBar

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Following our dynamic (shock wave) compression experiments on single walled (SW) carbon nanotubes CNTs [1] we probed the limit of structural integrity of CVD-grown double walled (DW) CNTs at shock pressures up to 0.5 MBar. In the different runs the pressure was ramped to a certain level between 6 and 52 GPa with a new CNT sample but from the same source batch. The recovered after shock material was characterized by Raman and HRTEM. Two distinct pressure ranges were identified: a steep increase of D/G-band intensity ratio at 30 GPa and a substantial altering of the spectrum at 52 GPa (2D-band shift and evolution of the D+G, 2G modes). By analogy to SWCNTs we associate the observed effects with the onset of extended structural damage and complete destruction of the DW CNTs respectively which is directly confirmed by HRTEM via observation of outer wall disruption, "unzipping" and shortening of the CNTs induced by shock. No CNT trace is detected after 52 GPa. Consequently, the DWCNTs demonstrate a remarkable resilience to the impact load. We compare SW- and DWCNT response to shock and analyze the products of CNT transformation.
[1] M. Noël, et al. Phys. stat. sol. (RRL), 8, 11, 935 (2014)

## THU 33
## Mechanically tunable strain fields in suspended graphene by micro electromechanical systems

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As graphene is only one atom thick, it is highly susceptible to external influences, leading e.g. to a crystal lattice that is easily distorted. These distortions, or strain variations, can induce pseudomagnetic fields, which allow for pseudospin flips that, in turn, limit the mobility in high-quality graphene devices (1). This shows the importance of understanding the electromechanical coupling of graphene. Thus, a precise control over strain fields in graphene is high up on the wish list of experimentalists. Here, we demonstrate the realization of controllable strain fields in suspended graphene by coupling it to Si-based electrostatic micro-actuators. An actuator can theoretically apply more than 10% of strain and can operate at cryogenic temperature, allowing the investigation of quantum effects in electromechanical systems.
By means of Raman spectroscopy we characterize various strain distributions (max. 0.5% strain) in graphene. The Raman analysis confirms the accurate tuning of ap-

plied strain by the actuators independent of doping effects. This precise control over strain distributions opens up a wide field of possible experiments, ranging from strain dependent transport to strain induced pseudomagnetic fields.
(1) Couto et al., Phys.Rev.X 4, 041019 (2014)

## THU 34
## Magnetic field induced electron-vibron coupling in a carbon nanotube quantum dot

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Quantum dots defined in suspended single wall carbon nanotubes define a nanoelectromechanical system where clear quantized harmonic oscillator behaviour becomes visible. We present transport measurements on a clean nanotube device tuned to the few electron regime, i.e., having a highly localized electronic system. Here, we demonstrate the emergence of Franck-Condon sidebands in single electron tunneling, corresponding to the longitudinal vibration, induced by a finite magnetic field along the carbon nanotube axis. The Franck-Condon coupling factor $g$ increases with magnetic field and saturates at $B \approx 5$T. The behaviour of the sidebands attached to different electronic quantum states is compared, and tentative models are discussed.

## THU 35
## Atomic vibrations in graphene: modeling, measurement and implications

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Graphene is an ideal material for precision studies of electron irradiation. Previously, to model atomic vibrations that activate low-probability processes due to the momentum of a vibrating target nucleus, a 3D Debye model [1] with an out-of-plane Debye temperature derived from phonon calculations [2] was used.
We develop a better justified model by considering the partition of kinetic energy due to the thermal occupation of phonon modes derived from DFT. This allows us to provide an accurate estimate for the mean-square velocity, and predict the knock-on cross sections. Comparing these to irradiation measurements of pristine $^{12}$C and $^{13}$C graphene allows us the assess the accuracy of DFT simulations.
The formalism is equally valid for modeling the mean square displacement (MSD) of atoms, which was recently measured for both the in-plane and out-of-plane directions via electron diffraction [3]. We analyze the data by separately considering each phonon mode, allowing us to disentangle their contributions and to clarify how the experiment is limited by crystallite sizes and the coherence of the beam.

[1] J.C. Meyer et al., PRL108, 196102 (2012)
[2] V.K. Tewary and B. Yang, PRB79, 125416 (2009)
[3] C.S. Allen et al., JAP118, 074302 (2015)

### THU 36

### Direct imaging of two-dimensional charge density wave phase in TaS2 single layers

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Truly two-dimensional many-body states are of fundamental importance as they can provide model systems for understanding the complex physics of interacting electron systems. Bulk TaS2 is known as a charge density wave (CDW) material with one of the richest electronic phase diagrams hosting CDW states stable high above the room temperature. However, several recent studies indicate that this collective phase is suppressed as we thin down the crystals towards the 2D limit. So far it was not clear whether this is due to the intrinsic three-dimensional nature of the correlated states or to the increasing disorder as we approach the atomically thin limit. Here we report the direct observation of a CDW phase in single layer TaS2 by atomic resolution Scanning Tunneling Microcopy measurements. Our measurements revealed a spectacular electronic phase transition as the crystal structure crosses the 3D/2D (bilayer/monolayer) frontier.Our results unambiguously prove the existence of two-dimensional collective electronic states, and open a new route towards engineering novel quantum phases by scaling down the thickness of materials to the single layer level.

### THU 37

### Hybrid van der Waals heterostructures of 0D and 2D carbon materials

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Van der Waals (vdW) heterostructures based on the stacking of atomically thin two-dimensional (2D) sheets represent a new class of layered nanomaterials with many promises in materials science and experimental physics. Here we present a modular and highly applicable approach to integrate other low-dimensional materials into

vdW heterostructures employing ∼1 nm thick bifacial Janus Carbon Nanomembranes (Janus CNMs) with distinct functional groups on their opposite faces as the elementary building block. We selectively functionalize the opposite faces of Janus CNMs with fullerenes (C60) or gold nanoparticles (Au NPs) and assemble them into layered stacks characterizing both chemical and physical properties by X-ray photoelectron spectroscopy, helium ion microscopy and mechanical bulge tests. We unambiguously show that the engineered Janus CNM/(C60-Janus CNM)n (n=1, 2 and 3) hybrid heterostructures possess high robustness, chemical homogeneity and can be assembled on the large scale (cm2). The developed approach paves the way to complex hierarchical layered materials for applications in nanoscience and nanotechnology.
Z. Zheng et al., Nanoscale 7 (2015) 13393-13397

## THU 38
## Functionalized-Graphene Enhanced Raman Scattering

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Surface enhanced Raman scattering (SERS) is a well-established technique, which enables measurement of very low molecular concentrations. In 2010 a concept of graphene enhanced Raman scattering (GERS) was proposed and demonstrated [1]. Contrary to SERS, GERS is suggested to offer better homogeneity of the enhanced signal because of the flatness of the graphene layer. Furthermore, it was demonstrated that GERS enhancement shows a strong molecular selectivity [2]. In this work we investigated the effect of GERS on Rhodamine 6G (R6G) test molecules using variously functionalized CVD-grown graphene samples: fluorinated, thiophenol functionalized and diazonium functionalized graphene. The enhancement of the R6G signal on the functionalized graphene was compared to the enhancement of the R6G on a pristine graphene samples, showing lower enhancement of fluorinated and thiophenol functionalized graphene, while diazonium functionalized graphene showed comparable enhancement to the pristine graphene sample.

(1) X. Ling, L. Xie, Y. Fang, H. Xu, H. Zhang, J. Kong, M. S. Dresselhaus, J. Zhang, Z. Liu, Nano Lett. 2010, 10, 553.
(2) S. Huang, X. Ling, L. Liang, Y. Song, W. Fang, J. Zhang, J. Kong, V. Meunier, M. S. Dresselhaus, Nano Lett. 2015, 15, 2892.

## THU 39
## Nanoscale Imaging of Charge Transport in Van der Waals systems

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Charge transport experiments are intrinsically limited by the finite number of terminals used (typically two or four). Hence, local resistance variations due to defects, discontinuities in the band structure, or other inhomogeneities cannot be resolved. Here, we present measurements on electrically contacted graphene (single to triple layer), for which we have overcome this limitation. For this, we have developed a new method, that allows us to locally determine the potential variations in a sample. Our contactless potentiometry method is based on low-energy electron microscopy (LEEM), an imaging technique for which the detected intensity depends sensitively on the electron landing energy. Specifically, we use the property that incoming electrons that are exactly resonant with (graphene) interlayer states show a minimum in reflection intensity [J. Jobst et al., Nature Comm. 6, 8926 (2015)].
In this meeting, we will present measurements on electrically contacted graphene as a prototype quasi-2D system. [J. Kautz et al. Sci. Rep. 5, 13604 (2015)]. Our method, however, is straightforwardly extendable to other quasi-2D systems, most prominently to the exciting class of layered van der Waals materials.

## THU 40

## Atomic and electronic structure of native point defects of MoS2 single layers

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Transition metal dichalcogenide single layers are in the focus of scientific attention due to their intrinsic direct bandgap and various intriguing properties. However, the presence of defects even at low concentration substantially affects the electronic properties [1]. In this work we provide a study of the atomic and electronic structure of point defects in single-layer MoS2 comparing STM topography data with density functional calculations. Our atomic resolution STM measurements on single layers of MoS2 prepared by a novel exfoliation technique [2] show various types of point defects at high concentration. Using DFT calculations sulfur vacancies are identified as the most often observed point defects with their characteristic defect states in the bandgap. Further point defects like disulfur vacancies are also observed and investigated.
Our results provide experimental and theoretical insight into the electronic properties of the native defects of 2D MoS2 crystals which is essential for understanding the operation of realistic devices based on MoS2 single layers.

[1] J.-Y. Noh, et al., Phys. Rev. B 89(2014) 205417
[2] G. Zs. Magda, et al., Sci. Rep. 5(2015) 14714

## THU 41
## Diamond growth on reticulated vitreous carbon foam from polyvinyl alcohol based solutions with nanodiamonds

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Polycrystalline diamond film represents a promising material for biological or electrochemical applications due to its inherent physical and chemical properties: thermal and chemical stability, stable surface when functionalized with biomolecules, chemical inertness, etc. Recently, porous self-standing diamond structures become highly attractive as electrically active scaffolds in microfluidic perfusion culture systems, sensitive gas sensors or supercapacitors. In this contribution we investigate the growth of diamond thin film on reticulated vitreous carbon foam. The effect of the concentration ratio of polyvinyl alcohol (PVA) and nanodiamonds (NDs) on the foam nucleation (seeds density, clustering) as well as the consecutive diamond growth mechanism (substrate etching, polymer transformation) will be presented. The PVA/NDs composite will be shown as an alternative treatment route for diamond growth on porous carbon foam. The obtained results underlines a technological importance of such a 3D polymer based nucleation on diamond growth rate and preserving foam base structure. The suitable proportion of the PVA/NDs lead to a formation of diamond coating on porous graphite based foam.

## THU 42
## Photoluminescence from Liquid-Exfoliated $WS_2$ Monomers in Poly(Vinyl) Alcohol Polymer Composites

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While liquid phase exfoliation can be used to produce nanosheets stabilized in polymer solutions, very little is known about the resultant nanosheet size, thickness, or monolayer content. The present study uses semiquantitative spectroscopic metrics based on extinction, Raman, and photoluminescence (PL) spectroscopy to investigate these parameters for $WS_2$ nanosheets exfoliated in aqueous polyvinylalcohol (PVA)

solutions. By measuring Raman and PL simultaneously, the monolayer content via the PL/Raman intensity ratio can be tracked while varying processing conditions. The PL can be maximized with polymer concentration. In addition, the monolayer content can be controlled via the centrifugation conditions, exceeding 5% by mass in some cases. These techniques have allowed tracking the ratio of PL/Raman in a droplet of polymer-stabilized WS2 nanosheets as the water evaporates during composite formation. No evidence of nanosheet aggregation is found under these conditions although the PL becomes dominated by trion emission as drying proceeds and the balance of doping from PVA/water changes. Finally, bulk PVA/WS2 composites are produced by freeze drying where $>$ 50% of the monolayers remain unaggregated, even at WS2 volume fractions as high as 10%.

### THU 43

### The effects of the number of layers and illumination on electrochemical properties of $MoS_2$

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The diverse electronic, optical, and mechanical properties of two-dimensional (2D) crystals make them highly suitable materials for electrochemistry-related applications, such as energy storage/conversion, electrocatalysis, and sensing. Understanding the key electrochemical behaviour of 2D crystals is critical for their successful implementation in these applications.

Molybdenum disulphide is one of the most promising and widely studied semiconducting 2D materials. Nevertheless, the electrochemistry of an isolated monolayer of $MoS_2$ has not been achieved to date. Using a unique microscale electrochemical probe, we measured the electron transfer kinetics and electric double-layer capacitance of pristine monolayer and few-layer $MoS_2$ and showed their strong dependence on the number of $MoS_2$ layers and illumination intensity. The differing relationships between the electron transfer kinetics and illumination power density of monolayer and bulk $MoS_2$ are rationalised based on the different light absorption and charge carrier diffusion mechanisms in these materials. This study highlights the opportunities for tuning of the electrochemical performance of $MoS_2$.

### THU 44

### Field Induced Dissociation of Excitons in $MoS_2$ Monolayer

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Despite the high exciton binding (>0.5 eV), monolayer $MoS_2$ transistors show a photovoltaic effect and potential as a photodetector. We exploit field assisted ultrafast spectroscopy to probe exciton dynamics and charge generation when an in-plane field is applied and charge injection is prevented by the appropriate gate voltage. In monolayer $MoS_2$, the starting photoexcited population is dominated by hot excitons that relax with a characteristic time of 800 fs, branching into mainly relaxed excitons and a smaller population of dissociated electron-hole pairs. An in-plane electric field around 8000V/cm increases the charge formation, detected as an enhancement of their characteristic photo-induced absorption features. The characteristic time of the exciton dissociation is 600 fs, slightly less than the exciton relaxation time without electric field. Hence the field-induced enhancement of the exciton dissociation is present during most of the relaxation.
Our results show that the limited yield of photoinduced free charges in $MoS_2$ can be significantly increased by applying a moderate in-plane electric field.

## THU 45

## Sideband cooling of tunable graphene optomechanical devices

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Nanomechanical resonators are excellent devices for high sensitivity detection of mass and force [1,2], and testing quantum mechanics phenomena [3]. In this work we report on a graphene nanomechanical resonator coupled to a superconducting cavity. By applying a DC voltage between the oscillator and a bottom gate electrode the mechanical properties can be tune and the optomechanical coupling can be increased by a factor 4. We perform sideband cooling on the graphene resonator lowering its thermal phonon occupation down to 7.2 phonons. In addition we are able to sense our mechanical vibrations with a sensitivity of 1.3 fm/$Hz^{1/2}$. Both phonon population and displacement sensitivity surpass by far previous results using graphene-based optomechanical devices.

References

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[3] F. Lecocq et al. Resolving the cacuum fluctuations of an optomechanical system using an artificial atom. Nat. Physics (2015)

## THU 46

## Two-dimensional fullerene peapods: a Raman spectroscopy and atomic force microscopy study

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Fullerene two-dimensional (2D) peapods represent a new type of bottom-up engineered material consisting of fullerenes sandwiched between graphene layers. Our 2D peapod was prepared by a sequential assembly of $^{12}$C single-layer graphene, $C_{70}$ fullerenes and $^{13}$C single-layer graphene. The isotope labelling of the graphene layers grown by chemical vapour deposition allowed us to address independently and locally the strain and doping in the top and the bottom layer of the peapod[1].

Using Raman spectral mapping and atomic force microscopy, we found an asymmetry in the strain and doping with respect to the top and bottom graphene layer of the peapod1. In addition, the local doping and strain of the top graphene layer was found to correlate with the local concentration of $C_{70}$ fullerenes. Finally, we performed temperature dependent Raman spectral mapping and observed, that the fullerenes act locally as a mechanical couplers between the bottom and top layer.

[1] V. Vales, T. Verhagen, J. Vejpravova, O. Frank and M. Kalbac, Nanoscale, 2015

## THU 47

## In-situ electrical measurements of Graphene Nanoribbons fabricated through Scanning Transmission Electron Microscopy

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We recently demonstrated a controllable and reproducible method to obtain suspended monolayer graphene nanoribbons with atomically defined edge shape [Q. Xu, et al., ACS Nano 7 (2), 1566-1572, 2013]. Our method exploits the electron-beam of a Scanning Transmission Electron Microscope (accelerated at 300 kV) to create vacancies in the lattice by knock-on damage and pattern graphene in any designed shape. The small beam spot size (0.1 nm) enables close-to-atomic cutting precision, while heating graphene at 600°C during the patterning process avoids formation of beam-induced Carbon deposition and allows self-repair of the graphene lattice. Self-repair mechanism is essential to obtain well-defined (zig-zag or armchair) edge shape and, if the electron beam dose is lowered, to perform non-destructive imaging of the graphene nanoribbons.

Drawing the electron-beam path with a software script, we were able to obtain reproducible graphene nanoribbons with sub 10 nm width. Using an in-house built microscopy holder equipped with electrical feedthroughs, we performed 2 and 4 wire measurements on several graphene nanoribbons, with different number of layers.

Early results show that our nanoribbons exhibit ohmic behaviour, with conductivity linearly proportional to the width.

### THU 48
### Controlled reduction of graphene oxide by ascorbic acid

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The chemical reduction is a one of the most convenient and commercially promising routes to produce graphene from graphene oxide (GO) with currently more than 50 types of reducing agents reported in the literature. There are several key characteristics of a “good reducing agent”: high reduction capability, healing the defective GO, improving the dispersion stability, affordability and environmentally friendly. One of such reducing agents is ascorbic acid (AA). The extend of GO reduction can be critical when it comes to dispersion stability and specific application.

Herein we systematically studied the effect of different reduction conditions on GO reduction using AA as reducing agent. Two GOs with different C/O ratios were used as starting material. The reduction reactions were performed at room temperature and 80C respectively, by varying the GO to AA ratio. We showed that, depending on the reduction temperature and AA amount, different states of rGO could be achieved: from viscous stable dispersion to hydrogels of different volumes and stability. This study allows the production of different forms of rGO, depending on the required application.

### THU 49
### In situ Raman spectroelectrochemistry of p- and n-type doped diamond

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In situ Raman spectroelectrochemistry with different laser excitation energies and electrolyte solutions was used to study two types of nanocrystalline diamond films: boron-doped diamond (B-NCD) with p-type conductivity and phosphorus-doped diamond (P-NCD) with n-type conductivity. In the case of B-NCD the Raman modes associated with boron incorporation into the lattice and the sp3 zone-center phonon exhibited no changes with the applied potential. This finding indicates a high stability of the diamond lattice with substitutionally incorporated boron [1]. On the other hand, the modes belonging to sp2 phases (D, G and D' band) change their intensities; they increase in cathodic direction and decrease in anodic direction. P-NCD films showed the same trend in the intensity changes of the peaks corresponding to sp3 and sp2 carbonaceous phases. Morphology studies (ex situ) and electrochemical measurements (cyclic voltammetry, electrochemical impedance spectroscopy) were performed to provide a complete picture of the prepared B-NCD and P-NCD films [2].

[1] Vlčková Živcová et al. Electrochim Acta 87:518 (2013)
[2] Vlčková Živcová et al. Diam Relat Mater 55:70 (2015)

### THU 50
### Graphene on single crystal diamond: synthesis and characterization

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The performance of electronic devices made of graphene substantially depends on the interactions of graphene with a substrate beneath, mostly silicon substrate covered with oxide layer. The reasons are numerous: remote phonon scattering, charge traps, adsorbed dopants, etc. Recently it was proven that changing silicon to diamond substrate significantly improved performance of the graphene devices. However, theoretical calculations of interactions at the graphene – diamond (GOD) interface vary and often contradict each other. Here we realize systems of graphene-on-diamond by different routes and investigate the atomic and electronic structures using HRTEM/STEM with atomic resolution. The GOD systems are further characterized by a number of spectroscopic techniques. The final goal is to understand the interactions between graphene and diamond and their relation to electronic transport.

### THU 51
### The interplay between intrinsic and external resonances in plasmon-enhanced Raman experiments on CNTs

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Plasmon-enhanced Raman scattering is a powerful technique to investigate vibrational and electronic properties of single molecules. The fundamental coupling mechanism between a plasmon and a non-resonant Raman scatterer, i.e. graphene, was studied recently. A quantum mechanical approach revealed that the plasmon gives rise to a broad enhancement profile with sharp resonance features. In new experiments we used carbon nanotubes as a Raman scatterer with an intrinsic resonance placed into a well-defined plasmonic system consisting of two gold nanodiscs (dimer). Enriched CNTs with a resonance energy matching to the plasmon resonance energy were used. The tubes were placed between the discs perpendicular to the dimer axis. The interaction between the plasmon resonance and the resonance of the CNTs was investigated. Due to the design of the plasmonic system, the plasmonic enhancement of the tube can be switched by turning the polarization. We measured the resonance behavior of a CNT with and without plasmonic enhancement. Wavelength and polarization dependent measurements of the G- and RB modes were performed.

### THU 52
### Strain engineering in monolayer of WS2, MoS2 and their heterostrustures

Xixiang Zhang[1], Xin He[1], Zhiyong Zhu[2], Yang Yang[2], Hai Li[3]
[1]Division od Physical Science and Engineering, King Abdullah University of Science & Technology, Thuwal
[2]Core lab, King Abdullah University of Science & Technology, Thuwal
[3]Institute of Advanced Materials (IAM), Nanjing Tech University (NanjingTech), Nanjing 210009, China

Mechanically exfoliated monolayers of MoS2, WS2 and their Van der Waals heterostructure (WS2/MoS2), have been made on the flexible substrates through which an uniaxial tensile strain can be applied on the 2D samples. The continuous tuning of the band structures of the materials upon applying strain has been investigated using micro-photoluminescence at room temperture. Excitons have been observed in monolayers of MoS2, WS2 and heterostructures of WS2/MoS2. However, charged excitons (trions) have only observed in both WS2 and WS2/MoS2 for their large binding energy. Both exciton and trion peaks are found to be redshifted with strain, indicating the decrease of band gaps. The redshift ratios of the exciton peaks are 55 meV/percent strain, 59 meV/percent strain and 49 meV/percent strain for MoS2, WS2 and WS2/MoS2, respectively; while the redshift ratios of the trion peaks are 56 meV/percent strain and 45 meV/percent strain for WS2 and WS2/MoS2, respectively. These results imply the potential applications of transition metal dichalcogenides in flexible electronics.

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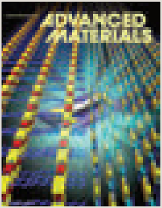

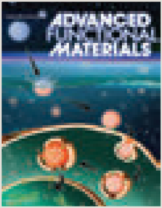

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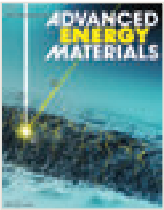

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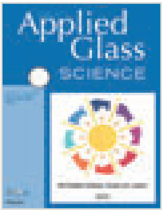

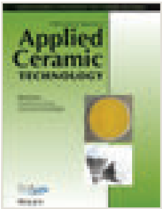

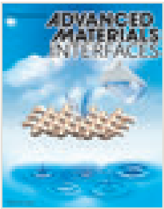

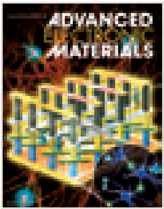

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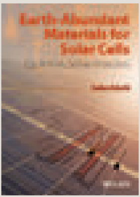

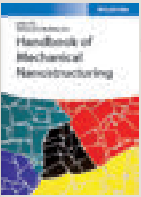

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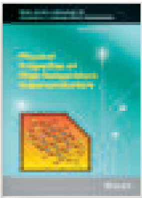

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| 08:30 – 09:00 | K. Ensslin, Zurich<br>*Measurement Back-Action in Stacked Graphene Quantum Dots* |
| 09:00 – 09:30 | P. Hakonen, Espoo<br>*Electron-phonon coupling in suspended mono- and bilayer graphene* |
| 09:30 – 10:00 | P. Makk, Basel<br>*Electron-Optics in suspended Graphene* |
| 10:00 – 10:30 | coffee break |
| 10:30 – 11:00 | M. Gibertini, Lausanne<br>*Engineering electron and hole wires in 2D materials through polar discontinuities* |
| 11:00 – 11:30 | Y. Shi, Riverside<br>*Symmetry-Broken Quantum Hall States in Bilayer and Trilayer Graphene* |
| 11:30 – 17:00 | mini workshops |
| 17:00 – 17:30 | Y. Kato, Tokyo<br>*Exciton physics in individual suspended carbon nanotubes* |
| 17:30 – 18:00 | L. Xian, San Sebastian<br>*Exploring novel 2D elemental materials with group IV elements* |
| 18:00 – 18:30 | A. Jorio, Belo Horizonte<br>*IWEPNM 2016 Conference Summary* |
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| 20:00 – 21:00 | Bauernbuffet – Farewell |

## 08:30

## Measurement Back-Action in Stacked Graphene Quantum Dots

Klaus Ensslin[1]
[1]Physics, ETH Zurich, Zurich

We present an electronic transport experiment in graphene where both classical and quantum mechanical charge detector back-action on a quantum dot are investigated. The device consists of two stacked graphene quantum dots separated by a thin layer of boron nitride. This device is fabricated by van der Waals stacking and is equipped with separate source and drain contacts to both dots. By applying a finite bias to one quantum dot, a current is induced in the other unbiased dot. We present an explanation of the observed measurement-induced current based on strong capacitive coupling and energy dependent tunneling barriers, breaking the spatial symmetry in the unbiased system. This is a special feature of graphene-based quantum devices. The experimental observation of transport in classically forbidden regimes is understood by considering higher-order quantum mechanical back-action mechanisms. The work has been done in collaboration with D. Bischoff, M. Eich, O. Zilberberg, C. Rössler, and T. Ihn.

## 09:00

## Electron-phonon coupling in suspended mono- and bilayer graphene

Pertti Hakonen[1]
[1]Department of Applied Physics, Aalto University, Espoo

Electron-phonon (el-ph) coupling is the basic means to control energy transport in a variety of devices which provide extreme sensitivity in calorimetry, bolometry, and radiation detection. For ultra sensitive detection at cryogenic temperatures, graphene is expected to have an advantage owing to its small heat capacity that allows fast operation even though its electron-phonon coupling becomes exceedingly small near the Dirac point.

This talk summarizes our results on el-ph coupling obtained using electrical transport experiments on both mono- and bilayer suspended graphene. In monolayer samples, we find strong "supercollision cooling" due to the presence of ripples in suspended graphene. In the high temperature limit, our results yield the first demonstration of the $T^5$ dependence for the el-ph heat transfer. In the low-$T$ limit, our results indicate quadratic dependence on the chemical potential $\mu$, which is in line with the cross-over, found at $T \sim \mu/k_B$, from the quintic high-$T$ behavior to cubic in the low-$T$ regime. On the contrary, we find that electron-optical phonon scattering dominates in bilayer graphene under similar measurement conditions. The connection of our results to the earlier work on substrates will also be discussed.

### 09:30
### Electron-Optics in suspended Graphene

Peter Makk[1], Peter Rickhaus[1], Romain Maurand[1], Ming-Hao Liu[3], Samuel Hess[1], Endre Tovari[2], Markus Weiss[1], Klaus Richter[3], Christian Schönenberger[1]
[1]Dept. of Physics, University of Basel, Basel
[2]Dept. of Physics, Budapest University of Technology and Economics
[3]Institute of Theoretical Physics, University of Regensburg, Germany

We realized electron optical elements in high-mobility suspended, ballistic graphene by utilizing local electrostatic gating [1]. In graphene gapless p-n interfaces can be formed showing a negative index of refraction and the effect of Klein tunneling. We demonstrate that with this technique a ballistic p-n junction can be formed [2] and in magnetic fields striking features appear due to the formation of “snake states” along the p-n interface [3]. We also show that electrons in ballistic graphene can be guided by gate potentials as photons in an optical fiber, and that Klein filtering increases the guiding efficiency [4]. Moreover, the guiding channel can be filled mode by mode. Finally, we demonstrate that tunable p-n interfaces can act as beam splitters [5].

[1] R. Maurand, P. Rickhaus, P. Makk, et al., Carbon, 79, 486 (2014)
[2] M.-H. Liu, P. Rickhaus, P. Makk et al., Phys. Rev. Lett. 114, 036601 (2015)
[3] P. Rickhaus, P. Makk et al., Nat. Comm. 6, 6470 (2015)
[4] P. Rickhaus, M.-H. Liu, P. Makk, et al., Nano Lett., 5819, 15 (2015)
[5] P. Rickhaus, P. Makk et al., accepted for publication and coverpage in Appl. Phys. Lett.

### 10:30

### Engineering electron and hole wires in 2D materials through polar discontinuities

Marco Gibertini[1], Giovanni Pizzi[1], Nicola Marzari[1]
[1]Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Unprecedented and fascinating phenomena have been observed at oxide interfaces between centrosymmetric cubic materials, where polar discontinuities can give rise to polarization charges and electric fields that drive a metal-insulator transition and the appearance of a two-dimensional electron gas. Lower dimensional analogues are possible, with polar discontinuities and electron or hole wires emerging at interfaces in honeycomb lattices. Here we suggest different realistic pathways to engineer electronic and hole wires in 2D materials and devices, and support these suggestions with extensive first-principles calculations. Several approaches are discussed, based on: (i) nanoribbons, where a polar discontinuity against the vacuum emerges; (ii) functionalizations, where covalent ligands are used to introduce polar discontinuities by selective or total functionalization of the parent systems; and (iii) structural interfaces, including inversion domain boundaries and phase-engineered interfaces. All the cases considered have the potential to deliver innovative applications in ultra-thin and flexible solar-energy devices and in micro- and nano-electronics.

### 11:00

### Symmetry-Broken Quantum Hall States in Bilayer and Trilayer Graphene

Yanmeng Shi[1], Petr Stepanov[1], Chun Ning (Jeanie) Lau[1]
[1]Department of Physics and Astronomy, University of California, Riverside, Riverside

Owing to the spin, valley, and orbital symmetries, the lowest Landau level in few-layer graphene exhibits multicomponent quantum Hall ferromagnetism. Using transport spectroscopy, we investigate the energy gaps of integer and fractional quantum Hall states in bilayer graphene (BLG) with controlled layer polarization, and explore the states and transitions at filling factors nu=1 and 2/3.

In another few-layer graphene system, ABA-stacked trilayer graphene consists of multiple Dirac bands, where crystal symmetry protects the spin degenerate counter-propagating edge mode. At even higher magnetic fields, the crystal symmetry is broken in by electron-electron interactions and the nu=0 quantum Hall state displays a rich phase diagram. Our findings indicate the role of crystal and spin symmetry in generation of topological phases in multiple Dirac bands.

### 17:00

### Exciton physics in individual suspended carbon nanotubes

Yuichiro K. Kato[1]
[1]Institute of Engineering Innovation, The University of Tokyo, Tokyo

Being a one-dimensional atomic-layer material, single-walled carbon nanotubes offer unique opportunities for investigating exciton physics. Here we discuss experiments aimed at highlighting the physics of tightly-bound excitons in individual suspended carbon nanotubes. The excitons are highly mobile along the tube, exhibiting diffusion for distances over a micron. Such a diffusion process occurs in a truly one-dimensional manner, as manifested in the exciton-exciton annihilation rates that scale to the third power of the density. By using gate voltages, it is possible to generate trions that are stable at room temperature. Simultaneous photoluminescence and photoconductivity spectroscopy show evidences for spontaneous dissociation, despite the expectation that free carrier generation from a tightly-bound excitonic state would be difficult. More recent measurements with increased sensitivity have revealed the fine structure of the excited excitonic states.

We acknowledge financial support from KAKENHI (24340066, 26610080), The Canon Foundation, and The Asahi Glass Foundation, as well as the Nanotechnology Platform and Photon Frontier Network Program of MEXT, Japan.

### 17:30

### Exploring novel 2D elemental materials with group IV elements

Lede Xian[1], Seymur Cahangirov[1,3], Peizhe Tang[1,4], Angel Rubio[1,2]
[1]NanoBio Spectroscopy Group and ETSF, Universidad del País Vasco, San Sebastian, Spain
[2]Theory Department, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
[3]UNAM - National Nanotechnology Research Center, Bilkent University, Turkey
[4]State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing, China

Following the success of graphene, considerable efforts have been given to exploring the two-dimensional (2D) structures of other group IV elements. Here, we employ first-principles methods based on density functional theory to investigate the structure and electronic properties of these novel 2D materials. We find that for freestanding silicene, germanene, and stanene, a 2D layer consisting of dumbbell units is energetic more favorable than the one with the buckled honeycomb structure. We show that one of the dumbbell structures for silicene may correspond to the $\sqrt{3} \times \sqrt{3}$ phase grown on silver surface. Moreover, we predict that a structure of stanene with dumbbell units is an intrinsic 2D topological insulator. Our studies give new insight into these low dimension materials and provide new directions for material synthesis. At last, we show that the substrate plays an important role in synthesizing 2D elemental materials. In particular, we identify the structure for germanene recently grown on gold surface as a planer honeycomb structure instead of the dumbbell structures. The electronic properties of the 2D materials grown on substrates, the effects of substrates, and the implications for the substrate selections for the growth will be discussed.

### 18:00

### IWEPNM 2016 Conference Summary

Ado Jorio[1]
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