

Name

XXIXth
International Winterschool
on Electronic Properties
of Novel Materials

Molecular Nanostructures

Program



Hotel Sonnalp
Kirchberg/Tirol
Austria

07 - 14 March, 2015



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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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Dear Friend:

Welcome to the 29th International Winterschool on:

Electronic Properties of Novel Materials: "Molecular nanostructures"

This Winterschool is a sequel of twenty-eight 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
Hans Tornatzky, Dirk Heinrich	accommodation
Amelie Biermann	finances
Asmus Vierck, Harald Scheel	website
Nils Scheuschner, Roland Gillen	technical assistance, video transfer, sponsoring
Sevak Khachadorian	announcements
Emanuele Poliani, Aurélie Pierret	technical assistance
Felix Kampmann	website assistance, visa applications
Felix Herziger, Christoph Tyborski	abstract booklet
Anja Sandersfeld	visa applications, general assistance

Also the managers of the hotel, Mrs. Mayer and Mr. Mayer, 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 Siegmur

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

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Scope

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

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

INFORMATION FOR PARTICIPANTS

Time and location

The IWEPNM 2015 starts on Saturday, 7 March, evening, at the hotel Sonnalp in Kirchberg/Tirol, Austria and extends to Saturday, 14 March, breakfast. There will be a reception party on 7 March, after dinner, and a farewell party including dinner on Friday, 13 March.

Transport

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

Addresses

The address of the Winterschool is:

IWEPNM 2015, Hotel Sonnalp, A-6365 Kirchberg/Tirol, Austria

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

All questions concerning the IWEPNM 2015 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 2015 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.

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 on Saturday evening.

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 and Nature Publishing Group.

Conference Publication

Invited and contributed presentations from IWEPNM 2015 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 2015: 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 2015 CHAIRPERSONS FOR THE ORAL SESSIONS

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

Sunday, 08.03.	morning	Kuzmany
	morning, after coffee break	Lotsch
	evening	Reich
Monday, 09.03.	morning	Ernst
	morning, after coffee break	Jorio
	evening	Obratzsova
Tuesday, 10.03.	morning	Thomsen
	morning, after coffee break	Backes
	evening	Haigh
Wednesday, 11.03.	morning	Rudolf
	morning, after coffee break	Berciaud
	evening	Skákalová
Thursday, 12.03.	morning	Kaiser
	morning, after coffee break	Andrej
	evening	Roth
Friday, 13.03.	morning	Krupke
	morning, after coffee break	Pichler
	evening	Hirsch

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, March 08			Monday, March 09		Tuesday, March 10		Wednesday, March 11		Thursday, March 12		Friday, March 13	
Topics	Carbon materials: design, growth, and applications	Graphene plasmonics, optics, and imaging	Two-dimensional materials and heterostructures	Graphene spectroscopy, topological materials	Graphene functionalization and nano-mechanics	Superconductivity, spins, and applications						
08:30	Growth of graphene: In-situ observations and chemical considerations SCHLÖGL	TUTORIAL: Exploitation of plasmon and phonon polariton modes for sub-wavelength confinement in graphene and polar dielectrics MAIER	TUTORIAL: The rise of van der Waals heterostructures GEIM	Artificial Atoms in Graphene ANDREI	Applications of Functionalized Carbon Nanostructures PRATO	Superconductivity in flatland: universal enhancement in 2D semiconductors at low doping MAURI						
09:00	Functional organic frameworks as platforms for light-driven hydrogen evolution LOTSCH			Topological Winding Number Change and Broken Inversion Symmetry in a Hofstadter's Butterfly BOCKRATH	Versatile and scalable approaches to chemical processing of nanocarbons SHAFFER	High T_c superconductivity in a single atomic layer of FeSe HOFFMAN						
09:30	Structure separation of SWCNTs by column chromatography using mixed surfactant TANAKA	Plasmons in nanographene and other atomic scale systems GARCIA DE ABAJO	Optoelectronics with 2D semiconductors MÜLLER	Electronic properties of functionalized 2D materials: graphene, boron nitride, transition metal dichalcogenides and phosphorene GRÜNEIS	Diversity of Oxo-Functionalized Graphene EIGLER	Nanosecond spin lifetimes in graphene-based spin-valves at room temperature BESCHOTEN						
10:00	Coffee break											
10:30	Optoelectronics with Aligned Carbon Nanotube Films KONO	Quantum interferences in plasmon-enhanced Raman scattering unraveled by graphene HEEG	Van der Waals heterostructures composed of thin 2D crystals sensitive to atmospheric exposure. GORBACHEV	Raman spectroscopy of graphene and transition metal dichalcogenides SAITO	Graphene growth on metallic and insulating surfaces RUDOLF	Spin phenomena in graphene materials FABIAN						
11:00	Manipulating the magnetic state of a carbon nanotube Josephson junction using the superconducting phase DEBLOCK	Ultrafast electronic readout of diamond nitrogen-vacancy centers coupled to graphene HOLLEITNER	Spin-valley Coupling in atomically thin Tungsten Dichalcogenides crystals CUI	Stokes-anti-Stokes correlation in Raman Spectroscopy JORIO	Coherent control of nanomechanical systems WEIG	Transport Studies in Black Phosphorus Field Effect Transistors ÖZYILMAZ						
11:30	Quantum Design in Carbon Nanotubes ILANI	Single-Walled Carbon Nanotubes and Graphene as Highly Efficient Hole Extraction and Transport Layer for Solar Cells MARUYAMA	Excitons and many-body phenomena in atomically thin 2D materials CHERNIKOV	Combined Raman spectroscopy and reflection/transmission measurements for graphene characterization PAILLET	Optomechanical coupling of a multilayer graphene resonator to a superconducting microwave cavity STEELE	Photo-Oxidation Promoted by Electronic Confinement in Exfoliated Black Phosphorus MARTEL						

PROGRAM

AND

ABSTRACTS

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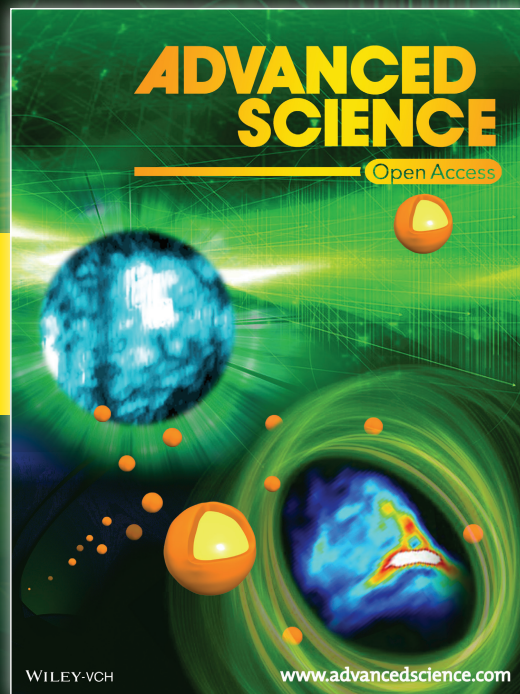
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- 08:30 – 09:00 R. Schlögl, Berlin
Growth of graphene: In-situ observations and chemical considerations
- 09:00 – 09:30 B. Lotsch, Stuttgart
Functional organic frameworks as platforms for light-driven hydrogen evolution
- 09:30 – 10:00 T. Tanaka, Tsukuba
Structure separation of SWCNTs by column chromatography using mixed surfactant
- 10:00 – 10:30 coffee break
- 10:30 – 11:00 J. Kono, Houston
Optoelectronics with Aligned Carbon Nanotube Films
- 11:00 – 11:30 R. Deblock, Orsay
Manipulating the magnetic state of a carbon nanotube Josephson junction using the superconducting phase
- 11:30 – 12:00 S. Ilani, Rehovot
Quantum Design in Carbon Nanotubes
- 12:00 – 17:00 mini workshops
- 17:00 – 18:30 Dinner
- 18:30 – 19:00 B. Yakobson, Houston
Why do nanotubes grow mostly chiral? Why would graphene grow not as hexagon?
- 19:00 – 19:30 K. Amsharov, Erlangen
Atomically Precise Synthesis of Carbon Based Nanostructures
- 19:30 – 20:00 F. Fischer, Berkeley
Molecular Bandgap Engineering in Bottom-Up Fabricated Graphene Nanostructures
- 20:00 – 20:30 P. Ruffieux, Dübendorf
Electronic and Optical Properties of Atomically Precise Graphene Nanoribbons

Sunday, March 08th

Carbon materials: design, growth, and applications

08:30**Growth of graphene: In-situ observations and chemical considerations**Robert Schlögl¹¹Fritz-Haber-Institut der MPG, Department of Inorganic Chemistry, Berlin, Germany

The growth of graphene has been the subject of many morphological and conceptual studies. Mostly morphological features and chemical properties evaluated post-growth were used as arguments to formulate several concepts of graphene formation. The chemistry of metallic supports as catalysts and transport phenomena at the growth surface were not frequently considered.

Owing to the ability to observe the growth of graphene in-situ by a chemical scanning electron microscope we were able to delineate processes of substrate transformations from those of graphene formation. The combination of microscopic studies with NAP-XPS experiments[1] performed under identical conditions allows drawing conclusions about the chemical state of growing graphene systems.

We discriminate three different modes of growth from the different control modes of carbon species. These modes are controlled by the choice of the metallic substrate acting in different ways as source of the carbon building blocks. The relation of these modes to the chemical and morphological quality of the final product will be discussed.

[1] R. Blume, P.R. Kidambi, B.C. Bayer, R.S. Weatherup, Z.-J. Wang, G. Weinberg, M.-G. Willinger, M. Greiner, S. Hofmann, A. Knop-Gericke, R. Schloegl, *Physical Chemistry Chemical Physics*, 16 (2014) 25989-26003.

09:00**Functional organic frameworks as platforms for light-driven hydrogen evolution**Bettina Valeska Lotsch^{1,2}¹Max-Planck-Institut für Festkörperforschung, Stuttgart²Ludwig-Maximilians-Universität München

The conversion of sunlight into storable chemical fuels has been identified as a viable strategy to alleviate future energy shortage. To this end, the development of efficient photocatalysts capable of splitting water into hydrogen and oxygen has become a major thrust in materials science.

While heterogeneous systems excel through their stability, homogeneous catalysts offer the potential to tune every step in the photocatalytic mechanism through molecular engineering. Combining the best of both worlds in molecularly defined heterogeneous systems therefore opens up new possibilities for the rational design of photocatalysts with optimized efficiencies.

In this talk, polymeric photocatalysts based on 1D or 2D carbon nitrides and covalent organic frameworks (COFs) will be highlighted and catalyst optimization strategies - through doping[1], exfoliation[2], functionalization[3], as well as hybridization with bio-inspired co-catalysts[4] - will be discussed.

[1] Angew. Chem. Int. Ed. 2013, 52, 2435;

[2] J. Am. Chem. Soc. 2014, 136, 1730;

[3] J. Am. Chem. Soc. 2015, 137, 1064;

[4] Angew. Chem. Int. Ed. 2014, 53, 11538.

09:30**Structure separation of SWCNTs by column chromatography using mixed surfactant**Takeshi Tanaka¹, Yohei Yomogida¹, Xiaojun Wei¹, Mayumi Tsuzuki¹, Atsushi Hirano¹, Shunjiro Fujii¹, Hiromichi Kataura¹¹Nanosystem Research Institute, AIST, Tsukuba, Japan

Single-wall carbon nanotubes (SWCNTs) are produced as a mixture of various structures, and the inhomogeneity hinders their fundamental research and applications. We have developed methods for single chirality and isomer separations of SWCNTs by overloading separation and temperature control separation using gel column chromatography (1). In this presentation, we show improved separation methods using mixed surfactant. The first separation method was combined overloading selective adsorption and stepwise elution using a mixed surfactant system. This method could separate not only chiralities but also isomers of SWCNTs at very high purities. The second separation method was combined different mixed surfactant systems for selective adsorption and desorption. This method is simpler than overloading method and enables us to achieve high-throughput separation up to mg/day production of (9,4) and (10,3) SWCNTs. This work was supported by KAKENHI No. 25220602.

(1) H. Liu et al.: Nature Commun., 14, 309 (2011), Nano Lett., 13, 1996 (2013), Nano Lett., 14, 6237 (2014).

10:30**Optoelectronics with Aligned Carbon Nanotube Films**Junichiro Kono¹¹Department of Electrical and Computer Engineering, Rice University, Houston

The one-dimensional (1D) character of confined carriers and excitons in carbon nanotubes (CNTs) leads to extremely anisotropic electric, magnetic, and optical properties. Individual metallic CNTs have been shown to be excellent conductors with long coherence lengths, while individual semiconducting CNTs have been shown to strongly absorb and emit light only when the light polarization is parallel to the tube axis. Even in macroscopic assemblies of CNTs, their anisotropic properties are expected to be preserved, but systematic optical, photonic, and optoelectronic studies have been limited. Here, we present results of a variety of electrical and optical measurements of large-area films of aligned single-wall, double-wall, and multiwall CNTs, demonstrating a rich array of phenomena promising for optoelectronic applications. In particular, we will provide a detailed description of their anisotropic response in the terahertz region of the electromagnetic spectrum due to their inherently 1D intraband carrier dynamics.

11:00**Manipulating the magnetic state of a carbon nanotube Josephson junction using the superconducting phase**R. Delagrangé¹, D. J. Luitz², R. Weil¹, A. Kasumov¹, V. Meden³, H. Bouchiat¹, R. Deblock¹¹Laboratoire de Physique des Solides, Orsay (France)²Laboratoire de Physique Théorique, Toulouse (France)³RWTH Aachen University and JARA, Aachen (Germany)

When a metal contains magnetic impurities, their associated moments can be screened by the conduction electrons, resulting in a singlet state. This many-body phenomenon is at the heart of the Kondo effect. If the metal is replaced by a superconductor, the singlet can be destroyed in favor of a magnetic doublet. This is accompanied by a sign change of the supercurrent in a junction geometry. This singlet-doublet transition was shown to depend on the relevant energy scales: the Kondo temperature and the superconducting gap, as well as the position of the impurity level. In the present work we show that the superconducting phase difference across a quantum dot can also control this magnetic transition of a Kondo impurity. We measured the relation between the supercurrent and the superconducting phase difference of a carbon nanotube Josephson junction. It exhibits distinctively anharmonic behavior, revealing the phase mediated singlet to doublet transition, in excellent agreement with finite temperature quantum Monte Carlo calculations and provides insights on the phase controlled level-crossing transition at zero temperature.

11:30**Quantum Design in Carbon Nanotubes**Shahal Ilani¹¹Weizmann Institute, Rehovot

Recent years have seen the development of several experimental systems capable of tuning local parameters of quantum Hamiltonians, including ultracold atoms, trapped ions, superconducting circuits and photonic crystals. These systems excel in studying the physics of bosons in disorder-free settings. A solid state analog, in which Hamiltonians of interacting electrons are designed and studied, remains a major open challenge, since in conventional solids electrons exist inside an imperfect host material that generates uncontrolled disorder. In this talk, I will describe our newly-developed platform for realizing in suspended carbon nanotubes such disorder-free, locally-tunable electronic systems. This platform becomes possible due to a new technique for nano-assembly of carbon nanotubes on complex electrical circuits without damaging their pristine electronic behavior. I will show a new experiment in which we have used this system to radically change the nature of interactions between electrons.

18:30**Why do nanotubes grow mostly chiral? Why would graphene grow not as hexagon?**Boris I. Yakobson¹¹Rice University, Houston, USA

In spite of similar edge dynamics of a tube or sheet, their topologies impact profoundly their morphology evolution. The closed loop of graphene edge by necessity contains different crystallographic orientations; the tube edge can preserve same crystallographic direction all around. Graphene flake can change shape on the fly; the tube helicity is locked after its cap is complete with 6 pentagons. The first title-?n is answered in 1991 paper by Iijima, yet it took decades to derive a formula, $R = \sin x$ (growth rate R , helical angle x). An alternative view - of which Smalley was loud proponent - is that thermodynamics favors the low energy armchair edge. A subtle balance of these views reveals sharply peaked abundance distribution $A = x \exp(-x)$ and explains the puzzling (n,n-1) types in many experiments [Artyukhov-Penev, Nature Comm. 5, 489, 2014]. To the second title-?n, DFT and MC modeling explain the shapes of symmetry lower than the symmetries of graphene and substrate. In equilibrium, edge energy variation dE manifests in slightly distorted hexagons. In growth, it enters as $\exp(-dE/kT)$, amplifying the symmetry breaking to triangle, ribbon, rhomb [Artyukhov et al. PRL, 2015].

19:00**Atomically Precise Synthesis of Carbon Based Nanostructures**Konstantin Amsharov¹¹Institute of Organic Chemistry II, Universität Erlangen-Nürnberg, Erlangen

Carbon based nanostructures such as fullerenes, nanotubes, nanographenes and nanoribbons attract considerable attention because of their unique properties and many potential applications. Since the diversity in properties strongly depends on the molecular structure, new methods for fabrication of these materials on atomically precise level are needed. Our methodology is based on the domino-like condensation of respective precursor molecules, which are pre-programmed for the construction of desired nanostructure exclusively. The approach allows access to isomer pure fullerenes, atomically precise nanographenes, and helicity pure nanotubes. The approach is not limited to the synthesis of fullerenes, carbon nanotubes and nanographenes but can be applied as well to the fabrication of various carbon based nanostructures including, but not limited to, exo-, endo-hedral, hetero- or open cage fullerenes, functional SWCNT, nanocones and many other related systems.

19:30**Molecular Bandgap Engineering in Bottom-Up Fabricated Graphene Nanostructures**Felix Fischer¹¹Chemistry, University of California Berkeley, Berkeley

Bandgap engineering has long played a vital role in technology by enabling semiconductor heterostructures to exhibit important behaviors such as resonant tunneling and enhanced solar conversion efficiency. As the dimensions of conventional electronic devices reduce further in size, however, their performance suffers due to short-channel effects and rough interfaces. Graphene-based molecular electronics has emerged as a possible candidate to overcome these obstacles by enabling control of electronic transport down to single-molecule scales. It has been predicted that bandgap engineering within single grapheme nanoribbons (GNRs) may be achieved by varying the width of covalently bonded GNR segments, but the experimental realization remains challenging. We demonstrate the rational bottom-up synthesis of width-modulated arm-chair GNR (AGNR) heterostructures, obtained by fusing segments of two different molecular building blocks. We study the resultant heterojunctions at sub-nanometer length-scales via scanning tunneling microscopy (STM) and spectroscopy (STS), and identify spatially modulated electronic structure that demonstrates molecular-scale bandgap engineering.

20:00**Electronic and Optical Properties of Atomically Precise Graphene Nanoribbons**Pascal Ruffieux¹¹nanotech@surfaces Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

Graphene nanoribbons (GNRs) are predicted to be semiconductors with an electronic band gap that sensitively depends on the ribbon width. This opens new ways for the design of GNR-based structures and heterostructures with specific and widely tunable electronic properties, but requires structuring at the atomic level.

Recently, we reported the successful bottom-up fabrication of atomically precise GNRs¹ based on surface-assisted synthetic routes using specifically designed precursor monomers. Here, I will review the bottom-up fabrication of prototypical GNRs and their electronic and optical characterization^{2,3}. An important handle for further tuning the electronic properties of GNRs is achieved by deterministic chemical doping. In particular, heterocycle containing precursor monomers can be used for the fabrication of nitrogen-doped GNRs and related GNR heterostructures⁴.

¹ J. Cai, *et al.* Nature **466**, 470 (2010)

² R. Denk, *et al.*, Nature Comm. **5**, 4253 (2014)

³ H. Söde, *et al.*, Phys. Rev. B, **in press** (2015)

⁴ J. Cai, *et al.*, Nature Nanotech. **9**, 896 (2014)

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- 08:30 – 09:30 **S. Maier, London**
Tutorial: Exploitation of plasmon and phonon polariton modes for sub-wavelength confinement in graphene and polar dielectrics
- 09:30 – 10:00 **J. García de Abajo, Barcelona**
Plasmons in nanographene and other atomic scale systems
- 10:00 – 10:30 **coffee break**
- 10:30 – 11:00 **S. Heeg, Manchester**
Quantum interferences in plasmon-enhanced Raman scattering unraveled by graphene
- 11:00 – 11:30 **A. Holleitner, Garching**
Ultrafast electronic read-out of diamond nitrogen-vacancy centers coupled to graphene
- 11:30 – 12:00 **S. Maruyama, Tokyo**
Single-Walled Carbon Nanotubes and Graphene as Highly Efficient Hole Extraction and Transport Layer for Solar Cells
- 12:00 – 17:00 **mini workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **U. Kaiser, Ulm**
Strategies of imaging low-dimensional electron-beam-sensitive objects with low-voltage aberration-corrected TEM
- 19:00 – 19:30 **K. Suenaga, Tsukuba**
Atomic Imaging and Spectroscopy of Low-Dimensional Materials
- 19:30 – 20:00 **S. Haigh, Manchester**
Cross sectional scanning transmission electron microscope imaging and analysis of multi-layered graphene based heterostructures
- 20:00 **Poster I**

Monday, March 09th

Graphene plasmonics, optics, and imaging

08:30**Exploitation of plasmon and phonon polariton modes for sub-wavelength confinement in graphene and polar dielectrics**Stefan Maier¹¹Physics, Imperial College London, London

Surface plasmon and surface phonon polaritons allow the two-dimensional confinement below the diffraction limit at interfaces between conductive and dielectric media. For the case of graphene, we will discuss the dynamics of hot electron generation mediated by localised surface plasmons of metal nanoparticle arrays, and evaluate the potential for ultrafast photodetection in hybrid graphene/metal nanoparticle structures. For polar dielectrics such as SiC, the confinement relies on the excitation of low loss phonon modes, allowing both high quality factors and ultrasmall mode volumes in the mid-infrared. This will be elucidated for the case of SiC nanopillar arrays. Lastly, hBN combines polar character with a natural multilayer structure due to weak van der Waals bonding between adjacent crystal planes. This leads to optical anisotropy and hence hyperbolicity. Arrays of nanocones of hBN therefore allow an intriguing avenue for creating truly three-dimensional sub-wavelength confinement in the mid infrared.

09:30**Plasmons in nanographene and other atomic scale systems**Javier García de Abajo¹¹ICFO - The Institute of Photonic Sciences, Barcelona

We will review recent advances in the control and understanding of plasmons in systems that have atomic dimensions along one or more directions. In particular, we will discuss plasmons in graphene, carbon nanotubes, and fullerenes, as well as thin metal layers and molecules such as polycyclic aromatic hydrocarbons. A simple, powerful, analytical eigenmode expansion formalism will be reviewed in the electrostatic limit, along with tutorial examples of application to the understanding of plasmons in these systems, including the derivation of approximate expressions for the plasmon frequencies and wave functions. Intrinsic advantages of plasmons in atomic-scale systems will be also discussed, and in particular, their large electrical tunability, their strong nonlinear response, and the possibility of reaching quantum strong coupling.

10:30**Quantum interferences in plasmon-enhanced Raman scattering unraveled by graphene**

Sebastian Heeg^{1,2}, Patryk Kusch¹, Christian Lehmann¹, Niklas Müller¹, Sören Wasserroth¹, Antonios Oikonomou², Nick Clark², Aravind Vijayaraghavan², Stephanie Reich¹

¹Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

²School of Materials, The University of Manchester, Manchester, UK

Plasmons are the collective excitations of free electrons in metals. They focus light into nanoscale volumes thereby enhancing local electromagnetic fields by orders of magnitude. A striking consequence is surface-enhanced Raman scattering, the giant enhancement of inelastic light scattering close to localized surface plasmons. We propose a quantum theory of plasmon-enhanced Raman scattering [1]. It is based on the quantum mechanical description of the Raman effect and predicts quantum interferences between scattering channels. Using graphene as a non-resonant Raman probe coupled to a plasmonic nanodimer, we demonstrate experimentally the predictions of our approach. At the dimer resonance, the G-mode of graphene is enhanced by 10^5 , but differs by a factor of two for the regimes of enhanced absorption and emission. In resonance, we further observe an altered polarization dependence of the G-mode and the appearance of defect-type modes in perfect graphene. Our results cannot be explained within the conventional framework of plasmon-enhanced Raman scattering: They verify the quantum nature of plasmon-enhanced Raman scattering. The proposed model provides a unified theory of surface- and tip-enhanced Raman spectroscopy.

[1] P. Kusch, S. Heeg, C. Lehmann, N. Müller, S. Wasserroth, A. Oikonomou, N. Clark, A. Vijayaraghavan, S. Reich, submitted (2015).

11:00**Ultrafast electronic read-out of diamond nitrogen-vacancy centers coupled to graphene**Alexander Holleitner¹¹Walter Schottky Institut and Physik-Department, Technische Universität München, Garching

We apply an ultrafast photocurrent spectroscopy to detect the non-radiative energy transfer from diamond nitrogen vacancy centers to graphene [1-4] with a time resolution of picoseconds [5,6]. Such centers are considered to play a fundamental role in new quantum information technologies. Our findings demonstrate that the transfer can be exploited as an electronic read-out process of the electron spin in the nitrogen vacancy centers. Furthermore, the ultrafast detection gives access to fast energy transfer processes, which are quenched in fluorescence measurements for short transfer distances [7].

We thank A. Brenneis, L. Gaudreau, M. Seifert, H. Karl, M.S. Brandt, H. Huebl, J.A. Garrido, and F.H.L. Koppens for a very fruitful collaboration and the ERC-grant "NanoREAL" for funding.

1. Z. Chen et al. ACS Nano 4, 2964 (2010).
2. X. Liu, et al. APL 101, 233112 (2012).
3. L. Gaudreau, et al. Nano Lett. 13, 2030 (2013).
4. J. Tisler, et al. Nano Lett. 13, 3152 (2013).
5. L. Pecht, et al. Nature Comm. 3, 646 (2012).
6. C. Kastl, et al. accepted (2015) arXiv:1501.07784.
7. A. Brenneis, et al. Nature Nanotechnology 10, 135 (2015).

11:30**Single-Walled Carbon Nanotubes and Graphene as Highly Efficient Hole Extraction and Transport Layer for Solar Cells**Shigeo Maruyama¹, Kehang Cui¹, Takaaki Chiba¹, Xiao Chen¹, Rong Xiang¹, Shohei Chiashi¹¹Department of Mechanical Engineering, The University of Tokyo, Tokyo

Structured single-walled carbon nanotubes (SWNTs) and millimeter-scale monocrystalline graphene are investigated as an advanced hole extraction and transport layer in various kinds of solar cells [1-4]. We found out that three-dimensional honeycomb structured SWNTs fabricated by breath figure directed self-assembly demonstrated higher fill factor and low serial resistance compared with random network. We also obtained a ten-fold increase in the power conversion efficiency (PCE) by using millimeter-scale monocrystalline graphene compared with polycrystalline graphene, with the PCE over 11% before any intentional doping process. The hole collecting and transport function of SWNTs was also demonstrated in perovskite solar cells [3] and organic solar cells [4] with high PCE. More importantly, all these solar cells have high stability in the ambient.

References:

- [1] K. Cui et al., J. Phys. Chem. Lett., 4 (2013), 2571.
- [2] K. Cui et al., J. Mater. Chem. A, 2 (2014) 11311.
- [3] T. Chiba, T. Sakaguchi, A.G. Nasibulin, E.I. Kauppinen, R. Xiang, S. Chiashi, S. Maruyama, (2015).
- [4] I. Jeon, K. Cui, T. Chiba, A. Anisimov, A.G. Nasibulin, E.I. Kauppinen, S. Maruyama, Y. Matsuo, (2014).

18:30**Strategies of imaging low-dimensional electron-beam-sensitive objects with low-voltage aberration-corrected TEM**Ute Kaiser¹¹Ulm University, Ulm

Structural and electronic properties of different low-dimensional electron-beam-sensitive crystalline (ion-implanted graphene, MoS₂, MoSe₂, SiO₂, CN, square water, transition-metal clusters) and amorphous (monolayer carbon, SiO₂) objects are obtained by analytical low-voltage aberration-corrected transmission electron microscopy following three main strategies:

(1) Theory and image processing: For exact calculation of the contrast of dose-limited high-resolution TEM images for low-Z materials at low voltages, image theory and image processing needs to be improved taking into account elastic and inelastic scattering.

(2) Sample preparation: We demonstrate our method to clean graphene. We show that sandwiching clean radiation-sensitive low-dimensional objects in-between two graphene layers or embedding them into single-walled carbon nanotubes allows to reduce electron-induced damage of the objects.

(3) Low-voltage transmission electron microscope: We outline our unique voltage-tuneable low-voltage (20-80kV) spherical and chromatic aberration-corrected TEM and show first results obtained from its prototype.

19:00**Atomic Imaging and Spectroscopy of Low-Dimensional Materials**Kazutomo Suenaga¹¹AIST, Tsukuba

In the Nanotube Research Center at AIST, we have been developing the top-level facilities of electron microscopy which enables the atomic resolution analysis of low-dimensional materials. Point defects and edge structures of graphene have been intensively studied with atomic precision in the last decade. Because the studies of atomic defects and boundaries are of general interest in the fundamental researches and becoming more and more crucial for technological applications of any nanoscale materials, the atomic scale studies can be also expanded to the other low-dimensional materials. Here I demonstrate some examples for atomic-scale imaging and spectroscopy of various low-dimensional materials with interrupted periodicities. Active 4/8 defects are most recently found to be responsible for plastic deformation of hexagonal boron-nitride (h-BN) layers. Vacancies and edges with radical bonds are also successfully assigned in h-BN. Doping and boundary behaviors of single-layered dichalcogenides (MX₂) are also intensively studied. More recently, the impurity atoms such as nitrogen and silicon are proved to affect the properties of graphene.

19:30**Cross sectional scanning transmission electron microscope imaging and analysis of multi-layered graphene based heterostructures**

Sarah Jane Haigh¹, Roman Gorbachev², Fred Withers², Aidan Rooney¹, Konstantin Novoselov², Andre Geim²

¹Materials, University of Manchester, Manchester, UK

²Physics, University of Manchester, Manchester, UK

By combining different two dimensional crystals within a Van der Waals heterostructure stack it is possible to produce devices with bespoke electronic bandstructures and advanced functionality. The individual crystal layers are produced by mechanical exfoliation and layered sequentially onto a Si substrate. Despite the necessity of employing polymeric support layers that are deposited and removed as part of the transfer procedure, our high resolution scanning transmission electron microscope (STEM) imaging has revealed that the heterostructure stacks form large areas of pristine synthetic crystal, free from hydrocarbon contaminants at the atomic scale (Haigh, et al. Nat Mater, 2012, 11, 764; Georgiou et al. Nat. Nano., 2013, 8, 100). More recently we have applied this technique to study devices incorporating transition metal dichalcogenides. For example, we demonstrate that STEM imaging is unique in being able to obtain critical information on the width of the h-BN tunnelling barriers as well as on the thickness and uniformity of MoS2 layers for a multiple quantum well LED heterostructure (Withers et al., Nat Mater, 2015, online).

MON 1**Hybrid Magnetic Systems based on 2D Materials: a Molecular Perspective**

Gonzalo Abellán^{1,2,3}, Eugenio Coronado³, Andreas Hirsch^{1,2}

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²Department of Chemistry and Pharmacy, University Erlangen-Nuremberg, Germany

³Institute of Molecular Science, University of Valencia, Paterna, Spain

Hybrid inorganic/organic materials have found many applications because they allow combining the properties of inorganic solids such as robustness, durability or mechanical strength with those introduced by the organic component such as functionality, tunability and convenient derivatization by synthesis. Recently, graphene (G) and related 2D materials have attracted a considerable attention due to their appealing electronic properties and the possibility to be tailored by chemical modification. In this sense, layered double hydroxides (LDH) are promising candidates for the development of hybrid functional materials due to their chemical versatility and the broad range of applications they exhibit. Herein we will show some examples of stimuli-responsive layered magnets[1,2], hybrid magnetoresistive nanocomposites[3,4] and multifunctional systems based on LDH and graphene building blocks.

G. A. thanks the EU for a Marie Curie Fellowship (FP7/2013-IEF-627386).

References:

[1] G. Abellán et al., Adv. Mater. 2014, 26, 4156.

[2] G. Abellán et al., Chem. Sci. 2015, DOI 10.1039/C4SC03460K.

[3] G. Abellán et al., Chem. Sci. 2012, 3, 1481.

[4] G. Abellán et al., ES Patent WO2013124503 A1.

MON 2**Hot carrier relaxation of Dirac fermions in bilayer graphene**

Jack A. Alexander-Webber^{1,2}, J. Huang², P. Braeuninger¹, T. J. B. M. Janssen³, A. Tzalenchuk³, T. Yager⁴, S. Lara-Avila⁴, S. Kubatkin⁴, R. L. Myers-Ward⁵, V. D. Wheeler⁵, D. K. Gaskill⁵, S. Hofmann¹, R. J. Nicholas²

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Hot carrier dynamics in bilayer graphene has considerable importance for a variety of applications including high power electronics, and quantum Hall metrology. By epitaxial growth on SiC a coverage of 1.5 graphene monolayers was achieved as determined by XPS. Through magnetotransport measurements of epitaxial bilayer graphene devices we reveal the hot-electron energy loss rate which follows a T^4 power-law behaviour at carrier temperatures from 1.4-100K due to electron-acoustic

phonon interactions. Additionally we observe a carrier density dependence $n^{-3/2}$, in contrast to the $n^{-1/2}$ dependence for monolayer, such that at low carrier densities the energy loss rates in bilayer graphene exceed those of monolayer graphene. However, in a number of applications the SiC substrate is unsuitable. Therefore, we have performed CVD growth resulting in large area ($40\mu\text{m}$) individual domains of bilayer graphene. Raman spectroscopy of individual bilayer regions has revealed that a significant proportion are Bernal-stacked, suggesting that large area CVD growth of bilayer graphene is within reach for use in high power applications exploiting the fast hot-electron energy-relaxation.

MON 3

Synthesis of vertically aligned single-walled carbon nanotubes with sub-nanometer-diameter using cobalt-copper binary catalyst

Hua An¹, Kehang Cui¹, Rong Xiang¹, Taiki Inoue¹, Shohei Chiashi¹, Shigeo Maruyama¹

¹Department of Mechanical Engineering, University of Tokyo, Tokyo

Single-walled carbon nanotubes (SWNTs) have been regarded as one of the most attractive materials for electronic devices because of their unique electronic structures and fascinating properties. Since the band gap of a semiconducting SWNT inversely depends on its diameter, small-diameter SWNTs are highly desired in the application. In this study, we used a novel combination of Co/Cu as catalyst to grow small-diameter SWNTs by alcohol catalytic chemical vapor deposition. We characterized the as-grown SWNTs by scanning electron microscopy, Raman spectroscopy, optical absorption spectroscopy and transmission electron microscopy (TEM). Compared with the conventional catalyst Co/Mo[1] and Co/Fe, the combination of Co/Cu can grow sub-nanometer vertically-aligned SWNTs. The diameter and yield of SWNTs can be further tuned by parametric modulation of the growth condition. The possible mechanism through detailed TEM analysis will also be discussed. We also discuss the preliminary result of SWNTs growth from sputtered W/Co binary metal catalysts for chirality controlled synthesis[2].

[1] R. Xiang et al., ACS Nano 6, 7472 (2012). [2] F. Yang et al., Nature 510, 522 (2014).

MON 4

Monte Carlo simulations of line width dependence of carrier transport properties in graphene nanoribbon interconnects with real space edge roughness

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²Low-power Electronics Association Project (LEAP)

Because of the high integration of ULISs, resistivity and reliability problems have become more and more serious in Cu interconnects in recent years. Graphene nanorib-

bons (GNRs) have attracted attention as a promising material for horizontal interconnects to replace Cu, because of their high electron mobility and high electro-migration tolerance. However, with the minimum feature size getting smaller, manufacturing variants, such as the edge roughness, cannot be avoided as long as lithography and dry etching processes are used. Because of the difficulties in experimentally fabricating the controlled edges of GNRs, we developed a novel simulation model for the GNR interconnects based on a semi-classical Monte Carlo particle method to investigate electron transport in multi-layered GNRs with edge roughness and the line width dependence of the transport properties [1]. We discuss the line width dependency of carrier mobility and the effect of edge roughness scatterings on the dependency, including the reproducibility of the simulation with a different set of random numbers.

[1] T. Misawa et al., Proceedings of Advanced Metallization Conference (ADMETA) 2014, 4-3 (2014)

MON 5

Spectroscopic metrics to determine monolayer content, mean number of layer and lateral dimensions of liquid exfoliated transition metal dichalcogenides

Claudia Backes¹, Jonathan N Coleman¹

¹School of Physics and CRANN, Trinity College Dublin, Ireland

Two dimensional nanomaterials beyond graphene such as transition metal dichalcogenides (TMDs) have received considerable attention the past years because of their interesting physical properties (such as indirect-direct bandgap transitions) and applications potential in a number of areas. In order for these materials to be used in a range of applications, large quantities need to be made available. Even though exfoliation in suitable liquids has proven to be an important production technique, it is limited by our inability to easily measure nanosheet sizes, thicknesses and monolayer content. As such, understanding of the exfoliation process and size selection techniques are also limited.

We have recently demonstrated that mean number of layers and lateral dimensions can simultaneously be obtained from an optical extinction spectrum due to edge and confinement effects.[1] We have used these metrics to understand and optimise the exfoliation process[2] and have now developed additional metrics based on the measurement of the Raman and photoluminescence in liquids to quantify the monolayer content in TMD dispersions.

1. Nature Commun, 5, 4576
2. Chem Mater, 10.1021/cm5044864

MON 6**Optical absorption induced dispersion of carbon nanotubes in a thermoplastic polymer and apparent Raman shifts in nanostructured materials**E Pavlenko¹, V Tishkova¹, P Puech¹, W Bacsá¹¹CEMES-CNRS and University of Toulouse, 29 Jeanne Marvig, 31055 Toulouse, France

We find that PEEK, a thermoplast polymer, in the vicinity of carbon nanotubes diffuses spontaneously into CNT agglomerates at the polymer fusion temperature. Enhanced diffusion in the vicinity of polymer molecules has the effect that the tubes disperse spontaneously. We find systematic differences of the dispersion for single, double and multi-wall tubes on a PEEK surface. We will present and discuss electron microscopy and Raman images as well as temperature dependent electric transport measurements. It has been recently shown that non-uniform illumination of the focal spot due to heterogeneity at the nanometer scale can lead to apparent Raman spectral shifts. We find on step edges how the partial illumination of the focal spot can lead to red or blue shifts as large as $1\text{-}2\text{ cm}^{-1}$ depending on which side of the focal spot is illuminated. This findings have important consequences when making interpretations of spectral shifts due local strain or doping. The fact that apparent spectral shifts have been overlooked so far, implies that published work on the optical spectroscopy of nano-structure surfaces needs to be reexamined.

MON 7**C60/Collapsed Carbon Nanotube Hybrids - A Variant of Peapods**Hamid Reza Barzegar^{1,2}, Eduardo Gracia-Espino¹, Aiming Yan², Claudia Ojeda-Aristizabal², Gabriel Dunn², Thomas Wågberg¹, Alex Zettl²¹Department of Physics, Umea University, 90187 Umea, Sweden²Department of Physics, University of California, Berkeley, CA 94720, USA

We examine a variant of so-called carbon nanotube peapods by packing C60 molecules inside the open edge ducts of collapsed carbon nanotubes. C60 insertion is accomplished through a facile single-step solution-based process. Theoretical modeling is used to evaluate favorable low-energy structural configurations. Overfilling of the collapsed tubes allows infiltration of C60 over the full cross-section of the tubes and consequent partial or complete reinflation, yielding few-wall, large diameter cylindrical nanotubes packed with crystalline C60 solid cores.

MON 8**Raman and electron microscopy study of C60 collapse/transformation to nano-graphene-based disordered carbon phase at high pressure/high temperature**

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Transformation of C60 polymers to superelastic hard carbon phase occurring in metal matrix in temperature interval 1000 K - 1100 K at a pressure of 5 GPa was studied by optical and scanning electron microscopy (SEM) and Raman spectroscopy. Using Raman mapping through T gradient in the sample allowed us to identify different stages of the structural transformation. We demonstrate nucleation character of the buckyballs collapse/formation of nanoclustered graphene phase (NGP) contrary to the recently proposed martensitic mechanism of this transformation [1]. Importantly, SEM and Raman show the NGP nucleation at the defects concentration sites in the parent fullerene structure that supports the proposed phase transition mechanism. The NGP-based composites exhibit further enhancement of the superior mechanical properties of the material synthesized from pure C60 [2] creating better prospective for practical applications.

[1] C. Lepoittevin, et al. Carbon (2013), 52, 278.

[2] O. Chernogorova, et al. Appl. Phys. Lett. (2014), 104, 043110.

MON 9**Probing electronic excitations in mono- to pentalayer graphene by micro-magneto-Raman spectroscopy**

Stéphane Berciaud¹, Denis M. Basko², Marek Potemski³, Clément Faugeras³

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We probe electronic excitations between Landau levels in freestanding N-layer graphene over a broad energy range, with unprecedented spectral and spatial resolution, using micro-magneto Raman scattering spectroscopy. A characteristic evolution of electronic bands from two up to five Bernal-stacked graphene layers is evidenced and shown to remarkably follow a simple theoretical approach, based on a one-electron, effective bilayer model [1].

In contrast, in monolayer graphene, the band velocity associated with the Raman active electronic excitations is found to depend on the index of Landau level involved, and to vary as a function of the magnetic field [1,2]. This contradicts the single-particle picture of non-interacting massless Dirac electrons, but is accounted for by

theory when electron-electron interactions are taken into account [2]. Raman active, zero-momentum inter Landau level excitations in monolayer graphene are sensitive to electron-electron interactions, due to the non-applicability of the Kohn theorem in this system, with a clearly non-parabolic dispersion relation.

[1] S. Berciaud et al. Nano Letters 14, 4548 (2014)

[2] C. Faugeras et al. arXiv:1412.0115

MON 10

Coulomb-induced Valley Coupling in Transition Metal Dichalcogenides

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Within a microscopic model we investigate the impact of Coulomb-induced intervalley coupling on the optical properties of transition metal dichalcogenides (TMDs). Our approach is based on the density matrix formalism and allows an analytical treatment of the excitonic absorption under the influence of intervalley coupling. We find that the strong Coulomb interaction in these atomically thin 2-dimensional materials couples resonant excitonic states in K and K' valleys [1]. This coupling leads to a splitting of excitonic absorption peaks in the range of the trion binding energy. We further investigate the impact of experimentally accessible parameters, such as doping, dielectric environment, and the detuning of resonant states in the K and K' valley, on the intervalley coupling. The gained insights are of crucial importance for the application of TMDs in valleytronics.

[1] Gunnar Berghäuser and Ermin Malic, "Analytical approach to excitonic properties of MoS₂", Phys. Rev. B 89, 125309 (2014)

MON 11

Functionalization of 2H-MoS₂ with metal acetate salts

Nina C. Berner^{1,2}, Claudia Backes^{1,3}, Xin Chen^{1,2}, Paul Lafargue^{1,2}, Pierre LaPlace^{1,2}, Mark Freeley^{1,2}, Conor P. Cullen^{1,2}, Georg S. Duesberg^{1,2}, Jonathan N. Coleman^{1,3}, Aidan R. McDonald^{1,2}

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Layered two-dimensional (2D) inorganic transition metal dichalcogenides (TMDs) have recently attracted great research interest due to their potential applications in catalysis, optoelectronics, and medicine. There is a growing need to improve the processing techniques and to find methods to functionalize 2D-TMDs in order to alter their surface chemistry and match it to the requirements of different applications. We have established a facile route towards the functionalization of 2D-MoS₂ which can be applied to both liquid exfoliated MoS₂ nanosheets in solution as well as to vapor-grown MoS₂ thin films and CVD-grown monolayers. We found that the reaction of 2D-MoS₂ with M(OAc)₂ (M=Cu, Ni, Zn; OAc=acetate) salts yielded

functionalized $\text{MoS}_2\text{-M}(\text{OAc})_2$ [1]. Importantly, this method successfully furnished the semiconducting 2H-polytype of MoS_2 , where all previously reported functionalization methods can only be applied to the metallic and unstable 1T-polytype.

[1] Berner, Backes et al., Angew. Chem. Int. Ed. 2015, doi:10.1002/anie.201409412R2

MON 12

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

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In the last decade, colloidal nanocrystals (NC) have attracted a lot of interest because their photoluminescence (PL) in the visible, UV and infrared spectrum. The possibility to synthesize NCs 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 in respect to conventionally used dyes in quantum yield, lifetime and narrow PL. 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 Raman spectroscopy and furthermore monitor the synthesis in real time in order to gather insights on the silica growth mechanism. While the optically active CdSe core remains almost unchanged, the CdS shell shows a defined shift, that occurs during the first hours of the experiment.

MON 13

Aligning graphite platelets in copper to enhance the thermal conductivity

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Lightweight composites with superior thermal transport properties promise great application as heat sinks for advanced electronic packaging. With the discovery of the extraordinary thermal conductivity of carbon nanotubes and graphene the interest in using these materials for heat dissipation applications has grown strongly. More specifically, using these materials to enhance the thermal properties of conventional materials such as metals or polymers. Here we present a study on refining the thermal properties of Cu by graphite platelet reinforcement. The high aspect ratio of the platelets leads to preferred orientation in the Cu matrix during the fabrication process. The degree of alignment depends on the lateral size of the platelets and

leads to anisotropic thermal conductivity of the composite which is up to 10 times higher along the graphite alignment compared to the perpendicular direction. The correlation between nanoplatelets alignment and their lateral size is quantitatively extracted from polarized Raman measurements. This information is used to derive the thermal interface resistance between Cu and graphite by means of effective medium approximation.

MON 14

Ultrafast electronic readout of diamond nitrogen-vacancy centres coupled to graphene

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The near-field interaction between fluorescent emitters and graphene exhibits rich physics associated with local dipole induced electromagnetic fields that are strongly enhanced due to the unique properties of graphene [1]. This interaction can be utilized to explore new limits of light-matter interactions. Recent fluorescent experiments have demonstrated that the fluorescence of nitrogen vacancy (NV) centers in diamond is quenched by the presence of graphene. We apply an ultrafast photocurrent spectroscopy [2,3] to detect the nonradiative energy transfer (NRET) from fluorescent emitters (NV centers) to graphene with a time resolution of picoseconds. Our findings demonstrate that the NRET can be exploited as an ultrafast, electronic read-out process of the electron spin in nitrogen vacancy centers in the diamond nanocrystals [4].

We thank the European Research Council (ERC) for financial support (Grant Nano-REAL, No. 306754).

[1] Gaudreau, L. et al. *Nano Lett.* 13, 2030 (2013)

[2] Auston, D. H. *IEEE Journal of Quantum Electronics* 19, 639 (1983)

[3] Preetel, L. et al. *Nature Communications* 3, 646 (2012)

[4] Brenneis, A. et al. *Nature Nanotechnology* (2015). doi:10.1038/nnano.2014.276

MON 15**Integration of graphene with atomic layer deposited Al₂O₃ dielectrics for future electronic devices**

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Atomic layer deposition (ALD) emerges as promising technique for deposition of thin oxide dielectric films on graphene without damage to underlying graphene lattice. However, ALD films do not form continuous layer on pristine graphene due to inert nature of the graphene surface. Consequently, additional surface functionalization is necessary to create functional groups for oxide film nucleation. In our contribution, Ni films with a thickness of 300 nm deposited on silicon using vacuum evaporation were used as a substrate. Graphene layers were prepared by chemical vapour deposition from methane atmosphere at temperature of 1000 °C. Thin Al₂O₃ films were prepared on top of the graphene films by ALD at temperatures 100 and 200 °C. Properties of graphene films before and after the ALD growth were studied using Raman spectrometry and scanning electron microscopy. Al₂O₃ films were characterised by capacitance-voltage and current voltage measurements. Ozone treatment has substantial influence both on graphene and Al₂O₃ dielectric properties and careful optimization should be performed for obtaining good quality dielectrics without degradation of graphene properties.

MON 16**Switching between different nitrogen forms by annealing/bombardment of CN_x nanotubes**

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As result of the synthesis, CN_x nanotubes usually contain different forms of nitrogen. The most common ones are graphitic nitrogen (direct substitution for carbon atom), pyridinic nitrogen (bonding with two carbon atoms) and pyrrolic nitrogen (location in a pentagonal ring). Here we show that ratio of these nitrogen forms can be tuned by annealing and bombarding CN_x nanotubes in a high vacuum. Aligned CN_x nanotubes have been grown vertically on silicon substrates and a post-synthesis treatment was done directly in a chamber of X-ray spectrometer. CN_x nanotube arrays were repeatedly bombarded by Ar⁺ ions with a kinetic energy of 0.5 and 1 keV and annealed at temperatures from 600°C to 1100°C. Electronic state of nitrogen in CN_x nanotubes before and after the treatment was probed using X-ray photoelectron and X-ray absorption spectroscopy. We found that with the annealing the content of graphitic nitrogen grows while it is impossible removing all pyridinic nitrogen. The final temperature after which the concentration of latter nitrogen form remains constant was determined. Effect of dominant nitrogen form on the field emission property of CN_x nanotubes was revealed.

MON 17**Light emitting devices based on organic spintronics**David Carroll¹¹Physics, Wake Forest University, Winston-Salem

Light emitting devices based on field-induced current injection have been shown to yield high intensity emission with very high power efficiencies. Such devices are typically activated using large AC fields across the nanometer scale thin film emitter organics. Recently, we have correlated the observation of high power efficiencies with the onset of negative magnetoresistance in the organic emitters suggesting that the internally coupled magnetic field of the device is playing a role in spin singlet selection of the injected currents. In this presentation we examine the insertion of 2D quantum dots (nanoplates) into the emitter. We show that the magnetic response of the additional nanophase can result in an additive effect on singlet selection in the emitter yielding a significant enhancement of the singlet to triplet population ratios. We believe such nanophase composites may present a potential route to realizing optical gain in electrically driven organic devices for the first time.

MON 18**Intra-layer potassium intercalation of multiwalled carbon nanotubes**Julio C. Chacon-Torres¹, S. Dzsaber², S. Vega-Diaz³, T. Pichler⁴, F. Simon², M. Terrones⁴, S. Reich¹¹Experimental Physics, Freie Universität Berlin, Arnimallee 14, Berlin, 14195, Germany²Faculty of Physics, Budapest University of Technology and Economics, Budafoki ut 8, Budapest, 1111, Hungary³Department of Physics, Department of Chemistry, Department of Material Science and Engineering and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, University Park, Pennsylvania 16802, USA⁴University of Vienna, Faculty of Physics, Strudlhofgasse 4, Vienna, 1090, Austria

We have obtained highly doped potassium intercalated multiwalled carbon nanotubes (MWNTs). This was only possible by using specific nanotubes uncapped at both ends, with intrinsic axial disruptions, and short length. Our results confirmed a full intercalation depicted by a change in color from black to brown-yellow in the MWNTs. The XRD analyses indicate the presence of K atoms between the layers of the MWNTs. Finally, the Raman spectra revealed a Breit-Wigner-Fano (BWF) line shape in the G-line region additionally to a Cz mode around 500 cm⁻¹ and a total vanishing of the 2D-line component.

We have found that the doping mechanism in MWNTs is highly similar to graphite intercalation compounds. Hence, the obtained Raman response is quite the same as in KC₈. The BWF Raman line shape and the XRD indicate a possible direct charge transfer mechanism from the intercalant to the rolled graphene layers of the nanotubes, which brings important implications to a potential superconducting phase.

Moreover, a successful complete intercalation in MWNTs will serve as a first step through an effective exfoliation process for bulk graphene nano-ribbon production. Funding DRS-Fellowship

MON 19

Temperature-dependent NEXAFS and HAXPES: charge carrier localization in the two-dimensional organic conductor (DOEO)₄[HgBr₄]TCE

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We investigated (DOEO)₄[HgBr₄]TCE crystals by near-edge X-ray adsorption fine structure (NEXAFS) and hard X-ray photoelectron spectroscopy (HAXPES). Experiments were performed at the WERA beamline of ANKA, Karlsruhe, and beamline P09 at PETRA III, Hamburg, respectively.

In (DOEO)₄[HgBr₄]TCE we found evidence of an antiferromagnetic phase existing below 40 K. We characterized occupied and unoccupied electronic states in the crystals. S2s and Cl2p HAXPES spectra were taken at different temperatures. They provide evidence of electron density redistribution in DOEO layers upon cooling and correlations between phase transitions and electronic states in the crystals. Furthermore, the S2p and O1s edges were investigated by NEXAFS, revealing fingerprints of charge carrier redistribution and localization below 50 K. Based on investigations of magnetic susceptibility, transport properties[1], electron spin resonance[2] and electron density distributions we propose a mechanism of localization with appearance of antiferromagnetic islands in (DOEO)₄[HgBr₄]TCE.

[1] A. Bardin et. al., Coord. Chem., 2006, 32, 88

[2] A. Chernenkaya, et. al., Phys. Sol. St., 2012, 54, 239

MON 20**H-terminated nanoribbons and coronene stacks inside and outside single-walled carbon nanotubes**

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Diameter of single-walled carbon nanotubes (SWCNTs) determines the possibility to encapsulate molecules and governs the type of structures that can be formed inside the tubes [1,2]. Differences between the encapsulated structures, such as coronene molecules stacks and graphene nanoribbons (GNR), were detected and studied via Raman and photoluminescence (PL) spectroscopies. We show the importance of the PL excitation mapping in a wide spectral range in order to clearly detect the spectral features specific to coronene stacks or GNR inside the nanotubes. We pay particular attention to the by-products that can be formed on the outside surface of nanotubes. Raman spectroscopy was used to study aggregates that were extracted from filled SWCNTs by sonication and density gradient centrifugation processes.

Funding by RFBR grants 13-02-01354, 14-02-00777 and MESRF grants 14.513.12.003, SP-7362.2013.3 is acknowledged.

[1] A.I. Chernov et al., ACS Nano 7, 6346 (2013)

[2] A.I. Chernov et al., Phys. Stat. Sol. (b) 251, 2372 (2014)

MON 21**Magneto-optical response of graphene on boron nitride: Dirac cone replica and Excitonic effects**

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Optical transitions between Landau levels provide precise information on the electronic structure of graphene, as well as substrate and many-body effects. In this work we calculate the magneto-optical response (optical conductivity) of large-size graphene flakes aligned on hexagonal boron nitride (BN) using a tight-binding approach. Recent experiments reveal satellite band gaps in the density of states away from the Dirac point induced by the BN substrate. These structures were interpreted as secondary Dirac cones. However, our calculations suggest that the satellites feature parabolic dispersion and the difference in interpretation arise as an artifact of measuring as a function back gate voltage [1]. We propose magneto-spectroscopy as a way to probe the satellite and Dirac Landau levels in terms of energy. In addition we include the magneto-excitonic correction to the main transition lines in first or-

der perturbation theory. Our approach yields a quantitative explanation of recently observed Landau-level dependent renormalizations of the Fermi velocity.

[1] L.A. Chizhova, F. Libisch, and J. Burgdörfer PRB 90 (2014) 165404

MON 22

Drawing Circuits with Carbon Nanotubes

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Controlling the orientations of nanomaterials on arbitrary substrates is crucial for the development of practical applications based on such materials. The aligned epitaxial growth of single-walled carbon nanotubes (SWNTs) on specific crystallographic planes in single crystalline sapphire or quartz has been demonstrated; however, these substrates are unsuitable for large scale electronic device applications and tend to be quite expensive. Here, we report a scalable method based on graphoepitaxy for the aligned growth of SWNTs on conventional SiO₂/Si substrates. The "scratches" generated by polishing were found to feature altered atomic organizations that are similar to the atomic alignments found in vicinal crystalline substrates. The linear and circular scratch lines could promote the oriented growth of SWNTs through the chemical interactions between the C atoms in SWNT and the Si adatoms in the scratches. The method presented has the potential to be used to prepare complex geometrical patterns of SWNTs by 'drawing' circuits using SWNTs without the need for state-of-the-art equipment or complicated lithographic processes.

MON 23

Non-linear luminescence and four-wave mixing from graphene, probed by femtosecond pulse shaping

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We investigated the non-linear emission of graphene for different layer thickness using confocal microscopy and a 15fs pulsed laser at 1.55eV with a pulse shaper. Ultrafast optical excitation leads to two main non-linear emission signals in the visible. The first contribution is described as incoherent non-linear photoluminescence (NLPL) [1]. Spectrally resolved autocorrelation scans revealed a continuously decreasing decay time of the NLPL from 1.2eV towards 2.8eV. Comparing the dynamics observed for different layers allows us to identify the influence of substrate induced doping.

The second results from near-degenerate four-wave mixing (nd-FWM) which is extraordinarily strong in graphene as compared to other materials. We show that in graphene nd-FWM is spectrally nearly uniform and dispersionless. Finally, we were able to separate a weaker third contribution induced by the microscopic polarization of graphene [2].

Financial support by the DFG through the Nanosystems Initiative Munich (NIM) and the ERC (NEWNANOSPEC) is gratefully acknowledged.

[1] C. H. Lui, T. Heinz et al., PRL 105 (2010). [2] T. Winzer, R. Ciesielski, M. Handloser et al., arXiv:1411.0531v1 (2014).

MON 24

Graphene integrated with silicon waveguides: a route to sensing

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There are distinct and obvious technological advantages to be gained by the integration of graphene with silicon photonics devices, but understanding the nature of the light-matter interaction in these systems is crucial if this potential is to be realised. Our immediate focus is on trying to understand the limitations on the practical sensitivity of silicon photonic cavities where graphene acts as a sensitization layer with improved reactivity over the bare silicon surface. We examined the near-IR light-matter interaction for graphene integrated cavity ring resonators based on silicon-on-insulator (SOI) race-track waveguides[1]. By measuring the TE mode linear absorption coefficient of graphene and combining this with a model of the variation in coupling strength with the graphene-waveguide separation, we are able to place limits on the graphene cavity length for optical sensing applications.

[1] - Crowe, I. F. et. al., Optics Express, 22, 15, 18625 (2014)

MON 25

Electrical tuning of spin-orbit interaction in InAs nanowires

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InAs nanowires are a promising platform to fabricate various quantum electronic devices. One of their attractive properties is their strong spin-orbit interaction (SOI). The controlled tuning of the SOI is desired property of spin based quantum devices. In this study we experimentally investigated the possibility of tuning the

SOI by electrostatic field. The sources of the electric field were backgate and two sidegates parallel to the wire axis. The strength of the SOI was analyzed by weak-antilocalization. We demonstrated that the SOI can be strongly tuned, by a factor of 3 with the electric field across the nanowire, while the average electron density in the nanowire was kept constant. Furthermore a simple electrostatic model was introduced to calculate the expected change of SOI and good agreement was found with the experimental results without fitting parameters.

MON 26

Stability analysis and improvement of HNO₃-doped graphene

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Although the charge carrier mobility of pristine graphene is high, its intrinsic charge carrier density is nearly zero. Doping is therefore necessary for industrial applications of graphene as a transparent, flexible conductor. Currently, it is possible to obtain a significant increase in conductivity, using for example nitric acid or iodine treatments, which are, however, not sufficiently stable for industrial applications [1]. A stable increase in conductivity can be obtained by evaporation of high work function oxides [1], but the improvement in conductivity in comparison to acid treatments is more modest. A combination of stable and strong doping is thus still elusive. Here we present a systematic analysis of the doping stability of nitric acid by electrical measurements, X-ray photoemission spectroscopy and Raman spectroscopy, for different treatments and under different environmental conditions. The analysed data is used to develop a procedure to stabilise the acid doping. This improvement in doping stability represents a step towards ITO replacement by graphene.

[1] D'Arsiè et al., APL (2014)

MON 27

High temperature molecular beam epitaxial growth of graphene on sapphire substrates

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Here we report the growth of graphene using a custom-designed dual chamber molecular beam epitaxy (MBE) system, based on the GENxplor from Veeco. The standard GENxplor has been specially modified by Veeco to reach growth temperatures of up to 1850°C in high vacuum conditions and is capable of growth on substrates up to 3 inches in diameter. Our estimate of the growth temperature is based on a thermocouple reading. In order to calibrate the temperature we have formed graphene on the Si-face of SiC by heating wafers to temperatures above 1400°C. To demonstrate

the scalability of the developed process, we have grown graphene on SiC substrate sizes ranging from 10x10 mm² up to 3-inch diameter.

We have also grown graphene layers on sapphire substrates using a SUKO-63 carbon sublimation source. Growth at substrate temperatures between 1000 and 1650°C have been investigated.

We report the results of a wide range of techniques (reflection high energy electron diffraction (RHEED), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), atomic force microscopy, scanning tunnelling microscopy and sheet resistance measurements) that we have used to characterise these layers.

MON 28

Vibrational properties of cove-shape edged graphene nanoribbons

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Recently, liquid phase processable graphene nanoribbons (GNR) with atomically precise edges were obtained by bottom up solution-mediated methods [1]. Here we report on ab-initio calculations [2] of the Raman spectrum for such novel structures with cove-shape morphology, where a C ring periodically decorates the zigzag edge. We consider a set of GNRs with different width and edge functionalization, finding very good agreement with experimental results [1]. We find that both the edge geometry and functional groups significantly impact the Radial-Like Breathing Mode (RLBM). The cove-shape morphology of the edge is instead mainly responsible for the activation of the D peak, which is not present in purely zigzag GNRs [3].

[1] Narita et al. Nat Chem 6, 126 (2014); ACS Nano 8, 11622 (2014)

[2] Giannozzi et al. JPCM 21, 395502 (2009)

[3] Gillen et al. PSSB 247, 2941 (2010) and references therein

MON 29

Light-emitting diodes by bandstructure engineering in van der Waals heterostructures

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The advent of graphene and related 2D materials has recently led to a new technology: heterostructures based on these atomically thin crystals. The paradigm proved itself

extremely versatile and led to rapid demonstration of tunnelling diodes with negative differential resistance, tunnelling transistors, photovoltaic devices, etc. Here we take the complexity and functionality of such van der Waals heterostructures to the next level by introducing quantum wells (QWs) engineered with one atomic plane precision. We describe light emitting diodes (LEDs) made by stacking up metallic graphene, insulating hexagonal boron nitride (hBN) and various semiconducting monolayers into complex but carefully designed sequences. Our first devices already exhibit extrinsic quantum efficiency of nearly 10% and the emission can be tuned over a wide range of frequencies by appropriately choosing and combining 2D semiconductors (monolayers of transition metal dichalcogenides). The range of functionalities for the demonstrated heterostructures is expected to grow further with increasing the number of available 2D crystals and improving their electronic quality.

F. Withers et al. arxiv.1412.762

MON 30

Investigation of contact properties and contact materials for graphene spin valve devices

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Although millisecond spin lifetimes have been predicted for graphene, the experimentally determined values are usually in the order of several hundred picoseconds in non local spin valve devices at room temperature. Previously, we showed that contact-induced spin dephasing is the main source of spin dephasing in devices where Co/MgO injection and detection electrodes were directly deposited on graphene (1). Here we demonstrate that the spin transport properties can be improved by fabricating Co/MgO electrodes on Si⁺⁺/SiO₂ and subsequently transfer the graphene on top of this structure. This reduces the coupling of the graphene to the electrodes and leads to spin lifetimes in the nanosecond range, spin diffusion lengths in the order of 10 μm as well as mobilities above 20,000 cm²/Vs (2). We present conductive AFM measurements of the Co/MgO interface to get an additional measure of the contact quality. Furthermore, first results using Al₂O₃ tunnel barriers are shown which are grown by atomic layer deposition.

(1) F. Volmer, M. Drögeler et al., Phys. Rev. B 88, 161405(R) (2013).

(2) M. Drögeler et al., Nano Lett. 14, 6050 (2014).

MON 31**ReS₂ interlayer bonding investigated through laser-pump x-ray probe spectroscopy**Ehren Mannebach², Friederike Ernst¹, Tony F. Heinz¹, Aaron Lindenberg²¹Columbia University, Department of Physics²Stanford University, Department of Materials Science and Engineering

ReS₂ is a transition metal dichalcogenide (TMDC) for which the Raman and photoluminescence response are similar between monolayer and bulk samples, contrary to the behavior observed in other TMDCs. A DFT study reports a small interlayer coupling strength of 18meV/ unit cell, less than 8% of that of MoS₂.^[1] Weak interlayer coupling may indicate that the individual layers behave like two-dimensional systems without the need for monolayers.

We conduct a laser-pump grazing-incidence x-ray probe study on monolayer-regime samples to investigate the structural changes induced by above band gap laser heating at the picosecond to microsecond scale. Structural changes are observed on two time scales. An initial drop in scattering intensity on the scale of 100ps is followed by a full recovery for laser fluences < 20mJ/cm² and a partial recovery for fluences > 20mJ/cm² on the scale of nanoseconds. These time scales support the weak interlayer coupling postulated in the DFT calculations.

[1] Tongay et al., Nature Comm. 5 3252 (2014)

MON 32**Doping of Carbon Nanotube Forests Using MoO₃**Santiago Esconjauregui¹, Lorenzo D'Arsiè¹, Yuzheng Guo¹, Cinzia Cepek¹, John Robertson¹¹Department of Engineering, University of Cambridge, Cambridge, UK

Carbon nanotube forests may find applications as interconnects in integrated circuits. However, to outperform the materials currently used in electronics, the tubes need to be grown at low temperatures, on conductive supports, and in the form of high-density forests with all the tubes holding metallic character. As control over structural selectivity has not been achieved yet, the forests show resistivity values orders of magnitude greater than that of Cu, regardless of the fact that nanotubes themselves can sustain much higher current densities. Here, we dope nanotube forests using MoO₃ and evaluate the doping stability at different conditions and its impact on the electrical properties of the tubes. By in-situ XPS, we first determine the minimum necessary MoO₃ thickness to dope a tube ensemble. We then study the variation of forest resistivity upon annealing in vacuum at various temperatures and times, and find that MoO₃-doped forests increase their conductivity at least two orders of magnitude thus reaching values comparable to that of Cu. As MoO₃ is CMOS-compatible, this report represents a step towards the use of nanotubes in interconnects of next generation electronics.

MON 33**Scaled Synthesis of Boron Nitride Nanotubes, Nanoribbons, and Nanococoons Using Direct Feedstock Injection into an Extended-Pressure, Inductively-Coupled Thermal Plasma**

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Boron nitride nanotubes (BNNTs), which are electrically insulating or semiconducting when properly doped, exhibit excellent thermal conductivity, great chemical inertness, high temperature oxidation resistance, and radiation-absorption properties, making them far superior than their carbon analogues for many applications. Unfortunately, scientific studies and industrial applications of BNNTs and related BN-based nanomaterials have been markedly limited by the lack of availability of synthesized material. Here we demonstrate the successful operation of a high-throughput, scalable BN nanostructures synthesis process whereby precursor materials are directly injected into a high-temperature, variable pressure (up to 10 atm) inductively-coupled thermal plasma system. The system can be operated in a near-continuous fashion and thus far has achieved a record output of over 35 g/h for pure, small diameter, few wall, highly crystalline BNNTs. Under suitable conditions, collapsed BN nanotubes (i.e., nanoribbons), and closed shell BN capsules (i.e., nanococoons) are also obtained. The process is adaptable to a large variety of feedstock materials.

MON 34**Revealing the properties of N-doped carbon nanomaterials synthesized by UHV-CVD**

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Herein we present the latest progress in the understanding of the properties and synthesis of Nitrogen doped Single Wall Carbon Nanotube (SWCNT) [1,2] and Graphene [3]. These materials doped with N show new different and interesting electronic properties, like having an n-type or p-type behavior correlated to the structure making them very interesting for several applications. Ultra-High Vacuum Chemical Vapor

Deposition (UHV-CVD) has been used to synthesize the nanomaterials with doping heteroatoms. Using a particular carbon feedstock and a set-up for the furnace it has been possible to achieve high quality nanomaterials. Raman spectra have typical shape of SWCNT with a very narrow diameter distribution. XPS confirmed the Nitrogen percentage and substitutional bonding environment. Using in situ Mass Spectroscopy additional understanding of the mechanism of growth detecting the different species was achieved during the growth.

TP acknowledges support from the (FWF Proj.Nr. I 943-N19), AMA support from DFG (MA 5215/4-1) and the EU (ERA-Chemistry)

[1] Ayala P. et al. Carbon 2010

[2] Ayala P. et al. Rev Mod Phys 2010

[3] Usachov D. et al. Nano letters 2014

MON 35

Prediction and theoretical investigation of new 2-D and 3-D periodical structures, having graphene-like band structures

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It is proposed and theoretically investigated the new general family of planar nanostructures having graphene's electronic band-structure. With help of general theory and using perturbation theory it is shown that the graphene-like planar structure consist of identical nanoparticles having relatively weak contacts should lead to the electronic band structure with the Dirac cones. Within DFT calculations using the VASP program the band structures of two different aforementioned structures consist of silicon nanoparticles having 71 or 114 atoms were calculated. The calculated electron velocity at the Fermi level near the Dirac cones were equal $1.05 \cdot 10^5$ and $0.53 \cdot 10^5$ m/s, respectively.

Also, by generalizing the theory it is proposed the family of 3-D structures having the band structures with the Dirac cones. As an example, the DFT calculation of a simple cubic lattice consist of identical silicon nanoclusters having 25 atoms shows that the band structure near the special surface of the form $(\cos(k_x) + \cos(k_y) + \cos(k_z)) = 0$ has a feature similar to the Dirac cones.

MON 36**THz-conductivity of CVD graphene on different substrates**

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We analyzed by THz-Time Domain Spectroscopy the conductivity of CVD graphene as grown and p-doped, deposited on different substrates: PET (Polyethylene Terephthalate), PEN (Polyethylene Naphthalate), quartz, glass and silicon, in the range from 0,1 to 2 THz. Graphene shows a superficial conductivity around 10 to 40 times the value of minimum conductivity at frequencies of THz, as previous studies have shown [1]. Our results show a noticeable dependence with the substrate at high frequencies. Flexible substrates like PET and PEN are interesting for applications as flexible electronic devices, including solar cells. We have developed an effective doping method for large area CVD grown graphene by UV-light irradiation under oxygen atmosphere. By Raman spectroscopy we can observe that doping occurs without a noticeable resistance increase and a slight mobility change, and is found to be stable and reversible. Superficial conductivity of p-doped graphene is slightly higher than pristine graphene; p-doped graphene presents an increase of electromagnetic absorption, compared to pristine graphene.

[1] W. Liu, R. Valdés Aguilar, Y. Hao, R.S. Ruoff, N.P. Armitage, J. Appl. Phys. 2012.

MON 37**Separation of Single-Walled Carbon Nanotubes with a Gel Permeation System**

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Recently we have shown that by altering the pH of the sodium dodecyl sulfate (SDS) eluent in a Sephacryl gel column that 15 different nanotube (n, m) single-walled carbon nanotubes (SWCNTs) species can be prepared from the HiPco raw material. By changing the pH of the SDS eluent we showed that hydrolysis of SDS leads to small quantities of 1-dodecanol being formed in solution, which become incorporated into the SDS micelle of the SWCNTs and alter the interaction with the gel. We now apply our approach to a gel permeation chromatography (GPC) system. In doing so we gain precise control over the pH of the SDS eluent and can utilize computer-controlled pH-gradients in the separation of (n, m) SWCNT species. This allows us to reproducibly elute different (n, m) species with control over when (time-based) different fractions should be collected. This automated procedure requires no pre-centrifugation, is scalable, and is found to yield monochiral SWCNT fractions of semiconducting SWCNTs with a purity of 61 - 95 %.

MON 38**Photoluminescence and Raman spectroscopy of N-layer MoTe₂**Guillaume Froehlicher¹, Étienne Lorchat¹, François Fernique¹, Stéphane Berciaud¹¹IPCMS, Université de Strasbourg and CNRS, France

Atomically thin transition metal dichalcogenides (TMDs, denoted MX₂), exhibit peculiar optical and electronic properties, which may be harnessed in novel optoelectronic devices. As compared to Mo- and W-based TMDs, Te-based TMDs remain less studied. Such compounds are expected to emit in the near-infrared range, thus extending the possible applications of TMDs over a broader spectral window.

Here, we present optical characterizations of N-(tri)layer molybdenum ditelluride (MoTe₂), from N=1 to N=10, by means of micro-photoluminescence (PL) and micro-Raman spectroscopy. As for other Mo- and W-based TMDs, a strong PL blueshift and PL enhancement are observed in monolayers, suggesting a transition from an indirect bandgap (~ 0.94 eV) in the bulk to a direct bandgap (~ 1.10 eV) for N=1. In addition, the low (breathing and shear modes, in the range 5-40 cm⁻¹) and high frequency Raman modes (in the range 150-300 cm⁻¹) of N-layer MoTe₂ are investigated by means of polarized Raman measurements. The frequencies of the shear and breathing modes are analyzed within a simple model based on a linear chain of oscillators and allow for an accurate determination of N.

MON 39**Investigation of carbon nanotube based field-effect transistors using atomistic quantum transport and numerical device simulation**Florian Fuchs^{1,2}, Andreas Zienert³, Jörg Schuster¹¹Fraunhofer Institute for Electronic Nano Systems, 09126 Chemnitz, Germany²now at Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany, and at Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany³Center for Microtechnologies, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Carbon nanotube based field-effect transistors (CNTFETs) are studied by use of two different approaches: numerical device simulation (NDS) based on the effective mass Schrödinger equation and atomistic quantum transport simulation based on the non-equilibrium Green's functions formalism (NEGF). The studied CNTFETs consist of n-doped source- and drain-electrodes together with an ideal wrap-around gate.

Using density functional theory, we extracted a parameter set for the NDS model. A band-to-band tunnel current is predicted by the NDS once the valence band edge is shifted to the Fermi energy, which increases the off-current and leads to slight ambipolar behavior. Using the NEGF instead, localized states inside the channel can be observed and the band-to-band tunnel current is suppressed, resulting in a high on/off ratio of about 10⁷. We illustrate the potential of the studied CNTFET for future applications by varying the channel length and find excellent properties

for a channel length down to 8 nm. Furthermore, the influence of the gate electrode is investigated, where good transistor behavior is observed even for a small gate of only 0.4 nm length.

MON 40

Reversible sublattice symmetry breaking in monolayer graphene nanomembranes using tip induced pseudomagnetic fields

Alexander Georgi¹, Peter Nemes-Incze¹, Ramon Carillo-Bastos², Daiara Faria², Silvia Viola Kusminskiy³, Marco Pratzer¹, Nancy Sandler², Markus Morgenstern¹

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Strain engineering in graphene might lead to a new generation of electromechanical devices, in particular due to its tunable pseudomagnetic field being a property of the unique sublattice degree of freedom within the honeycomb lattice. However, possibilities to tune the pseudomagnetic field on the nanoscale have not been realized so far. Here, we show that the forces of the tip of a scanning tunneling microscope can be used to switch local fields on and off by applying local strain, as visible by a relative change of the local density of states of the two sublattices up to 30 %. Comparison with tight binding simulations reveals that this contrast corresponds to a pseudomagnetic field of up to 500 T. We carefully rule out other possibilities for the apparent sublattice symmetry breaking such as buckling, a local Peierls transition, different lifting forces of the tip above different sublattices, or the correlation of electric and pseudomagnetic fields. Moreover, we show that model calculations of the van-der Waals forces between tip and graphene reproduce the observed effects quantitatively within 50 %.

MON 41

Graphene synthesis of crystalline precursor molecules

Kati Gharagozloo-Hubmann¹, Niclas Müller¹, Valerio Oddone¹, Stephanie Reich¹

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One of the most promising routes for the synthesis of graphene is the chemical vapor deposition. Common CVD-processes use gas phase carbon sources like methane as a building block. Recent synthesis via molecular building block received graphene from molecular precursor such as benzene or bianthryl, which are liquid and solid. The molecular structure and geometry of the starting compound (molecular precursor) for graphene production is a crucial factor that affects the crystal structure, lateral spreading, and the edges symmetry of resulting graphene. Different precursor molecules with different symmetries were used as starting material for graphene production. Subsequently, the resulting graphene crystals were investigated in respect of their 2-dimensional propagation geometry. We study the influence of the geometry

and the activity of the precursor molecules on the structure of the resulting graphene layers. The results will affect support the choice of the proper precursor structure for the gas phase production of graphene.

MON 42

Structure of Double Wall Carbon Nanotubes by combining a robust HRTEM approach and tight binding calculations

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Single-walled carbon nanotubes (SWNTs) have shown outstanding 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 could be to use double-walled carbon nanotubes (DWNTs), consisting of two concentric tubes, provided to know how they interact each other. To this aim, we have developed a systematic and robust procedure using acHR-TEM (aberration corrected Transmitting High Resolution Electron Microscopy) and image simulations to study the atomistic structure of over one hundred CVD made DWNTs. Using these tools, we have established some interesting statistics on helicities and diameters of inner and outer tubes of the DWNTs inspected.

Results reveal the existence of a strong coupling between the two concentric tubes, resulting in favoring high helicity angle configurations for DWNTs with outer diameters below 2 nm. The nature of the coupling and the observed selectivity are discussed with the help of energy calculations based on a tight binding approach.

MON 43

Assessing and improving the DFT+D3 method for van-der-Waals interaction in layered materials

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The novel physics in two-dimensional and/or layered materials gave rise to a recent advent of scientific publications with a variety of proposed applications. One demand on a theoretical study of such materials is the proper interclusion of non-covalent bonding effects between layers and/or adsorbed molecules to obtain the correct geometries and derived physical properties. A flexible description of such van-der-Waals interactions can be achieved by a posteriori corrections of semi-local density functional theory (DFT) in the recently proposed DFT+D3 scheme [1]. We have implemented this correction method in the freely available Quantum Espresso computational package and assessed its performance together with the highly accurate Jollet-Torrent-Holzwarth (JTH) set of high-throughout pseudopotentials on a range of layered and non-layered solids. Based on this assessment, we devised a sim-

ple fitting procedure based on a triquadratic model function and obtained a slightly altered set of parameters that led to further improvement of the predicted lattice constants and bond lengths compared to the originally proposed parameters.

[1] Grimme et al., J. Comput. Chem. 32, 1456 (2011).

MON 44

Non-perturbing, covalent functionalization of single walled carbon nanotubes

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The functionalization of carbon nanotubes (CNTs) has been widely exploited to attach dyes, switches and other molecules onto CNTs to tailor their optoelectronic properties. The attachment of the functional component can be realized by different approaches, such as non-covalent, covalent and sidewall functionalization, π - π stacking interactions, and endohedral filling. For optoelectronic studies non-covalent functionalization of CNTs had been the most favorable way, since it is a non-invasive and non-perturbing route to attach functional moieties onto CNTs [1,2]. Covalent functionalization on the other hand is known to be a rather harsh treatment, inducing great perturbations to the nanotube structure, resulting in altering the electronic properties of the CNTs. Here we introduce for the first time a non-invasive route to functionalize carbon nanotubes covalently, showing that the characteristic luminescence and Raman spectra remain unchanged upon functionalization.

[1] A. Setaro, P. Bluemmel, C. Maity, S. Hecht, and S. Reich, Adv. Funct.Mat. 22(11), 2425-2431 (2012)

[2] F. Ernst, T. Heek, A. Setaro, R. Haag, and S. Reich, Appl. Phys. Lett. 102, 233105 (2013)

MON 45

Liquid adhesion and capillary actions at the nanoscopic level: Direct observations of exceptional water-single WS2 nanotube interactions.

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The use of different nanostructures as fillers in polymer composite materials attracts an ever-growing interest. While the impact of nanoparticles (NP) on composite properties is well studied, the relations between individual NP and the host matrix are yet to be fully understood. In this work, we present a new technique for measurements of individual nanotube-liquid interactions using ESEM and AFM systems. Here the effect of WS2 nanotube morphology and structure on the interaction strength between different liquids and the nanotubes is assessed. These experiments in conjunction

with theoretical simulations show that the morphology of the WS₂ nanotube has a significant effect on the liquid-NT. The interaction energy of the nanotubes falls off dramatically with the diameter of the nanotubes and then levels off. These differences are currently attributed to the capillary interaction of the small hollow core nanotubes with the water. MD simulations show that the highly confined space results in large interaction energy between the water and the inner core of the nanotubes. These effects and the impact of the nanotubes surface chemistry on the interaction energy are presented and discussed

MON 46

Studying the interaction of phospholipids with graphene materials using a quartz crystal microbalance

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Studying the interaction of phospholipids with surfaces is important for the development of biosensors that accurately mimic or interact with cellular structures. Graphene is a promising material for such sensors due to its high sensitivity. One route to fabricate graphene/phospholipid biomimetic membranes is 'vesicle fusion' whereby small lipid liposomes (self-assembled spheres) are fused with a graphene surface to form a membrane. The interaction of liposomes with graphene can be followed in-situ using a quartz crystal microbalance. Using a graphene functionalized quartz crystal microbalance with frequency and dissipation measurements (QCM-D), the adsorption properties of phospholipid liposomes in aqueous solutions to various graphene surfaces is shown. The behavior of liposomes that come in contact with graphene depends strongly on the wettability of graphene to the lipids. Graphene oxide, with its hydrophilic surface, promotes the fusion of lipids whereas hydrophobic graphene causes liposomes to adhere but not fuse. The level of oxidation is important, as a trade-off between the loss of conductivity and stability of the membrane needs to be optimized to create efficient electronic sensors.

MON 47

Multiple subgap states in a superconductor - carbon nanotube hybrid device

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¹Department of Physics, University of Basel, Basel, Switzerland

Low-dimensional electronic systems coupled to a superconductor have recently gained much attention due to the search for exotic states like Majorana fermions [1], Cooper pair splitting [2,3], or Andreev bound states [4]. These seemingly different effects have in common that electron transport occurs at energies below the superconducting energy gap, leading to transport resonances where single electron transport should

be suppressed. Here we present detailed transport spectroscopy measurements on a carbon nanotube device contacted by a central superconducting Nb lead and two normal metal contacts. The most striking new features are up to 5 gate-tunable conductance peaks within the large energy gap of $\Delta = 1.2$ meV. We investigate these subgap states as a function of an external magnetic field and the temperature and interpret our results tentatively as the onset of a fully developed proximity effect of spatially varying strength in the superconductor-carbon nanotube system.

[1] V. Mourik et al., Science 336, 1003 (2012)

[2] L. Hofstetter et al., Nature 461, 960 (2009)

[3] J. Schindele et al., PRL 109, 157002 (2012)

[4] J-D. Pillet et al., Nat. Phys. 6, 965 (2010)

MON 48

Optomechanics with Graphene Mechanical Resonators

Johannes Guettinger¹, Peter Weber¹, Adrien Noury¹, Ioannis Tsioutsios¹, Darrick E. Chang¹, Adrian Bachtold¹

¹ICFO-Institute of Photonic Sciences, Barcelona

Graphene and Carbon nanotubes are attractive materials for nanomechanical devices because of their exceptional properties, such as high frequencies, quality factors, and low mass. These properties are employed to push the limits in mass and force sensing. The long lifetimes of excitations in mechanical resonators are also very promising for quantum applications. An outstanding challenge with carbon nanoresonators however, has been to obtain large coupling between the motion and external systems for efficient readout and manipulation. I will present our novel approach, in which we capacitively couple a high-Q graphene mechanical resonator to a superconducting microwave cavity [1]. We are able to use the coupling to measure cryogenic thermal motion and to cool the mechanical resonator. Additionally we strongly tune the mechanical properties by pulling on the resonator with a static electric force. This unique tunability in low-dimensional resonators opens up interesting new possibilities for optomechanical systems.

[1] P. Weber, J. Guettinger, I. Tsioutsios, D. E. Chang, A. Bachtold, Nano Lett. 14, 2854 (2014).

MON 49**Controlled folding of 2D materials: GraFold Printing**

Toby Hallam¹, Amir Shakouri², Emanuele Poliani³, Aidan P. Rooney⁴, Ivan Ivanov⁵, Alexis Potie¹, Hayden K. Taylor⁶, Mischa Bonn⁵, Dmitry Turchinovich⁵, Sarah J. Haigh⁴, Janina Maultzsch³, Georg S. Duesberg^{1,7}

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In the last few years significant inroads have been made into shaping, patterning, doping and processing of graphene to create novel technological applications. However, such approaches have generally ignored the ability of flat 2D materials to fold and crease. In fact, such deformations are typically considered to be undesirable. This is surprising, since the ability to fold is actually one of the properties that are specific to 2D materials.

We have developed a technique (GraFold) that uses elastomeric stamps with periodically varying adhesive properties to introduce structure and print folded graphene films. We report on an investigation of GraFold printed features with scanning probe microscopy, high resolution electron-microscopy and tip-enhanced Raman spectroscopy. The investigation highlights GraFold printing as a new technique which allows for significant modification of the properties of 2D materials without damaging or chemically modifying them. Furthermore, a finite element model is developed to show the fold formation process. Terahertz spectroscopy reveals induced anisotropy of carrier mobility along, and perpendicular to, the graphene folds.

MON 50**Improved integration process of individual SWNTs into sensors**

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One of the critical issues hindering the application of SWNTs in sensors is related to resist-based lithography applied during SWNT device fabrication. It induces contamination causing poor metal/SWNT electrical contacts [1]. To avoid this contamination we use alumina layer to protect the SWNTs during resist application. Removing alumina by H_3PO_4 is a residue-free process with no detectable change in the properties of SWNTs as verified by Raman spectroscopy [2]. To avoid resist residue redeposition onto the future contact area, oxygen plasma is introduced prior alumina etch. For a protective layer thicker than 30 nm no changes of nanotube Raman spectra due to the plasma are detected. Incorporating above mentioned processes into the CNFET fabrication, the median on-resistance of CNFETs was reduced by 66%

and its interquartile dispersion was narrowed by 88%, respectively. The developed process has been extended from chip to wafer level. The median on-resistance of 812 p-type CNFETs fabricated on the wafer was determined to be 64 k Ω for Cr/Pd contacts.

[1] W. Liu et al., Beilstein J. Nanotech. 5 (2014) 2202

[2] W. Liu et al., Sensors and Actuators B 198 (2014) 479

MON 51

Electron optics in suspended and encapsulated graphene

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We present two alternative ways how to fabricate a Veselago lens in graphene [1,2] - in suspended graphene using a resist technique (LOR) [3] and in graphene encapsulated in hexagonal boron nitride (hBN) using a dry-transfer technique [4]. Negative refraction is achieved by electrostatically gating the graphene seamlessly from n- into p-doping (or vice versa) using top-gates. For both techniques, point-contacts as small as 100 nm can be established. While the fabrication of top-gated devices on LOR works in a reproducible manner, the current annealing of multi-terminal devices with large top-gates turned out to be very demanding. On the other hand graphene encapsulated in hBN and contacted with side-contacts allows ballistic transport and high mobilities while allowing for versatile device-geometries. A reversed-order fabrication is introduced which holds the potential of improved side-contacts and at the same time simplifies the fabrication procedure.

[1] V.V. Cheianov et al. Science 315 1252 (2007)

[2] V. Veselago, Phys. Usp. 10 50 (1968)

[3] N. Tombros et al. J. Appl. Phys, 109 093702 (2011)

[4] L. Wang et al. Science 342 614 (2013)

MON 52

Electronic noise of carbon nanotube quantum dots

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We perform experiments with carbon nanotube quantum dots, which are coupled to an on-chip impedance matching circuit to account for the high device resistances [1]. In order to achieve high quality microwave circuits, we developed a nanotube

stamping technique to transfer them from the growth substrate to the pre-fabricated microwave circuit.

Our high-frequency setup built in a dilution refrigerator enables us to do two kinds of measurements. On one hand, one can measure the reflection coefficient around the resonance frequency of approximately 3 GHz, which is a fast and sensitive way to determine the real and imaginary part of the sample resistance [2]. But our main focus lies on detecting the current noise emitted by the device. In this situation, the impedance matching circuit acts like a band-pass filter with a bandwidth of a few Megahertz.

For the calibration of the setup, we use a noise source with a well-established Fano factor. Our choice is a gold wire in the hot-electron regime with a Fano factor of $\sqrt{3}/4$ [3].

[1] G. Puebla-Hellmann et al., APL 101, 053108 (2012)

[2] V. Ranjan et al., in preparation

[3] N. Bergeal, APL 100, 203507 (2012)

MON 53

Epitaxially driven molecular assemblies: from Kagome lattice to d- wave superconductor

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Surface mediated interactions have been utilized to pattern different structural assemblies of charge transfer salt such as (BETS)₂GaCl₄ (where BETS=bis(ethylenedithio) tetraselenafulvalene) on Ag(111). With a low deposition rate of less than 0.05 monolayer per minute, we find that the substrate temperature drive the molecular orientation and their packing geometry into insulating or superconducting phases. Orientation frustration occurs at 125K of deposition temperature, leading to the formation of Kagome lattice with BETS dimers crowding in triangular units. Using in situ STM tip functionalization, we map the spatial variation of the charge density with sub-molecular resolution on BETS dimers for the first time. When deposited at room temperature, the molecules retain their crystalline superconducting structure with their long molecular axis perpendicular to the substrate. Although the heteroepitaxial process increases the intra dimer separation to about 0.3Å larger than the bulk value, it is remarkable that superconductivity is robust down to a monolayer thickness and still preserves the signature of d-wave symmetry as its bulk counterpart.

MON 54**Controlled nitrogen-doping and carboxyl functionalisation of multi-walled carbon nanotubes**

Gergő Péter Szekeres¹, Krisztián Németh¹, Anikó Kinka¹, Melinda Magyar², Balázs Réti¹, Erika Varga³, Zsolt Szegletes⁴, András Erdőhelyi³, László Nagy², Klara Hernádi¹

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³Department of Physical Chemistry and Material Science, University of Szeged, Hungary

⁴Institute of Biophysics, Biological Research Centre, Hungarian Academy of Sciences, Hungary

Partial N₂ doping of MWCNT was performed during CCVD synthesis. A special reactor was created to enable the syntheses with different reaction conditions. Samples were analysed by TEM in order to provide information about the tubular morphology and their deformation gained after reaction conditions were changed. The N₂ incorporation was studied by XPS, meanwhile XRD and Raman spectroscopy showed the degree of graphitisation. Samples were then carboxyl functionalised in nitric acid solutions of varied concentration and then RC-26 protein was linked to the carboxyl groups in order to make the functionalisation's degree and location visible. Protein linked samples were characterized by UV-Vis spectroscopy and AFM. Results indicated that syntheses, carried out in the new reactor, were successful and resulted in CNTs partially doped with N₂. TEM studies revealed that the expected deformations are localized only in a defined segment of CNTs. The N₂ content in the samples represented in atomic ratios was between 0.9 and 2.9 %. The deformations help the functionalisation at that certain area thus the carboxyl groups' location can be determined.

MON 55**Electrical Properties of Palladium Carbide End-Contacts for Multi-Layered Graphene for Next Generation LSI Interconnects**

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¹Department of Electronics and Electrical Engineering, Keio University, Yokohama, Japan

²Low-power Electronics Association & Project (LEAP), Tsukuba, Japan

Multi-layered Graphene (MLG) has attracted great attention as a material for future LSI interconnects because of its extremely low resistivity. There have been several reports on the top contact electrode technologies for single-layered graphene FETs. However, a different type of contact configuration must be more suitable for MLG interconnects. An end-contact, in which a metal electrode comes into contact with the edges of the graphene layers, has been proposed, and a significant reduction in contact resistivity (r_c) has been demonstrated [1]. For this paper, on the basis of the considerations of carbonization and adhesion strength with nano-carbon materials,

we selected Palladium (Pd) as an end-contact material for MLG. After thermal annealing of 450°C, a 64 % reduction in r_c was obtained, and Pd-Carbide was found using XPS measurements. The minimum r_c reaches 1.8×10^{-7} ohm-cm², which is close to the lowest value ever reported for a pristine MLG [1]. It is worth noting that the r_c variation in Pd contacts is much better than that in Titanium contacts, which is probably because Pd is more resistant against oxidation than Ti.

Ref.:

[1] K. Ito et al., App. Phys. Exp. (2015)

MON 56

Study on Low Temperature CVD Growth Mechanism of Multi-layer Graphene on Single Crystal Ni(111) Wafer and Polycrystalline Ni Thin Film with Artificial Facets

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To develop graphene interconnect technologies for next generation LSIs, a low temperature ($T_g \leq 600^\circ\text{C}$) CVD growth mechanism for multi-layer graphene (MLG) is one of the most important subjects relating to high quality material growth under Si-LSI-compatible conditions. Y. Yamazaki et al. reported that graphene growth originates from crystalline facets with specific angles with respect to the crystalline orientation of catalytic metals [1]. To investigate a MLG growth mechanism, we performed MLG growth on a single crystal Ni(111) wafer and on polycrystalline Ni thin film with an etching step at a controlled angle ("artificial facet"). RF-plasma CVD with T_g of 60°C and SEM observations were employed. In the case of MLG growth on a single crystal Ni wafer, by removing the grown MLG with oxygen plasma, we found that connected facets had formed on the Ni surface along a contour of the removed MLG, suggesting the facet growth. From the experiments on MLG growth on artificial facets, we confirmed that MLG grew preferentially from the facets. Moreover, growth extension of MLG by additional CVD process was found after a growth interruption.

Reference:

[1] App. Phys. Exp. 5 (2012) 025101

MON 57**AC Characterization for Organic/Nanotube Thin-Film Transistors using Frequency-Dependent Current Hysteresis Measurements by Applying Sinusoidal Wave Signals**

Kazuhiro Watanabe¹, Ken Tanoue¹, Yasunori Taki¹, Kei Noda¹, Yuji Awano¹

¹Department of Electronics and Electrical Engineering, Keio University, Yokohama

Organic/Carbon nanotube thin-film transistors have attracted much attention as light, low cost, flexible, and printable devices in large-area electronics applications. However, their AC characteristics have not yet been well understood, and a measuring method for them has still not been established. Because of their high impedance, the conventional AC characterization methods for inorganic FETs, such as S-parameter extraction, are not suitable for them. The hysteresis effect in the I-V characteristics of OTFTs, which is observed very often and depends on the frequency of the AC applied voltage, should be eliminated for reliable and stable circuit operation even if its mechanism is still unknown. In this paper, we report a new measurement protocol for frequency-dependent current hysteresis phenomena in I-V characteristics by using a sinusoidal wave signal together with a measuring circuit considering the high device impedance. We reports current hysteresis changes in Pentacene TFTs depending on the frequency of the sinusoidal wave voltage signal input to the drain and source electrodes.

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- 08:30 – 09:30 **A. Geim, Manchester**
Tutorial: The rise of van der Waals heterostructures
- 09:30 – 10:00 **T. Müller, Vienna**
Optoelectronics with 2D semiconductors
- 10:00 – 10:30 **coffee break**
- 10:30 – 11:00 **R. Gorbachev, Manchester**
Van der Waals heterostructures composed of thin 2D crystals sensitive to atmospheric exposure.
- 11:00 – 11:30 **X. Cui, Hong Kong**
Spin-valley Coupling in atomically thin Tungsten Dichalcogenides crystals
- 11:30 – 12:00 **A. Chernikov, New York**
Excitons and many-body phenomena in atomically thin 2D materials
- 12:00 – 17:00 **mini workshops**
- 14:00 – 17:00 **special workshop**
Nano & Society
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **M. Glazov, St.-Petersburg**
Spin and valley dynamics of excitons in transition metal dichalcogenides
- 19:00 – 19:30 **J. Appenzeller, West Lafayette**
Two-Dimensional Layered Materials – Physics and Applications
- 19:30 – 20:00 **G. Duesberg, Dublin**
Vapour phase Synthesis and Functionalisation of 2D Transition Metal Films
- 20:00 **Poster II**

Tuesday, March 10th

Two-dimensional materials and heterostructures

08:30**The rise of van der Waals heterostructures**Andre Geim¹¹University of Manchester, Manchester, UK

Following the advent of graphene, many other one-atom or one-molecule thick crystals have been isolated. These 2D crystals have become one of the hottest topics in materials science and condensed matter physics. Moreover, isolated atomic planes can now be reassembled into designer structures made layer by layer in a precisely chosen sequence. The first but already remarkably complex heterostructures have recently been fabricated and investigated. I will briefly overview our progress in making such heterostructures with clean and atomically sharp interfaces and then illustrate how exceptionally rich in phenomena the research area is.

09:30**Optoelectronics with 2D semiconductors**Thomas Müller¹¹Institute of Photonics, Vienna University of Technology, Vienna

Two-dimensional (2D) atomic crystals, such as graphene and layered transition-metal dichalcogenides, are currently receiving a lot of attention for applications in (opto-)electronics. In this talk I will review our research activities on photovoltaic energy conversion and photodetection in 2D semiconductors. In particular, I will present a WSe₂ monolayer p-n junction, formed by electrostatic doping using a pair of split gate electrodes, and a MoS₂/WSe₂ van der Waals type-II heterojunction. Upon optical illumination, conversion of light into electrical energy occurs in both devices. I will present measurements of the electrical characteristics, the photovoltaic properties, and the gate voltage dependence of the photoresponse. In the second part of my talk, I will discuss photoconductivity studies of MoS₂ field-effect transistors. We identify photovoltaic and photoconductive effects, which both show strong photoconductive gain. We envision that the efficient photon conversion, combined with the advantages of 2D semiconductors, such as flexibility, high mechanical stability and low costs of production, could lead to new optoelectronic technologies.

10:30**Van der Waals heterostructures composed of thin 2D crystals sensitive to atmospheric exposure.**

Roman Gorbachev¹, Y. Cao¹, K. Khestanova¹, A. Rooney², A. V. Kretinin¹, P. Blake¹, G. L. Yu¹, A. Mishchenko¹, S. J. Haigh², A. K. Geim¹

¹Physics and Astronomy, University of Manchester, Manchester

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Of the many 2D layered materials known to exist only a precious few are completely stable in the ambient environment. Many more react with oxygen and atmospheric water and only survive due to self-passivation or surface reconstruction, which, in the case of atomically thin films leads to serious structural deterioration. I will describe how to prepare, protect and study these new materials in a specially designed clean argon environment. To demonstrate the technique we studied transport and optical properties of two selected materials: black phosphorus and niobium diselenide. We report, for the first time, transport in single layer black phosphorus. Starting from three layers we see quantum oscillations in magnetic field and determine the effective mass and g-factor. Niobium diselenide crystals in turn demonstrate superconductivity down to a monolayer that also has never been observed before with a relatively high T_c of a few Kelvin

11:00**Spin-valley Coupling in atomically thin Tungsten Dichalcogenides crystals**Xiaodong Cui¹¹Physics, University of Hong Kong, Hong Kong

The monolayers of group VI transition metal dichalcogenides feature a valence band spin splitting with opposite sign in the two valleys located at corners of 1st Brillouin zone. This spin-valley coupling, particularly pronounced in tungsten dichalcogenides, can benefit potential spintronics and valleytronics with the important consequences of spin-valley interplay and the suppression of spin and valley relaxations. In this talk we discuss the optical studies of WS₂ monolayers and multilayers. The polarized resolved photoluminescence spectra reveal a spin-valley coupling of 0.4 eV which suppresses interlayer hopping and manifests as a thickness independent splitting pattern at valence band edge near K valleys. (1) This giant spin-valley coupling, together with the valley dependent physical properties, may lead to rich possibilities for manipulating spin and valley degrees of freedom in these atomically thin 2D materials.

Reference:

(1) Bairen Zhu, Hualing Zeng, Junfeng Dai, Zhirui Gong, Xiaodong Cui, Anomalously robust valley polarization and valley coherence in bilayer WS₂, 111, 11606, PNAS, (2014)

11:30**Excitons and many-body phenomena in atomically thin 2D materials**Alexey Chernikov¹¹Department of Physics, Columbia University, New York

Since the discovery of graphene, a single sheet of carbon atoms, research focused on two-dimensional (2D) materials evolved rapidly due the availability of atomically thin crystals with intriguing physical properties. The 2D materials naturally inherit major traits associated with systems of reduced dimensionality such as strongly enhanced Coulomb interactions and highly efficient light-matter coupling. In particular, in the class of 2D semiconductors this leads to the emergence of strongly bound electron-hole quasi-particles, such as excitons, trions, and biexcitons, with unusually high binding energies and efficient light absorption.

In this talk, I will present a study of the excitonic properties of 2D semiconductors. The observation of exciton binding energies on the order of 0.5 eV and the marked deviation of the exciton Rydberg series from the hydrogenic model will be discussed. The results reflect both strong carrier confinement and the distinctive nature of dielectric screening in atomically thin materials. I will further describe how the presence of high carrier densities can profoundly alter the many-body interactions in these 2D systems.

14:00 - 17:00

Special Workshop (Panel discussion)

Nano and Society

Chair: Siegmur Roth

Panelists: David Carroll (Winston-Salem, USA)

Hui-Ming Cheng (Shenyang, China)

Georg Duesberg (Dublin, Ireland)

Peter Grambow (Nanoinitiative Bayern, Germany)

The goal of this workshop is to develop a feeling on how funding of nanotechnology R&D works in different parts of the world and on how well it works.

During the panel discussion, we may discuss topics like:

- 1.) Many funding agencies want to shorten the way from research to commercialization. Are there good examples for products having already come out from funded projects?
- 2.) In European cooperative projects often trans-regional cooperation is a goal by itself. Do you know success stories?
- 3.) Funding might not have led to a successful project as such, but the fact that companies do engage in attractive research may attract good people, and thus the business of the company might improve. Again, are there good examples?
- 4.) Do Flagship projects increase the creativity in a country or are they harmful by excluding many creative researchers from the community?
- 5.) Is it helpful that Europe, America, and China copy each others Flagships, so that the whole world works on the same topics, or would we prefer more global diversity?
- 6.) Is the 'grasshopper phenomenon' good or bad? (All scientists worldwide swarming from conductive polymers to superconductors to fullerenes to nanotubes to graphene). A big advantage might be an increased cooperation among scientists. However, does this lead to an "academic monoculture"?

All participants of the Kirchberg winterschool are welcome to attend this special workshop.

18:30**Spin and valley dynamics of excitons in transition metal dichalcogenides**Mikhail Glazov^{1,2}¹Ioffe Physical-Technical Institute of the RAS, St.-Petersburg, Russia²Spin Optics Laboratory of St.-Petersburg State University St.-Petersburg, Russia

The synthesis and studies of graphene, an atom-thick layer of Carbon, has opened up an era of novel truly two-dimensional materials. Such systems combine unusual optical and transport properties and attract a lot of interest nowadays. Monolayers of transition metal dichalcogenides (TMDCs) have, like graphene, hexagonal crystalline lattice, but, unlike graphene, possess direct band gaps (~ 1.7 eV) at the edges of the Brillouin zone, known as \mathbf{K}_+ and \mathbf{K}_- valleys. Extremely strong spin-orbit coupling in TMDCs yields the spin-valley locking: Spin components of individual charge carriers correspond to the given valley of the energy spectrum.

Recent experiments demonstrate valley-selective optical orientation, but the valley/spin polarization decays during several picoseconds. This is, at a first glance, unexpected, since spin-valley locking suppresses spin relaxation of individual electrons and holes. We develop the theory of the neutral exciton fine structure in TMDCs monolayers governed by the long-range exchange interaction between the electron and the hole. We show that this coupling is responsible for the rapid spin/valley depolarization in MoS_2 and WSe_2 .

19:00**Two-Dimensional Layered Materials – Physics and Applications**Joerg Appenzeller¹¹Electrical and Computer Engineering, Purdue University, West Lafayette

With 2D materials offering unique opportunities for future nano-electronics applications, the quest is to identify their useful properties and potential intrinsic performance benefits. While the most commonly studied 2D system, i.e. graphene, has excited scientists because of high achievable carrier mobilities, the absence of a band gap makes many device related applications very challenging. On the other hand materials as MoS₂, WSe₂, or WS₂, to just name a few, offer sizable band gaps at mobilities that cannot be achieved in bulk materials that are scaled down to similar thicknesses. In my presentation I will discuss the benefits of an ultra-thin body structure for scaled devices. I will also elucidate the critical impact of contacts to benefit from the intrinsic performance of MoS₂ based field-effect transistors (FETs). Our study supports the notion that a linear device Id-V_{ds} characteristic is by no means evidence of an ohmic contact and that contacts frequently mask the true mobility specs of novel low-dimensional materials. Moreover, I will present experimental results on the scaling properties of MoS₂ FETs and the impact of the layer thickness for device applications.

19:30**Vapour phase Synthesis and Functionalisation of 2D Transition Metal Films**Georg S Duesberg^{1,2}¹Chemistry, Trinity College Dublin, Dublin 2, Ireland²Centre for Adaptive Nanostructures and Nanodevices (CRANN) & Advanced Materials BioEngineering Research Centre (AMBER), Trinity College Dublin, Ireland

Transition Metal Dichalcogenides (TMDs) revealed exciting properties which have potential for electronic applications. In order to use TMDs in functional devices, reliable processes for large scale synthesis, functionalisation and integration must be developed. Here we present the thermally assisted conversion of various metal films and scalable CVD growth of TMD layers.[1] Characterization with Raman spectroscopy, photoluminescence, XPS and TEM are presented. We electrically addressed TMDs films to investigate their electrical viability in future electronics. In particular, a large scale p-n photodiode made from a MoS₂ layer on silicon is presented.[2] Further, we report their on-chip functionalisation.[3] Our approach, which uses large scale synthesis in combination with surface functionalization, is an important step towards integration of novel 2D materials with traditional technology; which may lead to significant advances towards TMD based electronics.

References

[1] O'Brien, M. et al. Scientific Reports 2014, 4.

[2] Yim, C. et al. Scientific Reports 2014, 4.

[3] Backes, C. et al. Angew. Chem. Int. Ed. 54, 9, 2015, 2638–2642

TUE 1**Optimizing Spin-transfer Torque in Graphene Spin Devices**

Chia-Ching Lin¹, Ashish V. Penumatcha¹, Vinh Quang Diep¹, Joerg Appenzeller¹, Zhihong Chen¹

¹ECE, Purdue University, West Lafayette

Graphene is an ideal channel material due to its long spin diffusion length, gate-tunable carrier density, and high carrier mobility. However, to further develop a graphene-based spin logic, spin transfer torque needs to be demonstrated in graphene devices to show that spin information can be communicated to the outputs. The first experimental measurement of spin transfer torque in graphene lateral non-local spin valve devices has been reported by us. Assisted by an external magnetic field, the magnetization reversal of the ferromagnetic receiving magnet is induced by pure spin diffusion currents from the input magnet. The magnetization switching is reversible between parallel and antiparallel configurations, depending on the applied charge current polarity. In this talk, I will show a new graphene spin device design to improve the spin absorption at the output magnet. The measured nonlocal spin valve signal has lower noise and its magnitude is comparable to a conventional graphene spin device. More importantly, the critical spin torque current density is greatly reduced.

TUE 2**Analysis of the double-resonant 2D Raman mode in bilayer graphene**

Felix Herzig¹, Matteo Calandra², Paola Gava², Patrick May¹, Michele Lazzeri², Francesco Mauri², Janina Maultzsch¹

¹Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany

²IMPMC, Université Pierre et Marie Curie, CNRS, Paris, France

We present a two-dimensional calculation of the double-resonant 2D-mode scattering cross-section in bilayer graphene. Based on a first-principles approach, we unravel the dominant contributions to the complex 2D-mode lineshape and demonstrate, in contrast to previous works, that so-called 'inner' processes are, by far, the most dominant processes [1]. Moreover, we show that the splitting between the two TO-derived phonon branches in bilayer graphene cannot be neglected for a consistent understanding of the 2D-mode lineshape. Additionally, we investigate the contributions from both TO branches to the symmetric and anti-symmetric scattering processes. Finally, we discuss the effect of the electronic broadening on the observed 2D-mode lineshape. Our results answer the long-standing question regarding the different contributions to the 2D-mode lineshape in bilayer graphene.

[1] F. Herzig, M. Calandra, P. Gava, P. May, M. Lazzeri, F. Mauri, and J. Maultzsch, Phys. Rev. Lett. 113, 187401 (2014).

TUE 3**Capacitive energy storage properties of large-area sprayed PEDOT:PSS transparent flexible films**

Thomas Higgins¹, Jonathan Coleman¹

¹School of Physics, Trinity College Dublin

To create a fully-integrated transparent/flexible device will also require energy storage and management systems. This role will almost certainly be played by batteries and supercapacitors.

In the absence of underlying current collectors, transparent supercapacitor electrodes based on disordered nanomaterial networks typically suffer from percolation effects, detrimental to both the resulting electrical and capacitive properties. Here we present transparent/flexible supercapacitors using PEDOT:PSS thin films, demonstrating a complete absence of percolation effects for film transmittance as high as $T=99\%$. In doing so, we have achieved the highest energy storage/unit area for technologically relevant transmittance (T greater than 90%).

TUE 4**Fabrication and characterization of thin film transistors based on semiconductor-enriched carbon nanotubes**

Jun Hirotani¹, Ryotaro Matsui¹, Shigeru Kishimoto¹, Yutaka Ohno^{1,2}

¹Graduate School of Engineering, Nagoya University, Nagoya, Japan

²EcoTopia Science Institute, Nagoya University, Nagoya, Japan

Carbon nanotubes (CNTs) have been widely recognized as a promising material for various electron device applications due to their remarkable electrical, thermal and mechanical properties. For their thin-film transistor (TFT) applications, the crucial issue is characteristic variation of the CNT thin film. The variation can be predicted to be reduced by increasing number density of CNTs in the channel. In the present work, we have investigated electrical performance and characteristic variation of CNT TFTs as changing number density of CNTs. Semiconductor-enriched ($\sim 95\%$) CNTs were used in this work. The vacuum filtration and transfer method were adopted to fabricate a uniform CNT film. We measured more than a hundred CNT TFTs for each CNT density, and obtained on/off ratio of $10^5 \sim 10^6$, and ON-current variation of $\sim 20\%$ in terms of a standard derivation divided by average ON-current. Our results indicate that as the CNT density increases, the variation in ON-current tends to be eliminated, while the variation is still larger than predicted by simulation.

TUE 5**Towards controlled, integrated manufacturing of 2D materials**

Stephan Hofmann¹, Sabina Caneva¹, Piran Kidambi¹, Robert S Weatherup¹, Andrea Cabrero-Vilatela¹, Bernhard C Bayer^{1,5}, Raoul Blume², Carsten Baecht³, Robert Schlögl⁴

¹Engineering, University of Cambridge, Cambridge

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³Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

⁴Fritz-Haber-Institut der Max-Planck-Gesellschaft

⁵Physics, University of Vienna

The first and foremost challenge for novel 2D materials is to develop integrated manufacturing and processing techniques. Chemical vapor deposition (CVD) has emerged as the most viable route to achieve 'electronic grade' 2D materials. Essential to growth control for 2D material CVD is an understanding of the underlying growth mechanisms, specifically the interactions of the precursors and growing 2D structure with the catalyst.[1,2] Here we focus on the growth of hexagonal BN [3,4]. By developing a detailed understanding of element-specific feeding mechanisms for various catalyst systems, we demonstrate the CVD of h-BN single crystals with lateral dimensions of ~ 0.3 mm as well as continuous h-BN films. Our study of rational catalyst design also includes the effects of oxygen during and after growth. We discuss the implications of these observations in the context of challenges in process integration and hetero-structure CVD.

1. Weatherup et al. JACS 136, 13698 (2014).
2. Blume et al. PCCP 16, 25989 (2014).
3. Kidambi et al. Chem. Mater. 26, 6380 (2014).
4. Caneva et al. submitted (2014).

TUE 6**Solution-processed MoS₂ for broadband ultrafast optical pulse generation at sub-bandgap photon energies**

Richard C. T. Howe¹, Robert I. Woodward², Guohua Hu¹, Felice Torrisi¹, Meng Zhang², Sergei V. Popov², J. Roy Taylor², Edmund J. R. Kelleher², Tawfique Hasan¹

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²Femtosecond Optics Group, Blackett Laboratory, Prince Consort Road, Imperial College London, London SW7 2AZ, UK

In fields such as manufacturing, spectroscopy and metrology, there is a considerable demand for wavelength-tunable ultrafast pulsed lasers. Carbon nanotubes and graphene have been used as saturable absorbers to produce such short optical pulses [1]. Here, we demonstrate saturable absorption from liquid phase exfoliated MoS₂. The ~ 25 μm free-standing MoS₂-polymer composite saturable absorber (SA) shows $\sim 6.3\%$ and $\sim 10.7\%$ modulation depth (change in optical absorption under intense

irradiation) at 1065 and 1565 nm, respectively. The SA is integrated into a fiber laser setup to produce short optical pulses by Q-switching and mode-locking, tunable from 1030 to 1070 nm [2, 3] and 1535 to 1565 nm [4], respectively. We propose that edge-state absorption from the MoS₂-nanoflakes could explain the saturable absorption observed at energies below the material bandgap.

[1] Hasan, T. et al., *Adv Mater*, 21, 3874 (2009)

[2] Woodward, R.I. et al., *Opt Express*, In Press (2014)

[3] Woodward, R.I. et al., in *Conference on Lasers and Electro-Optics (CLEO)*, DOI: 10.1364/CLEO_SI.2014.SM3H.6 (2014)

[4] Zhang, M. et al., *Nano Res*, DOI 10.1007/s12274-014-0637-2 (2014)

TUE 7

Low temperature inks of 2-dimensional crystals for inkjet printing

Guohua Hu¹, Richard Howe¹, Zongyin Yang¹, Tawfique Hasan¹

¹Cambridge Graphene Centre, University of Cambridge

Liquid phase exfoliation (LPE) allows production of dispersions of 2-dimensional (2d) crystals, typically in high boiling point solvents, *e.g.* N-Methyl-2-pyrrolidone (204°C). The dispersions can be formulated into functional inks for inkjet printing, making them promising for large-area, flexible devices. However, difficulties remain in removing the high boiling point solvents and achieving consistent and continuous coating on non-porous substrates.

We demonstrate production of graphene, MoS₂, WS₂ and MoSe₂ by LPE and formulate functional inks with suitable Z values (~ 12) for inkjet printing. Z is a figure of merit to characterize the jetting stability of inks with range $1 < Z < 14$ for stable jetting. The inks have low boiling points ($\sim 80^\circ\text{C}$) and surface tensions ($\sim 28\text{mNm}^{-1}$), making them ideal for a variety of substrates. We demonstrate uniform printed patterns of 2d crystals at high printing resolutions ($\sim 70\mu\text{m}$) on flexible glass, SiO₂/Si wafer, paper and polymers such as PET and even cling film. Our work promises a wide range of applications, including in photonics, (opto)electronics and sensors.

TUE 8

Efficient one-pot combustion synthesis of graphene sheets

Andrzej Huczko¹, Olga Łabęź¹, Agnieszka Dąbrowska¹, Michał Soszyński¹, Magdalena Kurcz¹, Michał Bystrzejewski¹, Piotr Baranowski¹, Leszek Stobiński^{2,3,4}, Artur Małolepszy⁵, Alexander Okotrub⁶

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⁶Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

The emerging graphene applications generate a high interest in a search for its large-scale production. Regarding graphene synthesis, thermal or chemical exfoliation of intercalated graphite seems to be the most promising route among various approaches because it enables high-volume production at low-cost, mostly for composite applications. We present here a combustion synthesis approach for the formation of few-layered graphene (FLG). The redox reaction between strong reducers (Mg, Si, Zn, Al) and fluorinated graphite CF_x and graphene oxide GO under neutral (Ar, He) and reactive (CO₂) atmosphere (at starting pressure 1 MPa) efficiently yields FLG. The products were purified and characterized by XRD, SEM, TEM, and Raman spectroscopy. This environmentally friendly method is simple, fast, economical and suitable for large-scale production of graphene.

Acknowledgement:

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TUE 9

Dielectric function and bandgap of graphene oxide

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Optical and electronic properties of graphene oxide (GO) depend on its oxidation state. Based on optical measurements, oxidised graphene is often considered a semiconductor with a wide bandgap of several eV that can be tuned down to almost zero upon reduction. However, this picture is not supported by electrical transport measurements which show rather small bandgaps in order of several tens of meV.

In our contribution, we present results of careful optical measurements of reflectance and transmittance in the visible and near-infrared of GO thin films on sapphire substrates. GO samples with a different level of oxidation were obtained by thermal reduction of a fully oxidised material. From the measurements, we have extracted the dielectric function (DF) in the 0.5 - 5 eV range without taking recourse to any particular model of DF. It has turned out the electronic structure of GO is rather similar to that of amorphous materials with no significant structures in the electronic density of states (DOS) in the energy range investigated. In particular, no sharp band edge in DOS has been found for any GO oxidation level in agreement with electrical conductivity measurements.

TUE 10**Diamond-coated three-dimensional GaN micromembranes**

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⁴Research Centre for Microtechnology, University of Applied Sciences, Hochschulstrasse 1, 6850 Dornbirn, Austria

In this work, we present technological issues on synthesis of diamond films as a back-side heat spreader for AlGaIn/GaN heterostructures. First, the AlGaIn/GaN circular membrane structures were obtained by a deep reactive ion etching of Si substrate (330 μm thick). The diamond growth was performed complementary in hot filament or microwave plasma CVD system, respectively. We found that standard nucleation techniques (ultrasonic seeding or bias enhanced nucleation) resulted in damaging or cracking of AlGaIn/GaN membranes, or low nucleation efficiency in the Z-depth of the structures. Therefore, we implemented a novel nucleation technique with PVA polymer consisting of diamond powder which led to coating of both at bottom and top membrane part, including side walls. Based on FEM simulation, the technological progress will be pointed out as potentially perspective issue for developing high temperature electronic devices working in harsh environments.

This work was supported by the grants 14-16549P and APVV-0455-12.

TUE 11**Theory of coherent light emission in graphene**

Roland Jago¹, Torben Winzer¹, Andreas Knorr¹, Ermin Malic¹

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Within the density matrix formalism we present a microscopic and full quantized theoretical description of the coupled carrier, phonon and photon dynamics in graphene implemented in a photonic crystal nanocavity. We demonstrate that under strong optical excitation a spectrally broad and long-lived population inversion can be achieved [1]. In the case of free-standing graphene non-radiative Coulomb-induced carrier-recombination on a femtosecond time scale prevents an efficient emission of coherent photons. To partially suppress this ultrafast recombination, we propose to support graphene on a substrate having high-dielectric screening. In this case, our calculations reveal a temporarily extended population inversion, that remains stable up to some tens of picoseconds under realistic conditions. In particular we observe the emission of coherent laser light suggesting graphene as gain medium for lasers [2].

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TUE 12

New Directions in Tip-Enhanced Near-Field Optical Microscopy

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The characterisation of nanostructures with high spatial resolution and detection sensitivity can be achieved by tip-enhanced near-field optical microscopy (TENOM) [1]. We report on our efforts to extend this method into further directions.

One direction is the application of tip-enhancement to photovoltaic and light-emitting devices. We obtained the first high-resolution photocurrent images of carbon nanotube devices using a metal tip to locally enhance optical-to-electrical transduction [2]. We show that the efficiency of the reversed process leading to electroluminescence can be increased as well.

We also implemented tip-enhanced near-field optical microscopy at low temperatures (5 K) and present a new microscope design based on a solid immersion lens configuration providing very high collection angles and efficiencies.

We acknowledge Financial support by DFG, NIM and the ERC (New-NanoSpec).

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TUE 13

Binary and Ternary Alloy Nanoparticles Prepared from Apoferritin towards Controlled SWNT Growth

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For controlled single walled carbon nanotube growth the composition, size distribution and density of catalyst particles on a substrate are crucial. It was demonstrated that by using bimetal and novel ternary alloy nanoparticles the yield, the average length as well as the diameter distribution of the grown tubes can be influenced. In this study, the nanoparticles were synthesized inside the protein cage apoferritin [1]. More specifically, Fe-Mo, Fe-Pt, Fe-Ni and Fe-Co as well as Fe-Mo-Pt and Fe-Mo-Ni nanoparticles were produced. For growth with acetylene the average CNT length from Fe-Mo particles could be enhanced by more than 250% in comparison to pure Fe catalysts. Similarly, Fe-Ni and Fe-Pt resulted in a threefold increase in yield. Fe-Mo-Ni displayed some narrowing in the CNT diameter distribution. Using a protein

cage implies that the elemental composition, size and the deposition density on the growth substrate can be controlled independently. As encouraging results were obtained, this approach is very promising to separately study the factors influencing the growth outcome and to synthesize SWNTs with targeted properties.

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TUE 14

Mono- and bi-layer WSe₂ as host of localised single – photon emitters

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Semiconducting transition metal dichalcogenides are attracting scientific attention due to its peculiar band structure. Under non-resonant excitation free/charged-exciton peak in monolayer (1L) WSe₂ is accompanied by a broad-band emission at lower energies which is associated with defect-bound exciton. Upon cryogenic temperatures $T = 4\text{K}$, the defect band becomes an origin of localised sharp emissions with average linewidth of $130\text{ }\mu\text{eV}$ and obeying single photon statistics (arXiv:1411.2449). In this work, we show that these lines appear and are localised only in the region where we measure large strain due to wrinkling, abrupt layer termination, or lithographically defined surface modulation. Unlike previous reports, these localised emitters are not only spectrally located in the range of defect-band emission but also extend to much lower energies. In order to characterise the emitters in depth we perform temperature- and polarization- dependent photoluminescence measurements. These findings suggest a promising future for role of strain in quantum optical investigations of spin-valley coherence in WSe₂ emitters and their potential for quantum information processing.

TUE 15

Confocal and tip-enhanced Raman spectroscopy on graphene nanoribbons

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Lithographic graphene nanoribbons (GNRs) on SiO₂ are studied by Raman spectroscopy in order to investigate influences from disorder and charge distributions. The nanoribbon width is obtained from atomic-force microscopy measurements providing a width distribution of each GNR.

The intensities of the defect-induced D and D' modes are compared to the G mode from bulk graphene giving an estimate on the defect concentration. A model, con-

sidering defective and non-defective regions of graphene in a GNR, is developed to quantitatively estimate the size of these regions. Previously used models for GNRs [1,2] and ion bombarded graphene [3] are discussed in comparison.

Our findings emphasize the need for nanospectroscopy, such as tip-enhanced Raman spectroscopy (TERS), as a suitable tool to study properties of graphene nanostructures. We present our recent progress in TERS on graphene nanoribbons.

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TUE 16

Picosecond photocurrents in single-walled carbon nanotubes

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¹Walter-Schottky-Institut and Physik-Department, Technische Universität München, Germany

The exciton dynamics in carbon nanotubes are typically detected in a time-resolved way by optical techniques such as transient absorption and photoluminescence spectroscopy. Many questions remain concerning the separation and transport of photo-generated charge carriers in optoelectronic devices. We address these questions by a novel ultrafast photocurrent spectroscopy, based on an on-chip THz time domain spectroscopy [1]. We find a combination of an optically induced ultra-fast displacement current, transport of photogenerated charge carriers at the Fermi velocity to the electrodes, and interband charge-carrier recombination processes to dominate the ultrafast photocurrent of the single-walled carbon nanotubes [2]. We further discuss optoelectronic effects in the carbon nanotubes which arise from an ultrafast optical excitation with a super-continuous light spectrum [3].

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

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TUE 17

Planar graphene tunnel field-effect transistor

V.L. Katkov¹, V.A. Osipov¹

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We propose a concept for a graphene tunnel field-effect transistor. The main idea is based on the use of two graphene electrodes with zigzag termination divided by a narrow gap under the influence of the common gate. Our analysis shows that such device will have a pronounced switching effect at low gate voltage and high on/off current ratio at room temperature.

TUE 18**Electrical property of highly aligned chirality selected single-walled carbon nanotubes assemblies**Hideki Kawai¹, Kai Hasegawa¹, Kazuhiro Yanagi¹¹Department of physics, Tokyo Metropolitan University, Tokyo

Conventional Single Wall Carbon Nanotube (SWCNTs) devices have been fabricated as random network where junctions between nanotubes strongly influence their transport property. Such junctions work as scattering centers where carriers are localized [1]. To reduce the presence of such scattering centers is of great importance for improvement of transport characteristics. In this context, development of techniques to produce aligned array or crystal-like assemblies of SWCNTs using the high purity SWCNTs is important. In this study, we report a string-like assembly of aligned SWCNTs, which prepared by controlling temperature of solution where SWCNTs were dispersed using surfactants [2]. In addition, we report production of assemblies of highly aligned chirality selected SWCNTs [3]. In this poster, we discuss the transport characteristics of the aligned assemblies.

Reference:

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[2] Kawai et al., Appl. Phys. Express 6, 065103(2013)

[3] Kawai et al., APL 105,093102(2014)

TUE 19**The effect of annealing on intrinsic defects in zinc oxide nano-crystals**Sevak Khachadorian¹, Rolland Gillen¹, Janina Maultzsch¹, Axel Hoffmann¹, Sumin Choi², Cuong Ton-That², Matthew R. Phillips²¹Institut für Festkörperphysik, Technische Universität Berlin, Berlin²School of Physics and Advanced Materials, University of Technology, Sydney, Sydney

The photoluminescence (PL) spectrum of ZnO exhibits a near-band-edge UV emission and generally a broad defect related visible emission. The origin of defect luminescence is still controversial. The optical and vibrational properties of zinc oxide nano-crystals (ZnO NCs), grown by vapor transport method, were investigated after the thermal annealing in oxygen-, argon- and vapor Zn-rich conditions. Raman scattering and other characterization techniques were conducted to show the effect of temperature annealing in various environments on the defect luminescence and local vibrational modes (LVM) of the ZnO NCs. Dramatic changes in the defect-luminescence and Raman LVMs were observed depending on the different annealing treatments. Scanning electron microscopy and X-ray diffraction methods were used to monitor the structural changes induced by the effect of annealing. The experimental results are complemented by density function theory (DFT) calculations using the SIESTA package to get a more detailed understanding of origin of intrinsic defects.

TUE 20**Synthesis and growth properties of inner tubes inside metallocene-filled single-walled carbon nanotubes**

Marianna V. Kharlamova¹, Christian Kramberger¹, Hidetsugu Shiozawa¹, Kazuhiro Yanagi², Takeshi Saito³, Thomas Pichler¹

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³AIST, National Institute of Advanced Industrial Science and Technology, Japan

The filling of SWCNTs and chemical transformation of encapsulated substances inside their channels are promising approaches to tailor properties of SWCNTs. In present work, we performed the filling of eDIPS SWCNTs of 1.7-nm mean diameter with nickelocene [1], cobaltocene and ferrocene [2] molecules and their further transformation into DWCNTs via thermal annealing in vacuum. Using multifrequency in situ Raman spectroscopy we investigated time-dependent inner tube growth in detail. We calculated growth rates and activation energies of the formation of inner tubes of different chiralities and diameters. We also performed DGU of the filled SWCNTs to study the inner tube growth properties inside metallic and semiconducting SWCNTs of certain chiralities and diameters. These results allowed us to achieve the comprehensive picture of the dependence of the physical properties of metallocene-filled SWCNT hybrids on tube diameter, chiral angle and metallocene type.

M.K. acknowledges the ÖAW for a DOC-fORTE fellowship.

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TUE 21**Probing Electrons in Carbon Nanotubes without Conduction**

Ilya Khivrich¹, Shahal Ilani¹

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The recent generation of carbon nanotube devices, which allow to engineer the potential landscape along a pristine one-dimensional system, forms a versatile playground for studying a large variety of correlated electronic ground states. While some of these ground states are conducting, others are fundamentally insulating, thus hindering their measurement via transport. Here we demonstrate a new method that allows us to directly measure these insulating states by probing the interaction between the electrons and the mechanical motion of the nanotube. The key feature of this method is a new capability to control and measure the nanotube's mechanical motion in the time domain while quickly switching between different electronic configurations. We can thus actuate the mechanical motion, let the electronic system of interest interact with it, and coherently measure the motion after the interaction took place by turning on the conductivity. We will demonstrate how this technique opens a new venue for observing electronic states that were previously impossible to probe.

TUE 22**A novel probe for local imaging of interacting electrons in 1D with minimal invasiveness**Ilanit Shammass¹, Sharon Pecker¹, Shahal Ilani¹¹Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel

Interacting electrons in a one dimensional channel are a unique physical system, which can exhibit a variety of correlated electron phases. Many of these phases, such as the quantum Wigner crystal, have a distinct signature in their real-space electronic structure. Recently, we have developed pristine multi-gate nanotube (NT) devices, which allow for precise engineering of 1D microscopic potentials along the NT, while maintaining strong electron interactions. This makes them ideal for realizing correlated electron phases, and calls for development of a local probe that can resolve their electronic spatial structure, without destroying it due to large potential modulations. For this purpose we created a novel experimental setup, where we use a second NT device as a sensitive charge detector in a scan probe microscope configuration. Its main advantage is that the probe invasiveness can be tuned, and is limited in principle only by the quantum back-action of single electrons in the detector. We will demonstrate how the invasiveness of the probe-NT can be controlled and drastically reduced. In addition, we will present initial results of wavefunction imaging using this platform.

TUE 23**Hydrogen storage in graphene related materials.**Alexey Klechikov¹, Guillaume Mercier¹, Alexandr Talyzin¹¹Physics, Umeå University, Umeå

Several studies reported recently that graphene adsorbs 3-10 fold more hydrogen compared to other carbon materials. Graphene powders with broad range of BET surface areas were prepared using thermal exfoliation/activation of Hummers and Brodie graphite oxides. Hydrogen sorption by samples with surface areas in the range 200-2800 m²/g was evaluated using gravimetric and volumetric systems at ambient temperature and 77K. It is found that hydrogen uptake of graphene samples shows precise correlation with surface area both at 295K and 77K, independently on type of GO precursor or activation methods. Maximal hydrogen uptake at 295K and 120 Bar H₂ pressure do not exceed 1 weight percent. Maximal value of H₂ uptake 5.6 weight percent was found for sample with 2800m²/g surface area at 77k. Hydrogen uptake versus surface area trends evaluated in our experiments for graphene are rather similar to those earlier reported for carbon nanotubes, activated carbons and metal organic framework materials. Graphene oxide framework samples synthesized using reaction of graphite oxide with boronic acids also showed no significant deviations from this "standard" trend.

TUE 24**Growth of high-quality monolayer WS₂ on graphite**

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Atomic-layer transition metal dichalcogenides (TMDCs) have attracted appreciable interest due to their tunable bandgap, spin-valley physics, and potential device applications. However, the quality of TMDC samples available still poses serious problems, such as inhomogeneous lattice strain, charge doping, and structural defects. Here, we report on the growth of high-quality, monolayer WS₂ onto exfoliated graphite by chemical vapor deposition. Unlike commonly-used substrates such as SiO₂/Si and sapphire, monolayer WS₂ grown on graphite presents a uniform, single excitonic photoluminescence peak with a Lorentzian profile and a very small full-width at half maximum of 21 meV at room temperature and 8 meV at 79 K. Furthermore, no additional peaks are observed for charged and/or bound excitons, even at low temperature. These results indicate that the cleaved graphite surface is an ideal substrate for the growth of high-quality, non-doped TMDCs, and such samples will be essential for revealing intrinsic physical properties and for future applications.

TUE 25**Atomic structure of 2D amorphous carbon membranes**

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Since over 80 years, the popular concept of the atomic structure of amorphous materials has been strongly influenced by the drawings of a random network by Zachariasen [1]. However, direct imaging of the atomic structure of a conventional glass has remained impossible. Only very recently, the first possibility to image the complete atomic structure of a disordered material appeared in the form of two-dimensional materials. So far, two different materials have been described: a truly 2D silica glass [2,3] and amorphized graphene [4,5]. Here, via atomic resolution scanning transmission electron microscopy, we compare the atomic arrangements in these materials to two other forms of amorphous 2D carbon: evaporated thin films and disordered membranes created via annealing of organic molecules on a metal substrate.

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- [3] Huang, P. Y. et al. *Nano Lett.* 12, 1081-1086 (2012)
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TUE 26

Low Dose Imaging of Organic Molecules on Graphene

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In conventional STEM beam induced damage is confidently hindering the imaging of small organic molecules with atomic resolution. Graphene is a notable support material that is not suffering beam damage at acceleration voltages as low as 60 keV. We demonstrate by simulations that the full atomic structure of organic molecules can be clearly resolved from large area ultra low dose (virtually dark) exposures on stochastic sub monolayers of organic molecules on a graphene support. By taking into account the full symmetry of the graphene support in a maximal likelihood image reconstruction even totally asymmetric planar molecules like Guanine can be fully resolved at an exposure as low as $10e^-/\text{\AA}^2$ or correspondingly 0.5 counts per graphene hexagon.

TUE 27

Correlations of RBM, G line, and D line frequencies of individual SWCNTs grown from carbon:nickel nanocomposite templates

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Carbon:nickel nanocomposite templates were used for CVD growth of separated, individual single-walled carbon nanotubes (SWCNTs) free of solvents or surfactants. The as-grown carbon nanotubes were characterized by laser-energy dependent Raman spectroscopy and atomic force microscopy. Raman spectra showing a single radial breathing mode (RBM) line were analyzed with respect to correlations of RBM, G⁺ line and D line frequencies for SWCNT diameters covering the range of 0.8 nm to 1.6 nm. Opposite line shifts were found for RBM and G⁺ lines of the individual SWCNTs. However, the line shifts of the G⁺ line are smaller than the standard deviation of the G⁺ position for SWCNTs with almost the same RBM frequency, i.e. 1 cm⁻¹ compared to ± 1 cm⁻¹ for the whole diameter range. The D line often shows

a complex shape including up to three components, which makes the identification of correlations with RBM frequencies possible only in selected cases.

TUE 28

Hydrodynamic Electron Flow in Graphene-Boron Nitride Heterostructures

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Electron transport in solid state systems is usually described, depending on sample dimensions and mean free path, by a diffusive or ballistic model where electron interactions are dominated by non-like particle collisions. Intrinsic graphene however has a very low electron-phonon coupling and as a result, at elevated temperatures, transport is dominated by electron-electron collisions where a hydrodynamic description may be more applicable. Theory has already predicted some interesting flow behaviour such as a high viscosity of the electron fluid, owed to the Dirac nature of the electrons. As a result of this viscous flow, whirlpools or vortices may form adjacent to the normal current flow. In this work we have studied high mobility encapsulated graphene and observed such whirlpools by measuring negative four-probe resistance in custom geometries.

TUE 29

Low temperature hydrogenation of diamond nanoparticles using diffuse coplanar surface barrier discharge at atmospheric pressure

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Diamond nanoparticles (DNPs) have attracted an attention of researchers due to their capability for applications as drug delivery, molecule labelling, spintronic, quantum computing. Commonly, high temperature processes (700°C) as hot-filament, microwave plasma or annealing in hydrogen gas atmosphere were used to passivate DNPs surfaces with hydrogen that defines the starting point for many functions and chemistries. Yet reliable mass hydrogenation of DNPs is still a challenging task. Here we report on a new approach to plasma assisted DNPs hydrogenation at temperatures below 100°C. As received detonation DNPs with size about 5 nm were annealed in air at 450°C for 30 min to reduce non-diamond carbon content. Then the annealed DNPs were plasma treated with atmospheric-pressure diffuse coplanar surface barrier discharge in pure hydrogen at power 1.2 W/cm². While IR spectra

of the annealed DNPs were dominated by oxygen containing functional groups, the hydrogenated DNPs revealed increase of bands of C-H stretching vibrations in the region 2800-3000 cm^{-1} after 5 min plasma treatment. No significant changes in IR spectra were observed for prolonged plasma treatments.

TUE 30

Cavity enhanced light emission from an electrically driven carbon nanotube

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Nanoscale photonic emitters are essential elements for on-chip networks and optical interconnects. Besides preferred electrical trigger capability, tailored optical properties are highly desirable to engineer application specific light sources. Recently we have shown how light from an electrically-driven carbon nanotube can be coupled directly into a photonic waveguide[1]. Here we demonstrate electrically driven nanoscale emitters with narrow linewidth based on carbon nanotubes embedded into nanophotonic circuits. A particular photonic emission wavelength is realized by engineering the photonic density of states of the dielectric environment of the CNT. Using one-dimensional photonic crystal cavities we spectrally select desired emission wavelengths and couple light into the underlying photonic network with high efficiency and reproducibility. Our approach holds promise for active photonic networks and localized sensing applications in a chipsale framework.

[1] S. Khasminskaya, F. Pyatkov, B. S. Flavel, W. H. P. Pernice, R. Krupke, *Advanced Materials* 26 (2014) 3465

TUE 31

Raman spectra of hydrocarbons formed in carbon nanotubes - a theoretical study

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The origin of several Raman bands which appear in ferrocene filled small diameter carbon nanotubes after annealing at 800 °C is still an open question. The most remarkable observation is the appearance of non-dispersive lines in the D-band region. The experimental details (including Raman- and mass spectra) are presented in the contribution of Kuzmany et al. We performed DFT calculations of structure, HOMO-LUMO transition energy and Raman spectrum with B3LYP functional for a large set of hydrocarbon molecules, including polyenes and polyaromatic hydrocarbons. To follow the effect of deuterization in the Raman spectra we varied the mass of hydrogen atom from 1 to 2 by 0.1 steps. With increasing mass the position of the

lines red shifted as expected. However in some rare occasions the intensity of the red shifted line dramatically decreased and at the same time an originally weak line gained large intensity at a nearby higher frequency. This can be interpreted in an experiment as an apparent blue shift. From a comparison of the calculations with experiments the dimer of the 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) is the most likely product of the annealing process.

TUE 32

The origin of non-dispersive Raman lines in the D-band region for ferrocene-@HiPco transformed at high temperatures

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For ferrocene (FeCp₂) in HiPco or small diameter DIPs new non-dispersive Raman bands appear in the D-band region after annealing at 800 °C. These bands can be very strong and are resonance enhanced in the red [1]. From Raman mapping a set of at least 6 lines, including a response from a C=C stretch vibration, was identified as belonging to the same source. Mass spectra from cold-trapped evaporation products revealed masses in the range of 450 to 700 Dt with an often observed species at 686 Dt. These values are typical for large hydrocarbon molecules. Isotope labelling of the FeCp₂ molecule showed that the new Raman lines originate from reaction products of FeCp₂. DFT calculations of Raman spectra were performed for a large set of hydrocarbon molecules, in each case with a stepwise increase of the hydrogen mass from 1 to 2. This allowed for a clear identification of the origin of the lines in hydrogenated and deuterated species. From a comparison of the calculations with experiments the dimer of the 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) (652 Dt) was found to give the best agreement.

[1] H. Kuzmany et al., Phys. Stat. Sol. B 251, 2457-2460 (2014)

TUE 33

One step production of MWCNT aerogels via catalytic CVD ethylene decomposition.

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Carbon nanotube (CNT) aerogels present a new bulk material which integrate unique properties of CNTs and specific properties of aerogels. Here we report one step MWCNT aerogel production by CVD process using preformed catalysts consisting of agglomerates of dispersed support particles with nano-sized oxide precursors of

iron group metal catalyst. In situ activation of the precursors in reaction conditions results in the formation of nano-sized metal particles which in turn provide multi center growth of MWCNTs. Growth of tangled MWCNTs provide the formation sponge structure of aerogel which volume increases a hundred times in comparison with a volume of preformed catalysts. Any form of MWCNT aerogels with density of 0.03-0.08 g/cm³ can be produced using different geometry of preformed catalysts (balls, cubes etc.). Aerogels demonstrate high electrical conductivity (several S cm⁻¹). Measurements of electric and magnetic polarizability in the frequency range of 8-12 GHz using open microwave resonator show that aerogel balls demonstrate electromagnetic properties close to that of metals. That makes them a perspective lightweight material for different EM applications.

TUE 34

Effect of temperature cycling on transconductance fluctuations in graphene

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The charge localization in quantum Hall regime can be captured by a simple measurement of transconductance. Transport measurements normally provide a macroscopic, averaged view of the sample, so that disorder frequently prevents the observation of fragile interaction induced states in the conductance. We demonstrated that these fluctuations reflect processes of charge localization [1]. A systematic study allows observing higher order fractional quantum Hall states. The fluctuations appear when conduction channels are influenced by the compressible quantum dots which form at hills or valleys of disordered potential landscape. The conductance fluctuations are found to be stable for months as long as the sample is kept at cryogenic temperature less than 15 K. However, the fluctuation curve change significantly once the sample is heated up to the temperature higher than 25 K and cooled down again.

TUE 35

Electrical and electromechanical properties of WS₂ nanotubes

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The electronic properties of dichalcogenide nanotubes (INT) and sheets and their incorporation into nanoelectromechanical systems (NEMS) is the subject of intensive research in recent years. INT-WS₂ possess superior mechanical properties and interesting stick-slip mechanical phenomena [1] and thus are a natural candidate for electro-mechanical devices.

We present here the first significant electro-mechanical response in pure inorganic nanotubes [2], field-effect mobility and surprisingly high current carrying capacity for the INT-WS2 [3]. The INT-WS2 conductivity exhibited a highly repeatable increase in response to strain and torsion. These results are in qualitative agreement with the theoretical torsional calculations presented here and previous theoretical predictions for strain. The high sensitivity to torsion and tension suggests INT-WS2 as promising components in NEMS such as gyroscopes and accelerometers.

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2. Levi,R.; Garel,J.; Teich,D.; Seifert,G.; Tenne,R.; Joselevich,E. In prep. 2015
3. Levi,R.; Bitton,O.; Leitus,G.; Tenne,R.; Joselevich,E. Nano Lett. 2013

TUE 36

Size quantization in graphene quantum point contacts

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Quantum point contacts form a cornerstone of mesoscopic physics as central building blocks for quantum electronic devices. Graphene shows a number of exceptional properties but the demonstration of graphene quantum point contacts has proven very challenging. Recent developments in the fabrication of high-mobility graphene-hexagonal boron nitride sandwich structures have improved the chances to observe quantum confinement of Dirac electrons in quasi-one dimensional graphene systems. Here we present joint experimental and theoretical work on ballistic transport of confined Dirac fermions in graphene nanoconstrictions. Reproducible kinks in the conductance are associated with size quantization in the quantum point contact. At high charge carrier densities, measurements agree excellently with theoretical simulations. Deviations from the expected linear behavior at low carrier densities emerge due to localized states at the edges, allowing the direct probing of trap states by transport measurements. Comparing the evolution of the observed kinks with magnetic field to theoretical predictions for one-dimensional confined states in graphene confirms size quantization as their origin.

TUE 37**Optical properties of highly-extended, ultrathin graphene nanoribbons in carbon nanotubes**

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Nano-templated growth of graphene nanoribbons (GNRs) at the interior spaces of the carbon nanotubes (CNTs) [1, 2] allows the possible construction of ultrathin ribbons with defined side edge configuration. However, due to the presence of the template tubes, less is known about the properties of GNRs inside. Herein, we report the optical properties of the extended GNRs, residing in single-wall CNTs. The GNRs were generated using coronene as precursors. Annealing at high temperature results in the extensive polymerization into ribbons of long length, as indicated by the Raman and TEM measurements. Signals generated from the outer CNTs were eliminated by using diazonium-based surface modification [3] to give clear optical absorption of the inner GNRs around 1.5 and 3.4 eV. The values are attributable to the first and second transitions across the energy gaps between the valence and conduction bands, in qualitative agreement with the first principle calculations.

References:

[1] H. E. Lim et al. Nat. Commun. 2013, 4, 2548.

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[3] M. S. Strano et al. Science 2003, 301, 1519-1522.

TUE 38**Multiphonon spectral analysis in bulk and monolayer MoS₂**

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We present a comprehensive multiphonon Raman and complementary infrared analysis for bulk and monolayer MoS₂ (1). For the bulk the analysis consists of symmetry assignment from which we obtain a broad set of allowed second-order transitions at the high symmetry M, K and Γ Brillouin zone points. The attribution of about 80 transitions of up to fifth-order processes are proposed in the low temperature resonant (with the A exciton) Raman spectrum. We conclude that the main contributions come from five phonons: A_{1g} (M), and two sets of single degenerate phonons at M with an origin of the two Brillouin zone center E_{2g} phonons. Consistent with the fact that at the M point only combinations with the same inversion symmetry are Raman-allowed, the contribution of combinations with the LA(M) mode is not dominant.

P and T dependent multiphonon Raman spectra will be analyzed in accordance with the above analysis.

For the monolayer MoS₂ the second-order phonon processes from the M and Γ Brillouin zone points are also analyzed and are discussed within similar framework to that of the bulk.

(1) T. Livneh and J.E. Spanier, 2D Materials (2015) in press ; arXiv: 1408.6748.

TUE 39

Synthesis and Electronic Properties of Li-doped Chemically Exfoliated Graphene

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Alkali atom intercalation of graphene leads to a conducting material which have both compelling fundamental properties and prospective applications. In particular, Li intercalation is expected to lead to a novel energy storage device. In addition, DFT calculations predict that the Li-graphene system is a superconductor with a critical temperature as high as 10 K. We produced Lithium doped Chemically Exfoliated Graphene (CEG/FLG) samples with the liquid ammonia solution method. This method is based on the good solubility of the alkali metal elements in liquid ammonia. The resulting samples were studied by Electron Spin Resonance Spectroscopy (ESR) and Raman spectroscopy. Upon doping, we observe an ESR line which is absent in the undoped samples. The line has a Dysonian lineshape which proves that this signal originates from itinerant electrons which thus come from the charge transferred electrons in graphene. Measurement of the ESR linewidth allows to determine the spin-relaxation time, which is important for prospective spintronics applications of charged graphene.

TUE 40

Theory of anomalous thermal expansion in 2D crystals

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The thermal expansion ath in layered crystals is a quantity of fundamental and practical interest. As suggested by I.M.Lifshitz 1952 a negative contribution to ath is due to anharmonic couplings between in-plane stretching and out-of plane bending, flexural, modes. Genuine in-plane anharmonicities give a positive contribution to ath.

A change of sign of α as a function of temperature T is a topic of current theoretical and experimental research. Here we present an analytical lattice dynamics approach for a 2D hexagonal crystal. The in-plane and out-of plane Grueneisen coefficients are calculated. The thermal expansion is studied as function of T and crystal size. The temperature T_a where α changes from negative to positive values decreases with decreasing crystal size. Renormalization of the flexural mode frequency leads to a further decrease of α . Numerical examples are given for graphene where the anharmonic couplings are determined from experiments. The theory is applicable to other monolayer crystals wherever the anharmonic couplings are known.

TUE 41

Photo-doping of MoS₂ revealed by Inelastic Light Scattering

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Two-dimensional layered 'van-der Waals' materials are of increasing interest for fundamental research as well as for device applications. For optical and optoelectronic applications as well as for studying fundamental optoelectronic properties, a comprehensive knowledge about the interaction of the 2D materials with light and the dielectric environment such as the substrate is essential.

We utilize inelastic light scattering for studying doping and heating effects of single- and multi-layer MoS₂. Using Raman measurements on top-gated field-effect transistor structures we demonstrate that the optoelectronic properties are strongly affected by the substrate. For mono- and bilayer MoS₂, we find a laser power induced change of the charge carrier density that is attributed to defects in the SiO₂-MoS₂ interface serving as trap states for photoexcited holes.

We acknowledge financial support by the DFG excellence cluster 'Nanosystems Initiative Munich'.

TUE 42

Potential of HCCNTs for nano-mechanical mass sensor applications

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We explore potential of helically coiled carbon nanotubes (HCCNTs) for applications as nano-mechanical resonators in mass and strain sensors. Using symmetry-based atomistic modeling, we consider both bridged and cantilevered configurations and also calculate fundamental frequencies of homogeneously deformed HCCNTs taking into account impact of the strain-induced deformations. Finally, we make comparative analysis of the performances of HCCNT-based and SWCNT-based nano-mechanical resonators.

TUE 43**High-energy plasmons in graphene and MoS₂ heterostructures**

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We investigate high-energy plasmons in layered 2D systems made of graphene and monolayer MoS₂. By direct comparison of momentum-resolved electron energy-loss (EEL) spectra and ab initio calculations, we want to gain insight into the influence of interactions between the individual layers.

Our EELS measurements have been performed using the low-voltage "SALVE I" TEM [1] equipped with a monochromator and an in-column energy filter. With simulations based on time-dependent DFT calculations for the graphene and MoS₂ layers, we find that regarding the investigated plasmons, only Coulomb interaction between the layers has to be considered. Whereas the spectra of multilayer graphene can be accurately described with homogeneous 2D layers in the layered electron-gas (LEG) model [2], we observe a discrepancy between LEG results and measured spectra of heterostructures involving MoS₂ layers. Calculations which account for the finite thickness of the MoS₂ layers may resolve this discrepancy, as corresponding calculations for bulk MoS₂ suggest.

[1] Kaiser et al., Ultramicroscopy 111, 1239-1246 (2011)

[2] Jovanović et al., Phys. Rev. B 84, 155416 (2011)

TUE 44**RF NEMS Based on CVD Multilayer Graphene**

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Silicon technology is currently dominant in the realization of nanoelectromechanical systems (NEMS), but the growing interest in graphene is paving the way to new devices with improved performance. Graphene is a promising candidate for NEMS applications due to its low mass, high mechanical stiffness, and high strength. For NEM switches, in particular, it brings the advantage of low actuation voltage and fast switching, while its hydrophobic surface avoids the surface stiction problem between the contacts, thus leading to better reliability. We discuss the prospect of graphene as a material for NEMS in the particular case of a NEM capacitive switch. We propose a novel design involving a suspended multilayer CVD-grown graphene membrane, doubly clamped on a coplanar waveguide (CPW). The fabrication consists in suspending the graphene membrane over the signal line of the CPW by etching the underlying sacrificial layer of oxide. We perform a thorough characterization of the NEMS between 1 and 40 GHz and discuss the potential for RF applications. Our results confirm that graphene is a good candidate for the fabrication of suspended membranes for fast-switching RF NEMS devices.

TUE 45**The role of quantum interferences in the plasmon-enhanced Raman scattering in graphene**

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Localized surface plasmon resonances in metal nanostructures can efficiently focus light into nanoscale volumes and generate very intense local fields. The Raman scattering cross section of a molecule in a plasmonic hotspot can be enhanced by several orders of magnitude - an effect that was discovered almost 40 years ago.

We present a new theory of plasmon-enhanced Raman scattering (PERS) that is based on a quantum mechanical description of the plasmonic enhancement. Quantum interference between different scattering channels significantly influences the excitation-energy dependence of the enhanced Raman cross section. Such PERS resonance profiles are explicitly calculated for graphene that is coupled to the plasmonic resonance of a gold nanocavity. Graphene is an ideal material for the investigation of PERS because of its constant Raman cross section. A formalism that is based on the second quantization of the collective electron excitations in the metal nanostructure is employed to calculate all relevant matrix elements. Our calculations explain the excitation-energy dependence of experimental PERS resonance curves, that were recorded with a tunable laser system.

TUE 46**Non-covalent Functionalization of Carbon Nanotubes**

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Single walled carbon nanotubes (SWNTs) are a material with extraordinary physical, chemical and electronic properties and a variety of possible and already implemented applications. The biggest hurdles one has to address concerning their processability, are their poor solubility and the polydispersity of the pristine material.

Commercially available detergents as well as specially designed surfactants have been extensively examined as means to disperse and even separate different types of SWNTs. However, usually no attention is paid to the effect of the temperature on the resulting dispersions. We demonstrate that the different behavior of detergents above and below their Krafft point is reflected in their selectivity and the dispersion efficiency.

Furthermore, we examine the interaction of tailor-made dyes with SWNTs and their capabilities concerning dispersion efficiency and individualization, depending on the size of their aromatic core and other structural motifs.

TUE 47

Synthesis and deposition of individual single-walled carbon nanotubes for applications and fundamental studies

Kimmo Mustonen¹, Patrik Laiho¹, Antti Kaskela¹, Hua Jiang¹, Esko I. Kauppinen¹

¹Department of Applied Physics, Aalto University School of Science, P.O. Box 15100, FI-00076 Aalto, Finland

We present a novel concept for the aerosol synthesis and direct deposition of predominantly individual single-walled carbon nanotubes for electronic applications and fundamental studies. The nanotube synthesis relies on iron catalyst particle generation in the range of 4 ± 3 nm via physical evaporation in a nitrogen driven spark discharge system. The aerosol catalyst particles are mixed with carbon monoxide (CO) and hydrogen and fed to a vertical laminar flow reactor tube held at 880 °C, where the SWCNTs form via catalytic decomposition of CO on the catalyst surface. The as synthesized nanotubes can be deposited on various substrates, including temperature sensitive ones, using a purpose-built thermophoretic precipitator. Based on atomic force and transmission electron microscopy studies, the as deposited SWNTs were up to 80% individual and of high quality and purity. The observed SWCNT mean diameters and lengths were 1.10 nm and 2.97 μ m respectively, and based on diffraction studies, 70% are semiconducting and 30% metallic. SWCNT transparent conductive films with sheet resistance of 65 ohms/sqr. @ 90%T and network transistors with On/Off current ratio up to 10^8 are presented.

TUE 48

Equilibrium concentration of singlet oxygen in photoreaction of reaction center/carbon nanotube bio-nanocomposites

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The primary events of photosynthesis take place in the reaction center protein (RC), where the energy of light is converted into chemical potential. When the photochemistry is oversaturated reactive oxygen species (singlet oxygen (1O_2), superoxide anion ($O_2^{\bullet-}$), and hydroxyl radicals ($\bullet OH$), with high cytotoxicity) are formed with

large probability. There is a large interest to reduce the formation of these components because they reduce the efficiency of photochemical energy conversion. The aim of our work is to create a system for efficient light energy conversion. We bind RC, to carbon nanotubes (CNT). 1,3-diphenylisobenzofuran was used to detect the concentration of the 1O₂. Although, CNTs are known as sensitizers, under our experimental conditions it is not probable that they play much role in generation of 1O₂, indeed, the main 1O₂ sensitizers are the RCs. However, CNTs can be sensitized by 1O₂ directly depending on the band structure and/or react chemically, typically through cycloaddition reactions. The equilibrium concentration of the 1O₂ is a result of the rate of the sensitization and the deactivation determined by the components and functions of the CNT/RC composite.

TUE 49

Self-assembly of Diamantane Chains inside Carbon Nanotubes from Functionalized Diamantanes

Yusuke Nakanishi¹, Haruka Omachi¹, Natalie A. Fokina², Ryo Kitaura¹, Peter R. Schreiner², Jeremy E. P. Dahl³, Robert M. K. Carlson³, Hisanori Shinohara¹

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Carbon nanotubes (CNTs), nanoscale cylinders composed of rolled-up graphene sheets, provide an ideal platform to create one-dimensional (1D) nanostructures. Precursor species are first filled into the cavities of CNTs, and then molded into linear structures via thermal annealing. To date, various kinds of 1D nanomaterials have been synthesized, including metal atomic wires, ultrathin boron-nitride nanotubes, and well-defined CNTs, which exhibit different properties from those of their bulk counterparts. As part of our exploring for novel 1D nanomaterials, we have been working on the synthesis of linear forms of crystalline diamond from diamantanes, the molecules in the diamond configuration.

Here we demonstrate that a string of diamantane can self-assemble from a functionalized diamantane within the internal cavities of CNTs. Transmission electron microscopy clearly shows that the diamantane cages are linked together inside CNTs. Using other analytical techniques, we succeeded at revealing the growth mechanism. This new class of diamond materials will offer a new direction for the nanodiamond research as well as a new strategy for the design and synthesis of 1D nanomaterials.

TUE 50**Starting 1985 - Thirty years of Winterschool contributions**Helmut Neugebauer¹¹Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Johannes Kepler University, Linz, Austria

According to the 30-years-anniversary of the authors's participation at the Kirchberg Winterschools, starting already 1985, a retrospective overview on the contributions is presented. In the early years, the work focused on spectroscopic and spectroelectrochemical studies on conjugated polymers, especially on polythiophenes and polyaniline using in-situ FTIR-ATR-spectroscopy. Doping induced infrared responses due to the strong electron-phonon coupling and their relation to structural and electronic properties were investigated. In the nineties and in the following decade, the focus changed to fullerenes, and the work became more device oriented. Especially photovoltaic devices with fullerenes in various molecular arrangements, like "double cable" polymers, molecular donor-acceptor-compounds and energy transfer systems were the main topics. In addition, novel infrared sensing properties and unusual transport phenomena in fullerenes were presented. Studies on oriented parasequiphenyl-needles, ellipsometric surface characterization and recently the presentation of ultrathin and lightweight organic solar cells with high flexibility rounded up the Winterschool contributions.

TUE 51**Contacts and Schottky Barrier Heights in MoS₂ and related 2D semiconductors**Yuzheng Guo¹, John Robertson¹¹Cambridge University, Cambridge, UK

MoS₂ and related Transition Metal Dichalcogenides (TMDs) have a band gap and so are suitable as semiconductors in FETs. However, their devices appear to be limited by the resistance of the electrical contacts, and also in the case of MoS₂ by the difficulty of making p-type FETs. Thus, a theory of Schottky Barrier Heights (SBH) in TMDs and van der Waals solids is needed. A key parameter is the SB pinning factor S , the rate of change of SBH vs. contact metal work function. A small S indicates many interface states and a pinned SBH, so that the contact resistance can be high. S approaching 1 indicates weak pinning, so that changing metal work functions allows n-FET or p-FET to be easily attained. We show that, against expectations, the standard metal induced gap state (MIGS) model of SBHs does work, despite the vdW bonding gap. The pinning factor S is evaluated as $S=0.3$. Additional anion vacancy defect states caused additional pinning, lowering S in some cases to $S=0.1$. Thus, extreme contact metal work function values are needed to scan the gap in MoS₂. Analysis finds that WSe₂ is better than MoS₂ for bipolar devices.

TUE 52**Fabrication and optical properties of transition metal dichalcogenide heterostructures**

Aurélie Pierret¹, Andreas Stegmaier¹, Janina Maultzsch¹

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Semiconductor transition metal dichalcogenides (TMD) are subject of increasing interest over the last years. In particular single layers of MoS₂ show strong photoluminescence associated with a direct-gap transition, in contrast to bulk. Heterostructures of TMDs will lead to modulations of their individual optical properties. It is expected from calculations that the band alignment of different monolayer TMDs are, for most of them, of type II, leading to spatially indirect excitons. Nevertheless, clear experimental evidence is still missing. It seems that the quality of the interface has a big influence on the results. Therefore, we investigate the fabrication of heterostructures by a dry transfer method, using a polymer stamp as an intermediate substrate, as proposed in Ref. [1].

Here we present, as a first step towards heterostructures, our results on the fabrication and optical properties of stacking of twisted few-layer MoS₂. We analyse the influence of the specific transfer method on the quality of the layers by Raman and photoluminescence spectroscopy.

[1] A. Castellanos-Gomez et al., 2D Materials, 1(1) 011002 (2014).

TUE 53**Tip-enhanced Raman spectroscopy of graphene folds**

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We studied a single vertically free-standing graphene fold by tip-enhanced Raman and micro-Raman spectroscopy. The folds are produced by GraFold printing [1] on SiO₂ substrate, forming out-of-plane, mono-dimensional deformations of graphene with 10 nm width and macroscopic length. Standard micro-Raman measurement can only give averaged information on the vibrational modes of the fold and of the surrounding area. However, the dependence of the Raman signal on the incoming light polarization shows interesting local anisotropic properties. Exploiting the evanescent field generated by localized surface plasmon polaritons at the apex of a bulk gold AFM tip, we are able to obtain a Raman map with 60 nm spatial resolution. The frequency shift of vibrational modes in relation to the fold morphology is used to calculate local variation maps of strain and doping. The top of the fold shows a variation of +0.3 compressive strain and $-10 \cdot 10^{12} \text{ cm}^{-2}$ hole doping compared to the flat region.

[1] Hallam, T.; Shakouri, A.; Poliani, E.; Rooney, A. P.; Ivanov, I.; Potie, A.; Taylor, H. K.; Bonn, M.; Turchinovich, D.; Haigh, S. J.; Maultzsch, J.; Duesberg, G. S. Nano Lett. DOI:10.1021/nl503460p.

TUE 54

Newly observed first-order resonant Raman modes in few-layer MoS₂

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We show measurements of two newly observed first-order Raman modes in few-layer molybdenum disulfide (MoS₂) with phonon frequencies of 286 cm⁻¹ and 471 cm⁻¹. These modes are strongly resonant and appear only at excitation energies above ≈ 2.4 eV. At 2.7 eV, in resonance with the *C* exciton, their intensity is comparable to the second-order Raman modes; their absence thus provides an easy and accurate method to identify single-layer MoS₂. At UV excitation, the intensity of the new modes is even larger than the typically examined A'_1/A_{1g} and E'/E_g modes. Using group theory, we provide a systematic analysis of the phonon modes, their symmetries, and their frequencies in few-layer materials, including the newly observed modes.

TUE 55

Raman spectroscopy on cation-exchanged XSe/CdSe (X=Pb, Zn) nanoparticles

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Colloidal nanoparticles have attracted much interest due to their electronic and optical properties. By controlling size, structure and stoichiometry one can achieve a higher photoluminescence quantum yield and control the fundamental transition energy. Due to these properties colloidal nanoparticles are expected to have a great impact on the development of optoelectronic devices.

XSe (X=Pb, Zn) nanoparticles of different size and shape were synthesized by wet chemical precipitation, a fast, cost-effective and well understood technique. XSe/CdSe composite nanoparticles were created by cation exchange, starting from XSe and exchanging the cation for Cd [1]. The cation exchange is a versatile method enabling the formation of composites which are not liable for direct synthesis. We present Raman measurements giving further insight into the mechanism of the exchange process and provide the possibility to further optimize process parameters to obtain nanostructures with desired properties.

[1] Marianna Casavola, Marijn A. van Huis, Sara Bals, Karel Lambert, Zeger Hens and Daniel Vanmaekelbergh, Chemistry of Materials, 24, 294 (2011).

TUE 56**UV Raman spectroscopy of graphene, graphite, and carbon nanotubes**

Christoph Tyborski¹, Roland Gillen¹, Felix Herziger¹, Janina Maultzsch¹

¹Institut für Festkörperphysik, Technische Universität Berlin, Berlin

We present Raman spectra of graphite, graphene, and carbon nanotubes with UV excitation energies. Using excitation energies above 5.0 eV we can observe the vibrational density of states of these carbon materials. We get access to regions of the first Brillouin zone that are not accessible with Raman spectroscopy in the optical visible range. By simulations of the phonon density of states of graphene and graphite, we can assign peaks in the UV Raman spectra to certain phonon branches and high symmetry points in the first Brillouin zone. Tuning the excitation towards lower energies activates double-resonant Raman scattering processes with ultra-short wavevectors. We analyze and explain the origin of the scattering processes by simulating corresponding spectra for various excitation energies.

TUE 57**Defect-induced zone-boundary acoustic phonons in individual carbon nanotubes**

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³Lehrstuhl für Angewandte Physikalische Chemie, Ruprecht-Karls-Universität Heidelberg

Raman spectroscopy on single-walled carbon nanotubes is often performed in dispersions or on ensembles of interacting tubes on substrates; such measurements, however, may average out subtle, highly dispersive features present in the spectra of individual tubes. Here, we studied perfectly aligned, mostly individual single walled nanotubes, grown on ST-cut quartz and transferred onto glass. We observe a new Raman mode emerging in the range of 350cm^{-1} to 500cm^{-1} , its second order overtone, and combination modes. We assign the new mode to the *ZA*-phonon derived phonon branch. We show that the *ZA* phonon mode becomes Raman-active due to defect-assisted double resonance close to the *K*-point, similar to the *D* mode. We present a theoretical evaluation of the diameter and excitation-energy dependence of the *ZA*, $2\cdot\textit{ZA}$ and $D\pm\textit{ZA}$ modes, which is in good agreement with our measurements and previous studies of the intermediate frequency region.

- 08:30 – 09:00 **E. Andrei, New Brunswick**
Artificial Atoms in Graphene
- 09:00 – 09:30 **M. Bockrath, Riverside**
Topological Winding Number Change and Broken Inversion Symmetry in a Hofstadter's Butterfly
- 09:30 – 10:00 **A. Grüneis, Köln**
Electronic properties of functionalized 2D materials: graphene, boron nitride, transition metal dichalcogenides and phosphorene
- 10:00 – 10:30 **coffee break**
- 10:30 – 11:00 **R. Saito, Sendai**
Raman spectroscopy of graphene and transition metal dichalcogenides
- 11:00 – 11:30 **A. Jorio, Belo Horizonte**
Stokes-anti-Stokes correlation in Raman Spectroscopy
- 11:30 – 12:00 **M. Paillet, Montpellier**
Combined Raman spectroscopy and reflection/transmission measurements for graphene characterization
- 12:00 – 17:00 **mini workshops**
- 17:00 – 18:30 **Dinner**
- 18:30 – 19:00 **B. Dora, Budapest**
Nematic, topological and Berry phases when a flat and a parabolic band touch
- 19:00 – 19:30 **H. Yeom, Pohang**
Soliton and Chiral Soliton of Atomic Wire Charge Density Wave
- 19:30 – 20:00 **S. Berciaud, Strasbourg**
Magneto-Raman spectroscopy of suspended graphene layers

Wednesday, March 11th

Graphene spectroscopy, topological materials

08:30**Artificial Atoms in Graphene**Yuhang Jiang¹, Jinhai Mao¹, Eva Y. Andrei¹¹Department of Physics, Rutgers University, Piscataway, NJ USA

Charged impurities are invisible to graphene's ultra-relativistic conduction electrons. This makes it difficult to localize and control its charge carriers and poses a problem for realizing graphene's promise as a building block in electronic applications. We show, using scanning tunneling microscopy and Landau level spectroscopy, that vacancies in graphene can host a so-called super-critical charge that is sufficiently strong to transform the local electronic properties. Such a charge traps electrons in a sequence of quantized states which resemble the bound states in an atom. This transformation is akin to the long sought-after phenomenon of super-criticality in ultra-heavy atoms. But unlike the 3D atom case, where super-criticality unleashes a chain reaction with electrons diving into the nucleus, emitting positrons and ultimately leading to atomic-collapse, we find that the artificial-atom created by a supercritically charged vacancy in graphene is stable and tunable.

09:00**Topological Winding Number Change and Broken Inversion Symmetry in a Hofstadter's Butterfly**Marc Bockrath¹¹University of California, Riverside

Recently several research groups have demonstrated accurate placement of graphene on hexagonal BN (hBN) with crystallographic alignment. Due to the resulting superlattice formed in the graphene/hBN heterostructures, an energy gap, secondary Dirac Points, and Hofstadter quantization in a magnetic field have been observed. Using aligned layer transfer we are able to produce graphene/hBN heterostructures with ~ 1 degree alignment accuracy, and measure the transport properties of the resulting systems. We observe an additional π Berry's phase shift in the magneto-oscillations when tuning the Fermi level past the secondary Dirac points, originating from a change in topological winding number from odd to even when the Fermi-surface electron orbit begins to enclose the secondary Dirac points. At large hole doping inversion symmetry breaking generates a distinct hexagonal pattern in the longitudinal resistivity versus magnetic field and charge density. This results from a systematic pattern of replica Dirac points and gaps, reflecting the fractal spectrum of the Hofstadter butterfly.

09:30**Electronic properties of functionalized 2D materials: graphene, boron nitride, transition metal dichalcogenides and phosphorene**Alexander Grüneis¹¹II. Institute of Physics, University of Cologne, Köln

Ionic functionalization of many layered materials by alkali and alkaline earth metals enables tuning of the charge carrier density into the superconducting regime. We investigate their electron energy band structure and spectral function with high-resolution angle-resolved photoemission spectroscopy (ARPES). For example, for Ca doped graphene this charge transfer can induce relatively large electron-phonon coupling constants of ~ 0.4 . This provides experimental support for the possibility to achieve superconductivity in graphene monolayers at $\sim 1.5\text{K}$. Regarding ionic functionalization of related layered materials, we investigate the interaction of alkali metals with epitaxial monolayer boron nitride and the bulk phosphorene and MoS_2 compounds. While boron nitride does not accept electrons, the band gap of the latter two materials is sufficiently small so that a semiconductor to metal transition can be induced by ionic functionalization.

10:30**Raman spectroscopy of graphene and transition metal dichalcogenides**Riichiro Saito¹, Eddwi H. Hasdeo¹, Ahmad R. T. Nugraha¹, Huaihong Guo¹, Teng Yang¹, Syahril Siregar¹¹Department of Physics, Tohoku University, Sendai

Recent works on Raman spectroscopy of graphene and transition metal dichalcogenides (TMD) in our group are presented. Asymmetric Raman spectra of G band of graphene which is expressed by Breit-Wigner-Fano (BWF) spectra are calculated as a function of the Fermi energy (E_F). The asymmetric factor ($1/q$) in the BWF function becomes the maximum at the Dirac point and decreases monotonically with increasing E_F . Raman spectra of MoTe₂ show some weak Raman spectra which are assigned by double-resonance Raman spectra of the M point phonon in the Brillouin zone. These double resonance peaks appear for other TMD materials, too, which are assigned either the K or the M point phonon. Raman spectra with use of the deep ultraviolet laser (266nm) show the absence of G' band, which is reproduced by calculation.

11:00**Stokes-anti-Stokes correlation in Raman Spectroscopy**Ado Jorio¹¹Physics, UFMG, Belo Horizonte

In this talk the correlation between the Stokes and the anti-Stokes processes in the light scattering by phonons will be discussed. This phenomena imposes corrections on the broadly utilized Stokes/anti-Stokes Raman intensity ratio, described theoretically by the boson statistics, and applied experimentally in the measurement of materials temperature. In diamond, the correlation is demonstrated by measuring the field correlation function ($g^2(0)$). Graphene was also explored, indicating that the phenomena can be made many orders of magnitude higher in this low dimensional system by exploring resonance conditions. The power dependence of the Stokes and anti-Stokes inelastic light scattering are theoretically described by an effective Hamiltonian. The photonic and phononic reservoirs are considered by including a Lindblad term in the density operator master equation.

11:30**Combined Raman spectroscopy and reflection/transmission measurements for graphene characterization**Matthieu Paillet¹¹Laboratoire Charles Coulomb, Université Montpellier 2, Montpellier

Raman spectroscopy (RS) of graphene-related materials (GRM) is being considered as a fast, versatile, powerful and non-destructive characterization technique. RS is sensitive to the number of layers, their stacking order, the nature and density of defects, the charge carrier density and in-plane strain variations. However, the positions, linewidths, profiles, intensities of the graphene/multilayer graphene (MLG) Raman bands are not only affected by all these perturbations but also depends on the uniformity across the probed area and on the substrate (through optical interference effects, dielectric screening...). An accurate interpretation of Raman spectra becomes then extremely complex and deserves the combined use of complementary diagnosis. We recently developed a RS set-up allowing to monitor simultaneously the laser power, transmission, reflection and Raman signal. In this contribution, we discuss the application of this tool for counting the number of layers of different kind of graphene/MLG samples with the aim to define standard procedures for GRM characterization on different substrates.

18:30**Nematic, topological and Berry phases when a flat and a parabolic band touch**Balazs Dora¹¹Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary

A (single flavor) quadratic band crossing in two dimensions is known to have a generic instability towards a quantum anomalous Hall (QAH) ground state for infinitesimal repulsive interactions. Here we introduce a generalization of a quadratic band crossing which is protected only by rotational symmetry. By focusing on the representative case of a parabolic and flat band touching, which also allows for a straightforward lattice realization, the interaction induced nematic phase is found generally to compete successfully with the QAH insulator, and to become the dominant instability in certain parts of the phase diagram already at weak coupling. The full phase diagram of the model, together with its topological properties, is mapped out using a perturbative renormalization group, strong coupling analysis, the mean-field theory. Interestingly, the Berry flux varies continuously in the single flavour limit with various control parameters.

19:00**Soliton and Chiral Soliton of Atomic Wire Charge Density Wave**Han Woong Yeom¹¹Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science, Pohang²Department of Physics, POSTECH

Solitons are important in understanding various quantum properties of low dimensional electronic systems. Solitons in charge density waves (CDW's) have drawn particular interest, since they have fractionalized electrons and are the edge mode of 1D topological insulators. While solitons were investigated for a long time, an individual soliton had not been directly observed until very recently. We review the recent breakthrough in observing directly solitons in commensurate and incommensurate quasi 1D CDW's with scanning tunnelling microscopy. The newly observed topological solitons in the commensurate CDW of indium atomic wires self assemble on silicon surface are discussed in details. This CDW wire is unique because each wire is composed of two In zigzag chains to yield four degenerate CDW states. This leads to not unique but various distinct solitons. We map this system into two interacting Peierls chains successfully. The topology of this system is unravelled as a rare realization of non-trivial Z_4 with the emergence of 'chiral' solitons. The exciting prospect of utilizing solitons and chiral solitons in future subnanometer scale scale electronics will be discussed.

19:30**Probing electronic excitations in mono- to pentalayer graphene by micro-magneto-Raman spectroscopy**Stéphane Berciaud¹, Denis M. Basko², Marek Potemski³, Clément Faugeras³¹IPCMS, Université de Strasbourg and CNRS, France²LPMMC, Université Grenoble 1 and CNRS, France³LNCMI-Grenoble, CNRS/UJF/UPS/INSA, France

We probe electronic excitations between Landau levels in freestanding N-layer graphene over a broad energy range, with unprecedented spectral and spatial resolution, using micro-magneto Raman scattering spectroscopy. A characteristic evolution of electronic bands from two up to five Bernal-stacked graphene layers is evidenced and shown to remarkably follow a simple theoretical approach, based on a one-electron, effective bilayer model [1].

In contrast, in monolayer graphene, the band velocity associated with the Raman active electronic excitations is found to depend on the index of Landau level involved, and to vary as a function of the magnetic field [1,2]. This contradicts the single-particle picture of non-interacting massless Dirac electrons, but is accounted for by theory when electron-electron interactions are taken into account [2]. Raman active, zero-momentum inter Landau level excitations in monolayer graphene are sensitive to electron-electron interactions, due to the non-applicability of the Kohn theorem in this system, with a clearly non-parabolic dispersion relation.

[1] S. Berciaud et al. Nano Letters 14, 4548 (2014)

[2] C. Faugeras et al. arXiv:1412.0115

08:30 – 09:00	M. Prato, Trieste <i>Applications of Functionalized Carbon Nanostructures</i>
09:00 – 09:30	M. Shaffer, London <i>Versatile and scalable approaches to chemical processing of nanocarbons</i>
09:30 – 10:00	S. Eigler, Fürth <i>Diversity of Oxo-Functionalized Graphene</i>
10:00 – 10:30	coffee break
10:30 – 11:00	P. Rudolf, Groningen <i>Graphene growth on metallic and insulating surfaces</i>
11:00 – 11:30	E. Weig, Konstanz <i>Coherent control of nanomechanical systems</i>
11:30 – 12:00	G. Steele, Delft <i>Optomechanical coupling of a multilayer graphene resonator to a superconducting microwave cavity</i>
12:00 – 17:00	mini workshops
17:00 – 18:30	Dinner
18:30 – 19:00	R. Baughman, Richardson <i>Powerful, Giant-Stroke Artificial Muscles From Twisted and Coiled Carbon Nanotube Yarns</i>
19:00 – 19:30	J. Ahn, Seoul <i>Graphene for Flexible and Wearable Electronics</i>
20:00	Poster III

08:30**Applications of Functionalized Carbon Nanostructures**Maurizio Prato¹¹Center of Excellence for Nanostructured Materials (CENMAT), INSTM UdR di Trieste, Dipartimento di Scienze Chimiche e Farmaceutiche, University of Trieste, Trieste, Italy

Our group has been involved in the organic functionalization of various types of nanocarbons, including carbon nanotubes, fullerenes and, more recently, graphene. The chemical functionalization represents an important and versatile tool for tuning the chemical and physical properties of the carbon nanostructures (CNS). For example, chemical functionalization can render CNS dispersible in different solvents. During this talk, we will summarize our most recent results in the chemistry and applications of functionalized CNS. In particular, we will focus on the use of carbon nanotubes and graphene as active interfaces in neurosciences and for the splitting of water.

09:00**Versatile and scalable approaches to chemical processing of nanocarbons**Milo Shaffer¹¹Department of Chemistry, Imperial College, London, UK

Chemical functionalisation is critical to a wide range of nanotube applications, but needs to be versatile and applicable at scale. Existing approaches rely on liquid phase reactions, often requiring damaging sonication or lengthy work up through filtration or centrifugation. The formation of individualized functionalised single wall nanotubes (SWNTs) is a particular challenge. One approach is to shift the modification reaction into the gas phase. We have developed a generic, scalable furnace treatment, based on the thermochemical activation of the CNTs, followed by reaction with functional organic monomers [1]. This approach allows the introduction of a wide variety of functional groups onto the CNT surface whilst maintaining the excellent properties of the untreated materials. The underlying mechanism of the reaction has been established and the distribution of the functionalised sites studied using tagging experiments. The reaction is extremely versatile and can be carried out with a variety of monomers. The reaction and the subsequent product purification can be carried out entirely in the gas-phase, simplifying work-up and improving scalability; the approach is compatible with the scale and equipment of many industrial CNT synthesis processes, and is applicable to multi-walled CNTs, SWNTs, and other carbon-based materials [6]. The surface properties of these products have been studied by direct wetting experiments on the nanoscale, dispersion studies, and inverse gas chromatography (IGC) [2]. Water dispersible materials with cationic, anionic, and non-ionic surface functionalities provide simple processing routes to a range of applications, and are particularly well suited to studying biological interactions [5,6]. A different approach to CNT processing, relies on reductive charging. Using a liquid ammonia process [3], pure nanotubides can be redissolved, purified, or optionally functionalised without sonication. A key step is to control the ratio of charge to carbons, as it determines the yield and the nature of the dissolved material. The G/D ratios observed during the dissolution sequence, as a function of metal:carbon ratio, demonstrate a new purification method for removing carbonaceous impurities from pristine SWNTs. A similar approach can be applied to graphene nanoplatelets [4]. The resulting nanocarbon ions can be chemically grafted for a variety of applications, depending on the reagent, charge density, and ionic concentration in the reaction medium [9]. The nature of the reactivity of charged graphenides is unusual, due to the continuum density of states of these otherwise molecularly discrete species [10]. The chemical charging agent can be avoided by a pure electrochemical process that yields CNT anions [5] and cations [8], suitable for purification, functionalization, or electrodeposition.

1. Menzel et al, Chem. Sci., 2010, 1, 603-8
2. Menzel et al, Langmuir, 2009, 25, 8340
3. Fogden al, ACS Nano, 2012, 6, 54-62
4. Milner et al, J Am Chem Soc, 2012, 8302
5. Chen et al, Biomaterials, 2014, 35, 4729
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09:30**Diversity of Oxo-Functionalized Graphene**Siegfried Eigler¹¹FAU Erlangen-Nürnberg, Fürth

Graphene (G1), a single layer of graphite is a platform for interdisciplinary research to discover new fascinating properties. However, the wet-chemical synthesis of pure G1 remains challenging because of the polydispersity of flakes of G1. Nevertheless, we synthesized oxo-functionalized graphene (oxo-G1) with a variable amount of functional groups and succeeded in the back-conversion of oxo-G1 to G1 with mobility values of charge carriers up to 1000 cm²/Vs for the best quality of flakes. Furthermore, only recently, we showed an enhanced method minimizing the average density of defects of the carbon framework, which can be as low as 0.04%. This is an unprecedented low average density of defects for wet-chemically prepared G1. Moreover, the carbon framework of oxo-G1 is thermally stable up to 100 °C and controlled transformations of chemical groups are possible. Thus, azide groups can be introduced or hydroxylated graphene can be prepared, what opens the ability for controlled chemical transformations.

10:30**Graphene growth on metallic and insulating surfaces**Petra Rudolf¹¹Zernike Institute for Advanced Materials, University of Groningen, Groningen

The epitaxial growth of graphene on catalytically active metallic surfaces via chemical vapour deposition (CVD) is known to be one of the most reliable routes toward high-quality large-area graphene. This CVD-grown graphene is generally coupled to the metal resulting in a modification of its intrinsic properties. Growth on oxides is a promising alternative that can lead to decoupled graphene. Here, I compare graphene on a pure metallic and on an oxidized copper surface, grown by a single step CVD process under similar conditions. Remarkably, growth on copper oxide, a high-k dielectric material, preserves the intrinsic properties of graphene; it is not doped and a linear dispersion is observed close to the Fermi energy. Density functional theory calculations give additional insight into the reaction processes and help explaining the catalytic activity of the copper oxide surface. I shall also present an alternative to CVD growth, namely growth from self-assembled monolayers of 1-1', biphenyl-4 thiol assembled on Cu and copper oxide, which were first polymerized with UV light and then heated to generate graphene. Best quality graphene from this SAM is obtained on copper oxide.

11:00**Coherent control of nanomechanical systems**Eva Weig¹¹Department of Physics, University of Konstanz, Konstanz

Nanomechanical resonators are freely suspended, vibrating bridges with nanoscale diameters. These nanostructures are receiving an increasing amount of attention, both in fundamental experiments addressing the foundations of quantum mechanics and for sensing applications, and show great promise as linking elements in future hybrid nanosystems. In particular, doubly-clamped pre-stressed string resonators are explored as high Q nanomechanical systems. Dielectric transduction by means of electrically induced gradient fields allows to actuate and probe these nanostrings, to tune their eigenfrequencies and to strongly couple their two orthogonal fundamental flexural modes. On resonance, the normal modes are described as a classical nanomechanical two level system, the state of which can be manipulated by radio frequency pulses. Full state control on the Bloch sphere is demonstrated by Rabi, Ramsey and Hahn echo experiments. Moreover, we find that all relaxation times T_1 , T_2 and T_2^* are equal. This indicates that energy relaxation is the dominating source of decoherence, such that not only T_1 but also T_2 can be increased by engineering larger mechanical quality factors.

11:30**Optomechanical coupling of a multilayer graphene resonator to a superconducting microwave cavity**Vibhor Singh¹, Sal Bosman¹, Ben Schneider¹, Yaroslav Blanter¹, Andres Castellanos-Gomez¹, Gary Steele¹¹Kavli Institute of Nanoscience, Delft University of Technology, Delft

The combination of low mass density, high frequency, and high quality-factor make graphene mechanical resonators very attractive for many quantum applications. Microwave optomechanics with superconducting cavities offers exquisite position sensitivity and enables the preparation and detection of mechanical systems in the quantum ground state. In this talk, I will present recent work [1] in which we demonstrate coupling between a multilayer graphene resonator and a high-Q superconducting cavity. We achieve a displacement sensitivity of $55 \text{ fm/Hz}^{1/2}$ and measure mechanical quality factors up to 220,000, both significantly better than shown before. Optomechanical coupling is demonstrated by optomechanically induced reflection (OMIR) and absorption (OMIA) of microwave photons, along with signatures of strong optomechanical backaction. We extract the cooperativity C , a characterization of coupling strength, quantitatively from the measurement with no free parameters and find $C=8$, promising for the quantum regime of graphene motion.

[1] Singh *et. al*, Nature Nanotechnology 9, 820 (2014)

18:30**Powerful, Giant-Stroke Artificial Muscles From Twisted and Coiled Carbon Nanotube Yarns**Ray H. Baughman¹¹Alan G. MacDiarmid NanoTech Institute, the University of Texas at Dallas, Richardson, TX, 75083 USA

Three successive generations of twist-spun artificial muscles are described that provide torsional and tensile actuation (1). Our first generation muscles are electrochemically powered twist-spun carbon nanotube yarns that provide torsional rotation speeds of 590 rpm, and torsional strokes that are 1000 times that for earlier artificial muscles. Our second generation muscles are electrolyte-free, guest-infiltrated carbon nanotube yarns that can torsionally actuate at 11,500 rpm, and deliver 85 times higher contractile power density than natural muscles. Our third generation muscles can rotate at 50,000 rpm, contract by up to 49%, lift 100 times heavier loads than the same size human muscle, or actuate at 7.5 cycles/s for millions of cycles.

(1) Collaboration between The University of Texas at Dallas, The University of Wollongong, The University of British Columbia, Hanyang University, and Namik Kemal University.

19:00**Graphene for Flexible and Wearable Electronics**Jong-Hyun Ahn¹¹Electrical and Electronic Engineering, Yonsei University, Seoul

With the emergence of unusual format electronics such as flexible and wearable devices, an effort has been made to integrate devices with various functions for providing enhanced convenience for the users. However, it is very difficult to accomplish such electronics with conventional, rigid electronic materials. Graphene has an extremely good mechanical property that should maintain a stable operation under a high strain and also possesses great electronic properties that make it a promising host for device applications. The recent advances in large-scale synthesis and fabrication technique of graphene films are expected to enable various applications for flexible and wearable electronics. In this talk, I present the application possibility of graphene films for flexible and wearable electronics including solid state lighting, strain sensor, transistor and energy harvesting/storage devices.

THU 1**Mechanical stability of empty and filled carbon nanotubes under high pressure**

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The mechanical stability of SWCNTs can be significantly influenced by filling with molecules or with inner tubes: It was shown by high-pressure resonant Raman spectroscopy that filling the SWCNT with another tube (DWCNT) or with argon results in the stabilization of the nanotube, whereas filling with fullerene molecules (peapods) or with iodine leads to the destabilization of the nanotube.

We discuss the mechanical stability of empty SWCNTs, C₆₀- and C₇₀-peapods, iodine-filled SWCNTs, and DWCNTs based on their optical response under hydrostatic pressure. The synthesis of the materials and their characterization by HRTEM, Raman and optical spectroscopy will be briefly described. The alterations of the electronic properties of the various nanotube materials under pressure were monitored by transmission measurements in the near-infrared and visible frequency range, where the characteristic absorption bands corresponding to optical transitions in the nanotubes can be observed. Anomalies in the pressure-induced shifts of the absorption bands can serve as indications for structural deformations and phase transitions.

THU 2**Raman spectroscopy as probe of nanometer-scale strain variations in graphene**

Christoph Neumann^{1,2}, Sven Reichardt¹, Marc Drögeler^{1,2}, Takashi Taniguchi³, Kenji Watanabe³, Slava V. Rotkin^{1,4}, Bernd Beschoten^{1,2}, Christoph Stampfer^{1,2}

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Confocal Raman microscopy has become a powerful and widespread tool in graphene research. Amongst other material properties such as carrier doping, short-range disorder and lattice temperature also mechanical strain can be extracted from Raman spectra. The spatial resolution of so-called Raman maps is on the order of the laser spot size, which, for confocal systems and typical laser energies, is usually around 500 nm. The extracted quantities such as doping or strain are in general averaged over the spot size. It is therefore important to distinguish between length scales significantly larger or smaller than the laser spot size. Here, we make use of a magnetic field and doping to control the influence of the electronic system on the line width of the graphene Raman G line. When Landau damping is minimized, we find a linear

dependence of the line widths of the G and 2D line, which reveals that different local strain conditions within the laser spot size make a significant contribution to the line widths (in particular of the 2D line). These nm-scale strain variations are hard to probe with other techniques, but are considered as important scatterers limiting electronic transport.

THU 3

Large-area fabrication and nanomechanical characterisation of suspended graphene membranes

Christian Nikolaus¹, Nicholas Clark¹, Aravind Vijayaraghavan¹

¹School of Materials, University of Manchester, Manchester

Nanoelectromechanical systems (NEMS) aim to explore the behavior and performance of mechanical devices in the nanometer regime. By reducing device dimensions, these systems demonstrate increased resonance frequencies and lower bending stiffness, thereby improving force and mass sensitivity. Graphene, the thinnest, stiffest, and strongest material known to date, has great potential for NEMS applications. Moreover, graphene is remarkably versatile in its processability. It can be grown over large areas, transferred onto arbitrary substrates and patterned by standard photolithography processes. However, the fabrication of suspended graphene membrane devices with minimal contamination and high yield over large areas remains a challenging issue. In this work we present a fabrication method that allows the construction of arrays of micrometer scale suspended graphene membranes over entire wafers. Furthermore, by either applying an electric field or a differential pressure across these suspended structures, whilst taking AFM measurements, we can study the electromechanical characteristics of graphene-NEMS devices.

THU 4

Coherent and squeezed states of phonons in single wall carbon nanotubes

A. R. T. Nugraha¹, E. H. Hasdeo¹, R. Saito¹

¹Department of Physics, Tohoku University, Sendai

In quantum mechanics, coherent states are known as a quantum state whose amplitude-phase uncertainty reach its minimum value. Moreover, we may generally increase the uncertainty in the amplitude and at the same time decrease the uncertainty in the phase, or vice versa, while still holding the minimum uncertainty principle. These states are the so-called squeezed states. Recently, there is a possibility to generate squeezed states of phonons in single wall carbon nanotubes (SWNTs) via ultrafast spectroscopy using less than 10 femtosecond pulses, in which the coherent oscillations of G' bands involving two-phonon process may be relevant as a particular example. In this work, we calculate the squeezed phonon amplitude of the G' band for a given SWNT and compare it with the coherent phonon amplitude of the G band. We find that the ratio between the G' band and G band intensities in ultrafast spectroscopy depend on the laser energy, laser pulse width, and SWNT chirality

(electron-phonon coupling). This result is useful for understanding the coherent control of phonon excitations, i.e. we may be able to selectively excite a certain phonon mode by adjusting some physical parameters.

THU 5

Chemical Vapour Deposition of MoS₂ and WS₂ via Close Proximity Precursor Supply

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Reliable chemical vapour deposition (CVD) of transition metal dichalcogenides (TMDs) is a highly pressing research field, as numerous potential applications rely on the production of high quality films on a macroscopic scale. Here, we show the use of liquid phase exfoliated and sputtered metal oxide precursor layers as solid precursors for CVD in a microreactor setup[1]. MoS₂ and WS₂ monolayers have both been synthesised in this way. Raman spectroscopy, photoluminescence, XPS, AFM, TEM, SEM and electrical transport measurements over large areas reveal the high quality of the TMD samples produced, with mobilities of up to 1.15 cm² V⁻¹ s⁻¹. This shows that large area CVD grown MoS₂ is potentially viable for electronic devices despite the presence of grain boundaries. Furthermore, through patterning of the precursor supply, we achieve patterned growth of monolayer TMDs in defined locations, which could be adapted for the facile production of electronic device components.

[1] O'Brien, Maria, et al. "Transition Metal Dichalcogenide Growth via Close Proximity Precursor Supply." Scientific reports 4 (2014).

THU 6

HRTEM and Optical Investigations of Ultrathin Graphene Nanoribbons Formed from Coronenes

Elena D. Obraztsova¹, Andrey L. Chuvilin², Alexander I. Chernov¹, Pavel V. Fedotov¹, Ekaterina A. Obraztsova¹, Vladimir L. Kuznetsov³, Andrew Fairbrother⁴, Roman Fasel⁴

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Flat one-dimensional graphene nanoribbons are interesting due to their band gap be-

ing inversely proportional to the ribbon width. One of the most reliable technique to form nanoribbons is to fill the nanotubes with coronene molecules and to treat them thermally [1]. A mechanism of transformation of coronene chain into nanoribbon has been theoretically modeled and then monitored by a high resolution transmission electron microscopy (HRTEM), Raman scattering and Photoluminescence techniques. A comparison of Raman spectra for the graphene nanoribbons inside single-wall carbon nanotubes and for the armchair graphene nanoribbons grown on metal surfaces [2] has been made.

The work was supported by RFBR-13-02-01354 project.

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THU 7

The Aharonov-Bohm effect in a graphene ring encapsulated in hexagonal boron nitride

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Recent developments in the fabrication of graphene-hexagonal boron nitride (hBN) heterostructures enable nowadays graphene devices on substrate with outstanding electronic properties. In state-of-the-art graphene devices mean free paths in the range of several micrometers as well as long phase coherence times are reported. The latter is an important quantity responsible for numerous mesoscopic phenomena such as the Aharonov-Bohm (AB) effect. Here we present low-temperature magneto-transport measurements on a high mobility graphene ring encapsulated in hBN. We show the existence of AB oscillations with high visibility as well as their dependence on charge carrier density. For low magnetic fields we observe focusing of charge carriers within the ring, where the cyclotron radius matches distinct sample-related length scales. From the crossover between quasi-ballistic transport and quantum hall effect (QHE) we extract relevant length-scales of our structure, consistently with the sample geometry. Finally, we report on the investigation of the AB effect in the crossover regime of emerging QHE at magnetic fields of a few Tesla and show qualitative agreement with earlier theoretical work.

THU 8**Biosensor applications of carbon nanotube thin film**Nguyen Xuan Viet¹, Shigeru Kishimoto¹, Yutaka Ohno^{1,2}¹Graduate School of Engineering, Nagoya University, Nagoya²EcoTopia Science Institute, Nagoya University, Nagoya

CNT have shown promising properties as electrochemical electrodes such as rapid electron transfer kinetics, wide potential window, biocompatibility, and manufacturing versatility. In this study, we demonstrate high-performance flexible microelectrodes based on a CNT thin film for electrochemical biosensor applications. The CNT microelectrodes were fabricated on a PEN film by the dry transfer method based on floating-catalyst CVD and standard microfabrication process. To minimize the process-originated contamination of CNT surface, the CNT surface was covered with an oxide film during the fabrication process. The electrochemical properties of flexible CNT microelectrodes were characterized by cyclic voltammetry with $K_4[Fe(CN)_6]$. The results showed that the fabricated CNT microelectrodes have high electron transfer rate. Electrochemical deposition of gold nanoparticles on electrode confirmed the excellent uniformity in electrochemical activity of the CNT film. We also demonstrate high sensitivity in detection of dopamine.

THU 9**Bottom-up assembly of suspended nanocarbon devices by dielectrophoresis**Antonios Oikonomou¹, Nick Clark², Sebastian Heeg², Andrey Kretinin³, Aravind Vijayaraghavan²¹National Graphene Institute, The University of Manchester, UK²School of Materials, The University of Manchester, UK³School of Physics and Astronomy, The University of Manchester, UK

Over the past few years, we have demonstrated that bottom-up device assembly of nanocarbons using dielectrophoresis (DEP) can achieve ultra-high integration densities, excellent FET device performance and can be combined with sorting to even produce single-chirality SWCNT device arrays. Recently, we have achieved the large-scale assembly of suspended single-walled carbon nanotube (SWCNT) and few-layer graphene (FLG) devices by bottom-up DEP assembly. Suspended device fabrication is associated with a range of new technological challenges which we have overcome. These devices are ideally suited for sensors and resonator applications. Our fabrication strategy resulted in ultra-flat devices and then to high-yield suspended structures as confirmed by atomic force microscopy (AFM) and scanning electron microscopy (SEM). Raman spectroscopy measurements highlighted the non-destructive nature of the fabrication process. These results further demonstrate the versatility of the DEP assembly technique for nanocarbon device fabrication and argue about the need of high quality materials dispersions in order to establish itself as an attractive device integration method.

THU 10**Electronic structure and optical properties of C_2F_x graphites**

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Interaction of graphite with a mixture of BrF_3 and Br_2 at room temperature produces bromine intercalated graphite fluoride with a composition of $C_2F_{x0.13}Br_2$, where x is less 1. The hosted bromine molecules are easily replaced by another intercalant. Optical spectra of absorption and luminescence were measured for samples with different fluorine contents. Obtained compounds can be considered as a stack of the fluorinated graphenes (FG). These FGs are large in area making it possible to study how the conjugated system is distributed on the basal plane. It was shown that fluorine atoms form short chains, while non-fluorinated carbon atoms are organized in very narrow ribbons and aromatic areas with a size smaller than 3 nm. These nanochains and nanoislands preserved after the fluorination process are likely responsible for the value of the energy gap of the compound of ~ 2.5 eV. Variation in the size and the shape of pi electron regions within the fluorinated graphene layers could be a way for tuning the electronic and optical characteristics of the graphene-based materials.

THU 11**Quantum Transport in Two-dimensional Transition Metal Dichalcogenides**

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Quantum spin Hall effect (QSHE) is a phenomenon which shows a great promise for quantum electronics. However, the materials that feature this effect do not live up to theoretical predictions and thus their applicability is limited. Recently, QSHE was proposed in 2D transition metal dichalcogenides [1]. This work is devoted to numerical quantum transport simulations in WTe_2 . Without strain, it is a semimetal with 0.1 eV band overlap, but if small strain is applied, the overlap can be removed. We prepared a tight-binding model in order to recreate low-energy band structure obtained from first principles calculations. It is used to study properties of the edge states, which reveals features such as a short decay length (about 5 nm). Quantum transport simulations for both free and strained material were performed and displayed the topological protection of the edge states from disorder, which results in quantized conductance for a broad range of disorder magnitudes, confirming the viability of this material in device application.

Reference:

[1] X. Qian, J. Liu, L. Fu, and J. Li, Science 346, 1344 (2014)

THU 12**Photocatalytic stability of single- and few-layer MoS₂ edge sites**

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MoS₂ is a promising two-dimensional "van der Waals" material with outstanding electronic, optical and catalytic properties that offers potential for many applications. The formation of a direct band gap in the visible range, together with a high catalytic activity makes single-layer MoS₂ a very promising material for solar energy conversion by photocatalytic hydrogen evolution.

In order to probe the photocatalytic stability, we perform spatially resolved μ -Raman spectroscopy of single- and few-layer MoS₂ in liquid environments. We find a significantly lower stability of edge sites compared to terrace sites. The decomposition on edge and defect sites can only be observed for excitations energies larger than the band gap energies, pointing towards the important role of photoexcited charge carriers. We discuss the increased stability in the single-layer case, the dependence on laser excitation power as well as preliminary results on electrochemically driven decomposition of single-layer MoS₂.

We acknowledge the financial support by the DFG excellence cluster "Nanosystems Initiative Munich" (NIM) and BaCaTec.

THU 13**Tailoring the interaction of separated SWCNT with NO₂ by advanced filling reactions**

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Our recent work on the interaction of ultrapure metallicity sorted SWCNT with NO₂ using a combination of high resolution XPS and XAS revealed a physisorption mechanism and a weak chemisorption with defects at 100 K [1]. Here we report on new experiments at the SUPERESCA beamline in ELETTRA showing how to tailor this interaction with NO₂ by advanced filling reactions using metalacetylacetylates containing Ni and Fe. We find a weak chemisorption at room temperature which is reversible after annealing at 150 C. We also were able to further fine tune the interaction by converting the filled molecules to Fe and Ni nanoclusters getting a fully reversible gas adsorption mechanism with a significant change in the density of states at the Fermi level at room temperature. The new results pave the way to get utmost sensitivity and selectivity for gas sensing at room temperature.

Work supported by the FWF and EU.

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

THU 14

Microscopic study of laser welded amorphous material

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The presented tests comprise bulk metallic glasses (BMG) with ferrous matrix characterized by two important properties—mostly very good magnetically soft ones and wear resistance. Because of their structure and properties metallic glasses can be used as monitoring equipment sensors or microelectromechanic systems. At present the elements made of BMG have small dimensions. The use of laser-beam fusion welding process will enable the increase of elements' diameter together with the enhancement of application abilities of new materials. To get exceptional properties of the material after welding process, its structure in the heat affected zone (HAZ), fusion zone (FZ) and parent material (PM) should be controlled. Because of the amorphous character of the welded material and small dimensions of particular fusion weld zones, TITAN 80-300 HRTEM and Hysitron TI950 Triboindenter nanoindenter equipped with QScope 250 microscopic attachment with Q-WM190 scanning probe were used for structure analysis. Probably in the presented work the atomic force microscope was used for the first time to examine the amorphous material after laser-beam welding process.

THU 15

Nanoindentation characteristic of Fe-based bulk metallic glass laser weld

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Fe-based bulk metallic glasses are characterized by good magnetic properties, high mechanical strength and corrosion resistance. Although, despite these properties, their using is limited because of small sample thickness that could be achieved by rapid solidifications. Therefore, one of the most prominent and promising process engineering which can be used for extending amorphous materials applications is laser beam welding. In this experiment, amorphous alloy of desired composition was prepared by melting high purity constituents. Fully amorphous plate was achieved by die pressure casting method. Next, the laser welding process was carried out by the use of TruLaser Station 5004.

In the present study, the influence of laser beam on the topography on the parent material, heat affected zone and fusion zone was investigated. Nanohardness and reduced Young's modulus of particular amorphous material fusion weld zones were examined with the use of Hysitron TI950 Triboindenter nanoindenter and with the

use of Berkovich's indenter. Examination of the nanostructure of particular weld zones by the use of TITIAN 80-300 high-resolution electron transmission microscope were carried done.

THU 16

Electron-phonon scattering and electron mobility in semi-conducting HCCNTs

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We consider model of helically coiled carbon nanotubes (HCCNTs) where pentagonal and heptagonal carbon rings are regularly incorporated into hexagonal carbon net [1]. Electron-phonon scattering rates are calculated out of electron and phonon dispersion relations [2,1], applying deformation potential approximation and evaluating electron-phonon matrix elements by means of extended tight-binding model based on density functional theory [3]. Electron drift velocities are obtained from one-particle Monte Carlo simulations where their motion is simulated as series of free flights interrupted by instantaneous electron-phonon scattering events.

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THU 17

Controllable fabrication of diamond thin films with active and inactive Si-related color centers

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In this paper we investigated the reproducible fabrication of Si-related color centers (Si-V) with a strong and homogeneous photoluminescence (PL) at 738 nm in diamond films deposited by microwave plasma enhanced CVD. The influence of process parameters (gas composition and concentrations of H₂/CH₄/CO₂/N₂ and substrate temperature) on the optical activity of Si color centers is studied. The activity of Si-V zero phonon line (ZPL) center is found similar for a broad substrate temperature range from 450 °C to 1100 °C with a FWHM of ~6 nm. For the lowest substrate temperature 350 °C the photoluminescence intensity decreased and the FWHM increased to 10 nm. For diamond films deposited at 5 % of methane in hydrogen, Si-V activity was still measurable for adding up to 0.5 % CO₂ or 1 % of N₂ to the hydrogen rich gas mixture while no shift of ZPL peak position of Si-V was observed. By the confocal PL setup we have measured about 10 000 Si-V centers in the focal spot. The comparison with monocrystalline diamond with ion implanted centers gives us

at least two orders of magnitude higher center intensity. This work was financially supported by the 14-04790S (GACR) project.

THU 18

Novel Functionalities in Electric Double Layer Transistors of CVD-grown Transition Metal Dichalcogenides

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Monolayer transition metal dichalcogenides have emerged as potential candidates for electronics and optoelectronics [1]. In particular, the combination of CVD-grown large-area samples and electric double layer transistors (EDLTs) leads to variety of functionalities due to extremely high carrier density accumulated at the electric double layer interface. In this paper, we fabricate EDLTs with various CVD-grown monolayers, such as MoS_2 , $MoSe_2$, WS_2 , and WSe_2 . As a result, we realized significant four functionalities of these devices, as shown in following list. (i) High mobility transistors and high-gain complementary inverters [2,3]. (ii) Highly flexible and fully stretchable transistors [4-6]. (iii) Novel light-emitting devices which can inject high current density at room temperature. (iv) Unique thermoelectric properties under continuous band filling.

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THU 19

Impact of differently long polyynes on the inner tube photoluminescence of double-walled carbon nanotubes

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Long linear carbon chains (lcc) can be grown inside the inner tubes of double-walled carbon nanotubes (DWCNT) by post-synthesis annealing of as-grown DWCNT in high vacuum. Growth yield and length distribution of the obtained polyynes depend sensitively on the growth temperature, with the longest chains being grown at 1460°C. The lcc alter the optical properties of the DWCNT: Photoluminescence (PL) of filled DWCNT is enhanced, depending on the inner tube diameter similar to the effect of filling SWCNT with ferrocene [1]. The optimum diameter for PL enhancement shifts towards smaller diameters when increasing the growth temperature which is linked to the thermal stability of long lcc. The physical process behind the

PL enhancement of the inner tube can be explained by a charge transfer between the excess charges located on the lcc ends and the nanotube. The amplitude of these excess charges varies with the lcc length which consequently leads to an optimum in the lcc length distribution for the PL emission intensity. We acknowledge the support of the FWF project P21333-N20.

[1] X. Liu et al., Adv. Funct. Mater., 22 (2012), 3202-3208

THU 20

Resist-free contacting and AFM nanolithography of graphene and transition metal dichalcogenides

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Contacting graphene and 2D layered transition metal dichalcogenides (TMDs) using conventional lithography techniques results in a poor quality device due to the difficulty in removing the resist after processing. The resist residue has an adverse effect on the electron mobility as well as further experimentation such as scanning tunnelling microscopy and atomic force microscope lithography (AFML). Here we present a shadow mask evaporation technique used to contact samples without a resist, resulting in a cleaner, better quality device. Shadow masks for 2, 3 and 4-terminal devices of various geometries were designed and made from thin Si wafers using deep reactive ion etching. The masks were used to fabricate devices for bulk and few layer graphene and TMDs, including MoS₂ and NbSe₂.

The absence of a resist residue allowed AFML to be performed on these devices to investigate local oxidation and hydrogenation. As in the literature, graphene was found to oxidise much more readily than to hydrogenate. Bulk MoS₂, previously unexplored in this area, behaved very differently from graphene, but the oxidation was still noticeably more reliable than the hydrogenation.

THU 21

Direct TEM observation on phase transition of aqueous solution sandwiched by graphene layers

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High-resolution transmission electron microscopy (HRTEM) provides real-time atomic-level structural information on nanomaterials. If HRTEM is applied to observation of liquids, nanostructures of liquids can directly be observed, which leads to a great impact on physical chemistry of liquids. One of the biggest problems for the realization of HRTEM observations of liquids is that samples have to be placed under a high vacuum condition, where almost all of liquids spontaneously vaporize. In our previous work, we have developed an HRTEM observation method of liquids, which incorporates encapsulation of liquids in graphene-sandwiched-type environmental cell. Using the graphene cell, we have found that water molecules encap-

sulated inside the graphene cell formed hexagonal ice at room temperature in high vacuum. In this work, we have applied the method to observe various solvents and solution of simple ions. We have observed the dynamics of various solutions by using graphene-sandwiched cell. At the graphene pockets, it can be seen the crystallization of solvent or hydrate salt. In this poster, details of sample preparation and results of TEM observations are addressed.

THU 22

A spectroscopic study of Ni clusters encapsulated in single-walled carbon nanotubes

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Investigating the electronic properties of metal clusters often poses several difficulties. To make their characteristics visible by spectroscopic methods environments are needed where clusters are protected from external influences.

Therefore, we filled ultra-clean SWCNT with Ni-acetylacetonate molecules and subsequently converted them to Ni clusters by high-temperature annealing where the cluster size is controlled directly by temperature and annealing time. X-ray absorption and (resonant) photoemission spectroscopy (RESPES) have been combined with X-ray diffraction and Raman analysis, where cluster sizes between 2 nm and 10 nm have been investigated. While higher annealing temperatures lead to formation of larger clusters it also reduces the Ni content in the SWCNT system. Smaller clusters show higher reactivity and therefore provide larger n-type doping to the SWCNT. RESPES shows the changes in the density of states of these Ni clusters, thereby providing insight into the effects caused by changing cluster size and doping.

In addition, this study provides another method to alter the properties of SWCNT in a precise and reproducible way.

We acknowledge funding by the FWF.

THU 23

Simultaneous, spatially-resolved optical and electrical measurements on mono- and few-layer MoS₂

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MoS₂ exhibits unique optical and electrical properties such as the transition from an indirect band gap to a direct band gap material for few and single layer nanosheets.

Due to their 2-dimensional structure paired with a direct band gap they are of great interest as a future material in solar cells. Despite recent success of using MoS₂ nanosheets in optoelectronic devices there is still a lack in the understanding of the interplay between the optical and electrical properties. Here, combined optical and electrical measurements can be helpful to further understand these interactions and improve future devices.

We present a novel method combining AFM and KPFM on one hand combined with scanning photocurrent and optical measurements on the other hand. Measurements were carried out simultaneously on single, free standing nanosheets as well as on contacted nanosheets. We investigate the effect of a local laser illumination on the charge state of individual nanosheets. Furthermore we correlate the local photocurrent with the local electronic properties as measured by scanning probe microscopy techniques.

THU 24

Orthogonal sorting of single-walled carbon nanotubes by ultracentrifugation

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The application of single-walled carbon nanotubes (SWCNTs) as source-drain channels in field-effect transistors requires semiconducting (sc) tubes with defined parameters. We present an orthogonal sorting method to separate SWCNTs according to electronic type and subsequently according to length by applying ultracentrifugation in a density medium. During the ultracentrifugation in a linear density gradient and in combination with different anionic surfactants, SWCNTs are sorted according to electronic type. We achieve an enrichment of sc-SWCNTs up to a content of 98% in two sorting steps. Afterwards these enriched sc-SWCNTs are separated according to length by performing ultracentrifugation without a density gradient. The challenge is to find appropriate anionic surfactants and conditions to combine successive the different sorting mechanisms. We use UV-Vis spectroscopy to measure the differences in the content of metallic and sc-SWCNTs between different samples and AFM to characterize the tube lengths.

THU 25**Covalent functionalization of single-walled carbon nanotubes with diazonium salts**

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Various routes of the covalent functionalization of SWCNTs were explored in the recent past. Diazonium cations react with nanotubes without previous activation by a radical chain mechanism, theoretically leading to a carbon species with an attached moiety and a positive charge. However, the latter has not been proven or investigated yet. We use analytical methods such as inert statistical raman spectroscopy and thermogravimetric analysis coupled with mass spectrometry and gas chromatography (TGA-MS or TGA-GC-MS) to examine the existence and the reactivity of these intermediately formed positively charged SWCNTs. These analytical methods are also used to characterize the products of further novel reaction pathways, like the reaction of brominated SWCNTs with nucleophiles and the reaction of potassium nanotubides with iodonium salts.

THU 26**Unraveling doping effects on SWNT light-absorption and emission by stationary and time-resolved spectroelectrochemistry**

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We have studied spectroelectrochemical properties of highly enriched semiconducting (6,5) single-wall carbon nanotubes (SWNTs) in organic suspensions using a home built setup. The experiment allows for quasi-simultaneous absorption and photoluminescence spectroscopy of SWNTs under potentiostatic control. We find that the absorption strength of the first and second excitonic transitions, as well as the photoluminescence intensity exhibit a strong but distinct dependence on the doping level. However, the overall oscillator strength in the VIS and NIR regions remains constant. The decrease of first and second subband exciton oscillator strengths is compensated by the development of new absorption features. Global analysis of our data identifies one of the features as a trion state, whereas a second feature appears to be due to light absorption by the well-screened free-carrier continuum.

Preliminary transient absorption measurements of SWNTs under potentiostatic control corroborate and complement the results from stationary absorption spectroscopy. Depending on the doping level we find a decreasing photobleach and vanishing photoabsorption signal in the first exciton subband range.

THU 27**Strong exciton-photon coupling in two-dimensional heterostructures**

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Monolayer films of transition metal dichalcogenides (TMDCs) are direct band gap semiconductors with large exciton binding energies and small Bohr radii, indicating great potential for development of novel optoelectronic devices. In this work we report strong exciton-photon coupling with these materials using a tunable open-access microcavity. TMDCs are embedded into the cavity via standard transfer methods of monolayer sheets of molybdenum diselenide (MoSe₂), placed on hexagonal boron nitride (hBN) at the planar DBR surface. A double quantum well (QW) heterostructure is produced by placing a second monolayer of MoSe₂, separated by 3nm thick hBN, on top of the first monolayer sheet. We observe a characteristic anticrossing between the tunable cavity mode resonances with the neutral exciton energy for the single and double QW showing a vacuum Rabi splitting of 20 meV and 29 meV respectively, displaying the expected dependence on the number of QWs. This work opens a new avenue in the field of polaritonics in a new material system of van der Waal crystals.

S. Dufferwiel et al. Appl. Phys. Lett., 104, 192107 (2014).

S. Schwarz et al. Nano Lett., 14, 7003 (2014).

THU 28**Bottom Surface States in Topological Insulators: AFM defined low-dimensional circuits**

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We optoelectronically investigate the bottom surface states in thin films of the topological insulator (Bi_{0.5}Sb_{0.5})₂Te₃ on SrTiO₃-substrates. In contrast to the top surfaces of the films, these buried topological states are encapsulated from environmental conditions. We introduce a dynamic plowing lithography based on an atomic force microscope to demonstrate that the bottom surface states are independent from the top surface morphology. We further verify a distinct optoelectronic response at the lateral edges of the circuits and in nano-plowed constrictions. We discuss photo-

thermoelectric currents in combination with potential fluctuations to explain the optoelectronic data.

THU 29

An interaction of lithium with fluorinated graphite via X-ray photoelectron and absorption spectroscopy

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To achieve the greatest efficiency of lithium batteries, it is necessary to get insight into the process of interaction of novel cathode materials with lithium. Here, we investigate the interaction of Li with originally fluorinated highly ordered pyrolytic graphite. The experiment was carried out in situ in perfect vacuum conditions for deeper understanding of the process. First time the breaking of the C-F bonds through LiF formation was directly observed in a process of Li penetration into the depth of fluorinated graphite by means of angle-resolved near-edge X-ray absorption spectroscopy (NEXAFS) of the C and F K-edge. Depth profiled information on elemental composition was derived by means of X-ray photoelectron spectroscopy (XPS) with different photon energies. During the Li intercalation into the material the layered structure is preserved, fluorinated carbon atoms with sp³ hybridization turn into the sp²-bonded ones and C-layers become conducting. We found also that the amount of the intercalated Li depends on the fluorine content. This result is important for finding the optimal composition of the fluorinated graphite as electrode material for primary lithium batteries.

THU 30

Effect of the close gold nanoparticles-carbon nanotubes proximity

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Recently, we have introduced a new class of nanohybrid systems obtained by encaging within the same micelle carbon nanotubes and gold nanoparticles to ensure their close proximity. The yielded hybrids exhibit enhancement of their linear and nonlinear optical response. Here we will show the effect of different coupling geometries onto the performances of the yielded hybrid systems; in particular, we will show the different approaches needed to couple the semiconducting carbon nanotubes with the near and the far field of the metallic particles.

THU 31**Fabrication of 2-D transition metal dichalcogenides using Atomic Layer Deposition**Akhil Sharma¹, N. Thissen¹, J.W. Weber¹, W.M.M. Kessels¹, A.A. Bol¹¹Dept. of Applied Physics, Eindhoven University of Technology, The Netherlands

Two-dimensional transition metal dichalcogenides (2D-TMDs) are an exciting class of new materials. Their ultrathin body, optical band gap and unusual spin and valley polarization physics make them very promising candidates for a vast new range of (opto-)electronic applications. So far, most experimental work on 2D-TMDs has been performed on mechanically exfoliated flakes made by the 'Scotch tape' technique. The major next challenge is the high quality and large-area synthesis of 2D-TMDs by a technique that ultimately can be used for commercial device fabrication.

In this contribution, a novel scalable process for the fabrication of 2D-TMDs using atomic layer deposition (ALD) has been explored. Ultra-thin films of HfO₂ and MoO₃ were deposited by ALD on SiO₂/Si substrates followed by thermal sulfurization at 1000°C. The formed nano-sheets were characterized by means of XPS, SEM, HRTEM, Raman spectroscopy and photoluminescence spectroscopy.

THU 32**Confined linear carbon chains: A route to bulk carbyne**Lei Shi¹, Philip Rohringer¹, Kazu Suenaga², Yoshiko Niimi², Jani Kotakoski¹, Jannik C. Meyer¹, Herwig Peterlik¹, Marius Wanko³, Seymour Cahangirov³, Angel Rubio^{3,4}, Kazuhiro Yanagi⁵, Paola Ayala¹, Thomas Pichler¹¹University of Vienna, Faculty of Physics, Strudlhofgasse 4, A-1090 Vienna, Austria²AIST, Nanotube Research Center, Tsukuba 305-8562, Japan³Nano-Bio Spectroscopy Group & European Theoretical Spectroscopy Facility (ETSF), Universidad del País Vasco, CFM CSIC-UPV/EHU-MPC & DIPC, 20018 San Sebastian, Spain⁴Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany⁵Department of Physics, Tokyo Metropolitan University, 1-1 Minami-Osawa, Hachioji, Tokyo 192-0397, Japan

The extreme instability and strong chemical activity of carbyne, the infinite sp¹ hybridized carbon chain, are responsible for its low possibility to survive at ambient conditions. We successfully synthesized extremely long linear carbon chains inside thin double walled carbon nanotubes (as nanoreactor and protector). Their existence, structure, lengths and yield have been proved by Raman, HRTEM, STEM and XRD. The results show that the single-triple bonded LLCCs including hundreds of carbon atoms have at least six new Raman lines, some of which are even stronger than the G-band. The optimum growth conditions, for example, diameter of the host tubes, annealing temperatures and time were carefully studied. The interaction and charge transfer between the LLCCs and their host nanotubes were explored using resonance

Raman, low-temperature Raman and also DFT calculations. Extracting the LLCCs from the nanotubes was done by density gradient ultracentrifugation method, and the separated solutions were measured by Raman and absorption spectroscopies.

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THU 33

Reduced graphene oxide/polyaniline composites for energy storage devices

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Reduced graphene oxide/polyaniline (rGO/PANI) composites were prepared by simply mixing the dispersions of graphene oxide (GO) and polyaniline (PANI), followed by in situ chemical reduction of GO. Here we report the morphological and spectroscopic characterizations of the rGO/PANI composites, and their electrochemical performance. The obtained results are promising for development of energy storage devices such as batteries and supercapacitors. Optical images combined with atomic force microscopy and Raman spectroscopy clearly show that GO nanosheets are uniformly dispersed in the composite matrix. This can be associated to the good stability of the individual components and the electrostatic interaction (positively charged polymer chains and negatively charged GO nanosheets). Raman spectra show an increase of the relative intensity of the D band, which confirms the in situ reduction of GO in the composite. Moreover, they confirm that PANI remains doped in the rGO/PANI composite. Electrochemical performances of the composites are being assessed by cyclic voltammetry and galvanostatic charge/discharge cycles, and will be correlated to their structural and morphological aspects.

THU 34

Optically detected magnetic resonance in single-wall carbon nanotubes

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Understanding the photophysics of SWCNTs is important for potential applications in light-harvesting and light-generation. Excited states of SWCNTs are known to form bound electron-hole pairs, excitons. Only excitons with a singlet spin state can be excited optically but they can form triplet excitons with a low probability in a process known as intersystem crossing. The triplet excitons decay to the ground state with a long relaxation time as the spin conservation is again violated in this process. Understanding the details of the singlet-triplet excited state energy levels and the excitation and decay dynamics is of great importance for the potential applications. We present optically detected magnetic resonance (ODMR) on SWCNTs at 77 K

and 9 GHz. We developed a unique ODMR spectrometer for this: light source is a tunable laser, detection is in the NIR in a spectrally resolved manner. Usual ODMR instruments operate in the visible range with a single laser source and without spectral resolution of the emitted light. We identify light emission from the triplet states and determine the triplet binding energy.

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THU 35

Raman spectrum of two-dimensional silica glass on graphene

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A two-dimensional (2D) silica glass was synthesized on top of graphene during the CVD process. With help of atomic-resolution transmission electron microscopy, the 2D nature of the new structure is visualized in its amorphous as well as crystalline forms with the crystalline lattice constant 5.3 Å, roughly 2.14 times that of graphene and it was identified as a bilayer of SiO₂. Ab-initio calculations indicate that van der Waals interaction with graphene energetically favors the 2D structure against the bulk SiO₂. Raman spectrum acquired from 2D silica glass shows a specific very narrow peak at 1050 cm⁻¹. The calculation of the phonon spectrum indicates that the mode at 1050 cm⁻¹ originates from antisymmetric stretching displacements. These results demonstrate a new class of 2D structures that, in principle, can be produced and applied in layered graphene devices.

THU 36

Calculating core level binding energies for graphene and azafullerenes

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X-ray photoelectron spectroscopy (XPS) combined with first principles modeling is a powerful tool for determining the chemical composition of novel materials. We have calculated the carbon 1s core level binding energy of pristine graphene [1] using two methods based on density functional theory total energy differences: a delta Kohn-Sham calculation with a frozen core-hole (KS) [2], and a novel all-electron extension of the delta self-consistent field (SCF) method. Although the binding energy depends on the chosen exchange correlation functional, using the Perdew-Burke-Ernzerhof functional we find a value remarkably close to what has been measured for graphite. As a first application, we have analyzed XPS measurements of free-standing powders of C₆₀ and C₅₉N fullerenes using such core-level calculations [3]. This has allowed us to propose a model for oxygen impurities and to quantify the effect of C₅₉N dimerization on its N 1s core-level shift (-0.4 eV), with implications for interpreting measurements of other nitrogen-doped systems.

[1] T. Susi et al., arxiv:1411.3874 (2014)

[2] T. Susi et al., doi:10.3762/bjnano.5.12

[3] D. Erbahar, T. Susi et al., submitted

THU 37

Generating photocurrent by nanocomposites based on photosynthetic reaction center protein

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There is a large interest these days in binding photosynthetic proteins purified from plants (PS-I and PS-II) and from purple bacteria to nanostructures while their functional activity is largely retained. Current researches are focussing on finding the best bio-nanocomposite sample preparations and experimental conditions for efficient energy conversion and for the stability of the systems. Photosynthetic reaction center protein (RC) purified from purple bacterium *Rhodobacter sphaeroides* was bound successfully to functionalized multiwalled carbon nanotubes (MWCNTs) then this complex was immobilized onto the surface of indium tin oxide (ITO) by using specific silane crosslinker and conducting polymer. Structural and functional measurements have shown that RCs were bound effectively to the functionalized carbon nanotubes. The complex has high stability and generates photocurrent in wet and

dried condition as well. Several hundreds of nA photocurrent was measured with fully active RCs when the RC turnover was reconstituted by the electron acceptor quinones. The study of possibility for generating photocurrent in organic solar cell based on RC protein is also under process.

THU 38

Structure of graphene oxide membranes in solvents and solutions.

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Structural modification of graphite/graphene oxide (GO) under conditions of hydration/solvation is the key parameter for understanding of GO membrane permeation and filtration properties. It is believed that solvent and solute molecules travel through the network of interlayers between graphene oxide sheets of GO membranes in process of permeation. In situ synchrotron X-ray diffraction study demonstrated that GO membranes exhibit expansion (swelling) swelling properties which are distinctly different compared to precursor graphite oxide powder samples. Intercalation of several liquid solvents into GO membrane structure occurs with maximum one monolayer insertion (Type I), in contrast with insertion of 2-3 layers of these solvents into graphite oxide structure. However, examples of GO membrane structure expansion similar to precursor graphite oxide are also found (Type II). It can be anticipated that Type II solvents will permeate GO membranes significantly faster compared to Type I solvents. It is found that inter-layer distance of GO structure can be modified in a broad range of values up to several nanometers due to intercalation and chemical modification of the membranes.

THU 39

Separation of Metal and Semiconducting Single-Wall Carbon Nanotubes using Automatic Gradient Elution-Gel Filtration

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Single-wall carbon nanotubes (SWCNT) are excellent materials for electronic devices. However, due to the varying properties from metallic (m-SWCNT) to semiconductor (s-SWCNT), conventional as-grown SWCNT have limited uses for electronic devices. Obtaining single type of either m-SWCNT or s-SWCNT therefore is essential to optimally utilize SWCNT as electronic device materials.

Our work focused on separation of m-SWCNT and s-SWCNT by a simple gel filtration. For elution of SWCNT, we chose two surfactants as eluent: sodium dodecyl sulfate (SDS) and sodium cholate (SC). Metallic SWCNT are collected during first elution with SDS solution while semiconductor SWCNT are collected during second elution with SC solution. Fractionation during SC elution helps improving the pu-

urity of the collected s-SWCNT. Finally, we developed an automatic gradient elution (AGE) system which change the eluent composition from SDS to SC over time. By utilizing AGE system, further purity improvement of s-SWCNT is obtained. Furthermore, diameter-based separation and length-based separation of SWCNT have also been achieved simultaneously by the optimized AGE system.

THU 40

Carbon nanotube thin films from liquid crystal phase polyelectrolytes

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Thin films of carbon nanotubes have been widely reported and the potential applications of such films are numerous and varied. However the commonly used preparation methods of spray deposition or vacuum filtration from surfactant stabilised suspensions produce either sparse 'spiderwebs' with poor homogeneity and large void spaces on the nanoscale, or extremely rough and opaque films. As well, the extended ultrasonication required invariably shortens the nanotubes and introduces defects into the sidewalls which irreparably alters the electronic and optical properties of the pristine material. An area of recent research interest in the nanotube community is in the production of thin films in which the nanotubes are very highly aligned in one direction parallel to the surface and it is expected that such films will exhibit much improved properties compared to their randomly aligned counterparts. A new method to fabricate such films will be presented, based on the deposition of nanotubes from polyelectrolyte inks having a liquid crystal phase, and measurements of the films and from some devices which use them will clearly demonstrate their superiority.

THU 41

Synthesis and characterization of TiO₂/C nano-materials: Applications in water treatment

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The TiO₂ deposition on high surface possessing supports can increase the photocatalytic efficiency of the semiconductor. This effect has been resulted the high adsorption capacity of the support which can help to enrich organic substrate around the catalyst, promoting the charge transfer process between the pollutants and the photocatalysts. In this study the synthesis of TiO₂-carbon composite photocatalytic materials have been investigated. Titanium tetrachloride (TiCl₄) was used as the precursor, while graphite, activated carbon and carbon aerogels were chosen as carbon supports. These have different surface properties and various surface textures, thus obviously can lead to distinct photocatalytic performances. An optimization of the synthesis method was proposed by varying the molar ratio titanium / carbon (Ti/C). The obtained materials were characterized by XRD and DRS. The specific surface area, pore volume and pore size distribution were evaluated by nitrogen adsorption/desorption. The photocatalytic activity was investigated by the photodegradation of Diuron which was a model pollutant.

THU 42

Raman analysis of strain in ¹²C graphene/fullerenes/¹³C graphene system

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Strain engineering has been proposed as a powerful technique for modifying the electronic properties of graphene [1]. It has been shown recently that strain and doping in graphene cause different shift of G and 2D Raman bands [2]. Therefore it is possible to separate both effects by a correlation analysis of G and 2D positions.

In our work we sandwiched fullerenes in between two layers of graphene in order to induce strain in graphene. Isotope labelling [3] was used to distinguish the top and the bottom graphene layers in the measured Raman spectra. We analysed the Raman maps of isotopically labelled graphene-fullerene sandwiches and estimated the effect of the fullerenes on graphene layers. The results were compared to the AFM images of the surface topography.

(1) S.-M. Choi, S.-H. Jhi, Y.-W. Son, Effects of strain on electronic properties of graphene, Phys. Rev. B. 81 (2010) 081407.

(2) J.E. Lee, G. Ahn, J. Shim, Y.S. Lee, S. Ryu, Optical separation of mechanical strain from charge doping in graphene., Nat. Commun. 3 (2012) 1024.

(3) O. Frank, L. Kavan, M. Kalbac, Carbon isotope labelling in graphene research, Nanoscale 6 (2014) 6363.

THU 43**Quartz crystal microbalance gas sensor with nanocrystalline diamond sensitive layer**

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In this contribution we present a gas sensor for ammonia (NH₃) detection at room temperature. The sensor is based on a bulk acoustic quartz crystal microbalance (QCM) piezoelectric device coated with nanocrystalline diamond (NCD) as a sensitive layer. Diamond film was directly grown on the QCM by pulsed linear antenna MWCVD process from the H₂/CH₄/CO₂ gas mixture at the deposition temperature lower than 400 °C. The QCM coated with the NCD showed a twofold increase in the frequency shift compared to virgin QCM sensor for the NH₃ gas detection. The frequency shift for 50 ppm NH₃ at room temperature was about 10 Hz. Due to the NCD large surface area the response time was very fast (5 s). Further, it was found that the response and recovery times were varied with the NH₃ concentration (10 and 50 ppm) as well as for different detection/purging times. Moreover, the sensor showed a good selectivity to NH₃ gas over CO₂ (2500 ppm) and promising response for the relative humidity detection at room temperature. In summary, such QCM/NCD platform provides a promising gas sensor with good response, reasonable selectivity, high stability and promising repeatability at room temperature.

THU 44**Wet Chemical Exfoliation of Graphene: The Solvent Effect**

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The covalent functionalization of graphene represents a main topic in the growing field of nano materials. Since the pioneering work of Pénicaud and Drummond, graphite intercalation compounds (GICs) have been exploited as highly activated species for a subsequent covalent functionalization of the individualized carbon layers. Intercalation of alkali metals in graphite has shown to be a controllable procedure which can be monitored in situ by Raman spectroscopy. For the exfoliation of high quality graphene, absolute and inert solvents are required for a defect-free stabilization of the intermediately charged layers.

Under high vacuum conditions, stage 1 GICs were exposed to various common solvents via vapor pressure control. In order to observe the interaction of the inter-

calation compound, four common solvents were investigated: 1,2 dimethoxyethane, tetrahydrofurane, dimethyl sulfoxide and acetonitrile. Applying in situ Raman spectroscopy to the air sensitive ternary system GIC-solvent, a detailed study of these solvents let us conclude about the quality of each solvent by the spectroscopic signatures in situ prior to the exposure to air.

THU 45

Low temperature induced uniaxial and biaxial strain in CVD grown monolayer graphene

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Using strain engineering, the range of remarkable properties of graphene can be further extended. To observe these predictions experimentally, a well-defined strain direction and a rather large magnitude of the strain is needed, which are not straightforward to realize.

Different thermal expansion coefficients of graphene and its supporting substrate result in the introduction of strain when heating or cooling the sample. Although a relatively large strain is needed to observe changes in the band structure of graphene, it is important to understand the type and magnitude of the strain which is induced in graphene due to thermal cycling.

Here, we study how strain is induced in CVD grown graphene, transferred on a Si/SiO₂ substrate, by varying the temperature between 300 K and 4 K. As Raman spectral mapping is used, we follow an area on the CVD grown graphene sheet where growth induced ripples are clearly present. In this way, we can follow how graphene and the ripples behave when the temperature is varied. Using the correlation analysis, we clearly see a difference between the uniaxial strain in the ripples and biaxial strain in graphene.

THU 46**Large-scale multiplex functionalization of graphene using dip-pen nanolithography**

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¹School of Materials, University of Manchester, Manchester

²Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Karlsruhe, Germany

The application of graphene for sensors relies on engineering selectivity and sensitivity through chemical modification of graphene. Non-covalent chemical modification allows efficient charge-transfer interaction between molecules and graphene as well as not significantly disturbing the electronic structure of graphene. Recently, we have shown that dip-pen nanolithography (DPN) can be used to pattern self-assembled phospholipid membranes on graphene, which mimic biological membranes.[1]

Here we present further developments to this work. Firstly, we demonstrate how single-pen DPN can be scaled up to multi-pen DPN, where a 1-dimensional array of cantilevers can be used to simultaneously write arrays of lipid patches on graphene. Each probe can carry a different lipid mixture, allowing multiplex functionalization. This can then be extended to simultaneous writing over a 2-d surface using a 2-d array of polymer probes, using a technique called polymer-pen nanolithography (PPN).

Secondly we demonstrate how proteins can be incorporated into the graphene supported biomimetic membranes for biosensing applications.

1. Hirtz, M.; et al; Nature Communications, 2013, 4, 2591

THU 47**Bottom-up assembly of 2-dimensional materials devices**

Antonios Oikonomou¹, Aravind Vijayaraghavan¹

¹School of Materials, The University of Manchester, Manchester

We have previously demonstrated that dielectrophoresis (DEP) can be used to assemble carbon nanotubes and graphene into large-scale integrated device arrays. This approach is compatible with sorted materials such as single-chirality SWCNTs, resulting in single-chirality device arrays. Such devices are ideal for certain applications like sensor arrays. In this work, we extend this approach to a variety of other 2-dimensional materials. 2-d materials can be produced by ultrasonic exfoliation in a variety of solvents including water and NMP. We show that MoS₂, WS₂, MoTe₂, MoSe₂ and phosphorene can be assembled from their respective dispersions into functional devices using bottom-up DEP. The assembly of individual flakes can be confirmed by scanning electron microscopy with EDX, scanning probe microscopy and Raman spectroscopy measurements. As previously observed with graphene, we obtain predominantly few-layer devices due to the nature of the starting dispersions which contain a majority of few-layer flakes. The devices are shown to be functional

using electronic transport measurements and compared to devices produced by other methods.

THU 48

Nanostructures of Bismuth Chalcogenide Topological Insulators: A Computational Study

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Surface states of three-dimensional Z_2 topological insulators (TIs), such as the layered bismuth chalcogenides Bi_2Se_3 and Bi_2Te_3 , are defined by a Dirac cone band dispersion with a helical spin texture. Low-dimensional nanostructures of TIs represent a promising avenue for exploring and harnessing the topological protection of these surface states due to the increased surface-to-volume ratio. Aside from the much explored low energy (0001) surface, bismuth chalcogenide nanostructures possess other higher energy facets. A systematic ab initio investigation of these facets was performed. Calculations find several stable surfaces and, depending on the chemical potential value, allow the prediction of conditions favouring nanoplate and nanowire morphologies. Surface orientation is found to significantly affect the band dispersion and spin polarization of the topological surface states. Furthermore, 1D nanowires and nanoribbons of Bi_2Se_3 were constructed and investigated using a tight-binding model. The band dispersion and spin texture of the surface states, stemming from their circumferential confinement in 1D nanostructures, is discussed.

THU 49

Electrochemical Degradation of Legal and Illegal Drugs in Waste Water by Boron Doped Diamond Electrode

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Water is a crucial resource for human beings and the environment. Conventional waste water treatment plants cannot degrade the majority of new types of pollu-

tants. Hence the powerful methods for the decontamination of drugs, psychoactive substances and antibiotics waste have received increasing attention over the past decade. The Boron doped diamond (BDD) anode is the best electrode with low adsorption properties, remarkable corrosion stability even in strongly acidic media and extremely high O₂ evolution overvoltage. In this study, we investigate the application of polycrystalline BDD thin films in the field of water micropollutants degradation. Extreme effective degradation process of the most "popular" legal and illegal drugs in water (Methamphetamine, Cocaine, Cotinine, Tramadol, Diclofenac, etc.) is presented. We compare the efficiency of BDD and Fenton system degradation techniques analyzed by LC-MS/MS in waste water from the input of a sewage treatment plant on Danube River in Bratislava.

This work was financially supported by the grants of No. 1/0785/14, Slovak Research and Development Agency under the contract No. APVV-0365-12.

THU 50

Nanostructured boron doped diamond films for detection of erythromycin in water samples

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Nowadays, many studies are focusing on various pollutants emerging in the environment, including in waste-waters and in drinking water, whose presence is continuously increasing. These pollutants include different chemical species such as drugs, personal care products, endocrine disruptors and many other chemicals that are used daily worldwide. Risk assessment of these chemicals and of new products in the environment requires a comprehensive understanding of their degradation behavior and persistence, respectively, which is becoming a field of increasing interest. It is known that the important degradation paths of xenobiotics in the environment usually involve a redox reaction mechanism. In our experimental work we were concerned with optimization of electrochemical conditions for analysis of erythromycin in water samples. We used square wave voltammetry (SW) for analysis. Our BDD electrodes provided oxidation peak at potential 0.87 V at trace concentration level (umol/L). Commercial glassy carbon paste electrode provided no signal in this concentration range.

This work was financially supported by the grant of the Slovak Research and Development Agency (APVV-0365-12).

THU 51**Highly conductive carbon nanotube fibers**

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Carbon nanotubes (CNTs) exhibit metallic or semiconducting properties, depending on their chirality and diameter. In generally, the electrical conductivity of the macroscopic fibers without doping is only 103~105 S/m, which is 2-4 order in magnitude lower than that of the individual tubes. Here, we demonstrate our recent advance in preparing highly conductive CNT fibers from controlling growth of metallic CNTs to making near ideal fibers. We first prepare CNT fibers with conductivity higher than stainless steel from macroscopic and semiconducting-rich CNT films by using industrial wire-drawing method. The curving CNT bundles are straightened and aligned along the fiber axis under tension, which reduce inter-tube contact resistance and cross-sectional area of the fibers. The fiber has an electrical conductivity of 1.5×10^6 S/m which is one fold higher than that of the fibers without drawing. By controlling the catalyst and gas, we can increase the content of metallic CNTs in the samples. The metallic-rich CNT fibers have electrical conductivity above 6×10^6 S/m. The highly conductive CNT fibers have great potential applications in replacing copper wires in the future.

THU 52**In situ Study of Metal Induced Crystallization Processes for Low-Dimensional Materials Synthesis**

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Metal induced crystallization (MIC) is a promising technique for 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. However this technique lacks depth resolution and is therefore unable to track diffusion and layer exchange.

Here, the Si/Ag and C/Ni bilayer systems are studied. The samples are annealed at temperatures of up to 750 °C. Simultaneously, depth profiles of the elements are investigated by in situ Rutherford backscattering spectroscopy revealing the diffusion kinetics. The changes in the phase structure are explored by in situ Raman spectroscopy. Both the quick initial nucleation and ensuing growth processes are in-

vestigated. Scanning electron microscopy provides insight to the surface morphology.

THU 53

Catalyst-free growth of nanographene on oxides by various CVD methods

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Since its first isolation by mechanical exfoliation, graphene has been attracting broad interest due to its outstanding physical properties.[1] In recent years, great progress has been made on catalyzed CVD growth of graphene.[2] To make use of this kind of graphene, the important issue is that a transfer process is needed, which dramatically degrades graphene.[3] Therefore, there is an increasing demand to growth graphene on dielectric substrates - normally oxides such as SiO₂, especially under a low temperature by remote plasma CVD. [4, 5]

In this study, we demonstrate the growth of nanographene on oxides by various CVD methods including thermal CVD (quartz tube style furnace), modified microwave-plasma assisted CVD and modified DC-plasma assisted CVD. These successful approaches also promote our understanding of the catalyst-free growth mechanism of nanographene.

[1] Geim, A. K, Novoselov, K. S. Nat. Mater. (6) 2007, 183.

[2] Bae, S., et al. Nat. Nanotechnol. (5) 2010, 574.

[3] Li, X., et al. Nano Lett. (9) 2009, 4359.

[4] Zhang, L. C., et al. Nano Res. (4) 2011, 315.

[5] Kim, Y. S., et al. Nanoscale (6) 2014, 10100.

THU 54

Fabrication of Thermoelectric Devices using Precisely Fermi Level Tuned Single Wall Carbon Nanotubes by Electric Double Layer Carrier Injections

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¹Department of Physics, Tokyo Metropolitan University, Tokyo

Thermoelectrics are a very important technology for efficiently converting waste heat into electric power. Hicks and Dresselhaus proposed two important approaches to innovate the performance of thermoelectric devices. One approach involves using low-dimensional materials, and the other approach involves properly tuning the Fermi level because the Seebeck coefficient strongly depends on the Fermi Level. Here we report across-bandgap p-type and n-type control over the Seebeck coefficients of semiconducting single wall carbon nanotube (SWCNT) networks through an electric double layer transistor setup using an ionic liquid as the electrolyte. All-around gating characteristics by electric double layer formation upon the surface of the nanotubes enabled the tuning of the Seebeck coefficient of the nanotube networks by the shift in gate voltage, opening the path to Fermi-level-controlled three dimensional thermoelectric devices composed of one-dimensional nanomaterials. Moreover, by

freezing the motion of the ionic liquids, we fabricated thermoelectric devices using the precisely p-type and n-type tuned semiconducting SWCNTs.

Reference: Yanagi et al., Nano Lett. 14, 6437 (2014)

THU 55

Magneto transport properties of three-dimensional flexible and conductive interconnected graphene networks

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In this work we present the study of magneto-transport properties of the three-dimensional flexible and conductive interconnected graphene networks. The magnetoresistance (MR) as a function of applied magnetic field was measured in different configurations: a) magnetic field being perpendicular to both the foam plane and the current; b) magnetic field being parallel to the foam plane and the current; and c) magnetic field being perpendicular to the current, but angle between the magnetic field and normal direction of the foam plane being changed. As large as 300 percent of magnetoresistance was observed in two both configurations of (a) and (b). More importantly, the observed MR is not only very large, but also nearly temperature independent over the whole temperature range. This characteristic of the MR qualifies the graphene foam as a potential material candidate for the field sensors operating in both wide temperature range and with magnetic field range. Another very interesting observation is that an anisotropic MR was observed in the third configuration, which was not expected for three dimensional nature of the material.

THU 56

Few-layer-thin Two-dimensional Metallic Niobium Disulfide Nanosheets: Preparation, Optical Characterization and Transport Properties

Sihan Zhao¹, Takato Hotta¹, Takumi Sawazaki¹, Mitsuhiro Okada¹, Hisanori Shinohara¹, Ryo Kitaura¹

¹Department of Chemistry, Nagoya University, Nagoya

The semiconducting two-dimensional (2D) transition-metal dichalcogenides (TMDs), such as MoS₂, WS₂ etc., have recently been studied intensively, however, research work on 2D metallic TMDs, such as NbS₂, NbSe₂ etc., which show superconductivity and charge-density-wave (CDW) states in bulk, has been limited. In this contribution, we report a direct chemical vapor deposition (CVD) growth of ultra-thin 3R-NbS₂ nanosheets down to 3 layers on the exfoliated hexagonal boron nitride (hBN) flakes. AFM data show that most of NbS₂ samples grown are very thin with an average lateral size of ca. 2~3 μm . Detailed Raman spectroscopy studies on layer number-identified NbS₂ samples reveal a systematic shift of out-of-plane vibration mode (A_{1g}), which offers a reliable and rapid optical method for layer number identification. Two-terminal devices on thin-layered NbS₂ were also fabricated and show

a metallic transport behavior as predicted by DFT calculations. The metallic nature of thin-layered NbS₂ has also been supported by absence of PL peaks regardless of number of layers. Exploration of 2D superconductivity and CDW states in this system is an on-going work.

- 08:30 – 09:00 **F. Mauri, Paris**
Superconductivity in flatland: universal enhancement in 2D semiconductors at low doping
- 09:00 – 09:30 **J. Hoffman, Cambridge**
High T_c superconductivity in a single atomic layer of FeSe
- 09:30 – 10:00 **B. Beschoten, Aachen**
Nanosecond spin lifetimes in graphene-based spin-valves at room temperature
- 10:00 – 10:30 **coffee break**
- 10:30 – 11:00 **J. Fabian, Regensburg**
Spin phenomena in graphene materials
- 11:00 – 11:30 **B. Özyilmaz, Singapore**
Transport Studies in Black Phosphorus Field Effect Transistors
- 11:30 – 12:00 **R. Martel, Montréal**
Photo-Oxidation Promoted by Electronic Confinement in Exfoliated Black Phosphorus
- 12:00 – 17:00 **mini workshops**
- 17:00 – 17:30 **F. Kreupl, München**
High Performance X-ray Transmission Windows Based on Graphenic Carbon
- 17:30 – 18:00 **S. Garaj, Singapore**
Ion selectivity and water flow in graphene-derived membranes
- 18:00 – 18:30 **C. Stampfer, Aachen**
IWEPNM 2015 Conference Summary
- 18:30 – 20:00 **break**
- 20:00 **Bauernbuffet – Farewell**

08:30**Superconductivity in flatland: universal enhancement in 2D semiconductors at low doping**Francesco Mauri¹, Matteo Calandra¹, Paolo Zocante¹¹Universite Pierre et Marie Curie / CNRS, paris

The occurrence of superconductivity has been reported in several two-dimensional (2D) semiconductors, such as transition metal dichalcogenides or cloronitrides (ZrNCl, HfNCl). In these systems, a metallic state can be achieved and controlled by intercalation or by gating in a field-effect transistors. Unexpectedly, in the layer compound LixZrNCl, the superconducting transition temperature (T_c) increases by decreasing the doping (x), reaching a maximum of 15 K at the metal-insulator transition. In 2D multivalley semiconductors, at low doping, the electron-electron interaction enhances the response to any perturbation inducing a valley polarization. If the valley polarization is due to the electron-phonon coupling, the electron-electron interaction results in an enhancement of the superconducting critical temperature. By performing first principles calculations beyond DFT, we prove that this effect accounts for the unconventional doping-dependence of T_c and of the magnetic susceptibility measured in LixZrNCl. Finally we discuss what are the conditions for a maximal T_c enhancement in weakly doped 2-dimensional semiconductors.

Work to be published in PRL, arxiv:1408.6502

09:00**High T_c superconductivity in a single atomic layer of FeSe**Jennifer Hoffman¹¹Physics, Harvard University, Cambridge

The remarkable discovery of superconductivity above 100 K in a single atomic layer of FeSe (compared to the relatively mundane $T_c = 8$ K in bulk FeSe) prompts tremendous excitement and numerous pressing questions. What is the mechanism of the order-of-magnitude T_c enhancement in FeSe? What is the pairing symmetry? Could FeSe be a topological superconductor? What applications might one envision with such a 2D superconductor? I will review current experimental progress towards addressing these questions, then discuss our own growth (via molecular beam epitaxy) and imaging (via scanning tunneling microscopy) of single layer FeSe. We use quasi-particle interference imaging to access the band structure of filled and empty states, and to explore the pairing symmetry.

09:30**Nanosecond spin lifetimes in graphene-based spin-valves at room temperature**Bernd Beschoten¹¹2nd Institute of Physics, RWTH Aachen University, Aachen, Germany

By successive oxygen treatments of graphene nonlocal spin-valve devices we achieve a gradual increase of the contact-resistance–area products $R_c A$ of Co/MgO spin injection and detection electrodes. With this manipulation of the contacts, the spin lifetime can be increased by a factor of seven in the same device reaching values larger than 1 ns at 300 K. This demonstrates that contact-induced spin dephasing is the bottleneck for spin transport in devices with small $R_c A$ values [1].

Spin transport properties can further be enhanced by improving both the electrode-to-graphene and graphene-to-substrate interface. In these devices, Co/MgO spin injection electrodes are first fabricated onto $\text{Si}^{++}/\text{SiO}_2$. Thereafter, a graphene–hBN heterostructure is mechanically transferred onto these prepatterned electrodes. Room temperature spin transport in single-, bi-, and trilayer graphene devices exhibit spin lifetimes of several ns with spin diffusion lengths reaching $10\mu\text{m}$ combined with carrier mobilities exceeding $20,000\text{ cm}^2/(\text{V s})$ [2].

[1] F. Volmer et al., Phys. Rev. B 88, 161405(R) (2013).

[2] M. Drögeler et al., Nano Lett. 14, 6050 (2014).

10:30**Spin phenomena in graphene materials**Jaroslav Fabian¹¹Physics, University of Regensburg, Regensburg

Intrinsic spin-orbit coupling in graphene is relatively weak, some tens of micro eVs. On one hand, this is nice, as the projected intrinsic spin relaxation is also slow, on the order of microseconds. On the other hand, a greater value for the spin-orbit interaction is desired for spin manipulation and spin-orbit induced phenomena, such as the (quantum) spin Hall effect. In this talk I will review basics of the spin-orbit physics in graphene and show how to effectively increase the value of the spin-orbit interaction by adding adatoms. Examples will be hydrogen, fluorine, and copper adatoms. I will present first-principles results as well as phenomenological model Hamiltonians which are useful to study model spin transport and spin relaxation. I will also discuss the spin relaxation problem in graphene: experiments get the spin relaxation times of 100 ps, orders of magnitude below what is theoretically expected. The cause appears to be extrinsic, due to impurities. I will argue that the mechanism is resonant scattering by a small concentration of magnetic moments (wherever they come from). I will also present graphene-TMC heterolayers as promising systems for spin optoelectronics

11:00**Transport Studies in Black Phosphorus Field Effect Transistors**Barbaros Özyilmaz^{1,2}¹Physics, National University of Singapore, Singapore 117546²Centre for Advanced 2D Materials, National University of Singapore, Singapore 117546

Unlike graphene, Ultrathin black phosphorus (BP), is a semiconductor with a sizeable band gap that allows both high carrier mobility and large on/off ratios. Its excellent electronic properties make it attractive for applications in transistor, logic, and optoelectronic devices. However, it is also the first widely investigated two dimensional electronic material to undergo degradation upon exposure to ambient air. Therefore a passivation method is required to study the intrinsic material properties, understand how oxidation affects the physical transport properties and to enable future application of phosphorene. I will show that atomically thin graphene and hexagonal boron nitride crystals can be used for passivation of ultrathin black phosphorus. I will also discuss experiments where we characterize few-layer black phosphorus field effect transistors on hexagonal boron nitride (BN) and compare with results obtained with BP fully encapsulated with BN.

11:30**Photo-Oxidation Promoted by Electronic Confinement in Exfoliated Black Phosphorus**

Alexandre Favron¹, Etienne Gaufres^{1,3}, Anne-Laurence Phaneuf², Frederic Fossard³, Pierre Levesque¹, Annick Loiseau³, Richard Leonelli¹, Sebastien Fracoeur², Richard Martel¹

¹Université de Montréal, Montréal, Canada

²École Polytechnique, Montréal, Canada

³Laboratoire d'Etude des Microstructures, UMR 104 CNRS-Onera, Châtillon, France

Exfoliated Black phosphorus (P(black)), a lamellar crystal of P atoms that can be exfoliated down to few layer 2D-phosphane (also called phosphorene), has recently been highlighted for their 2D semiconducting properties, such as tunable bandgap with thickness and high carrier mobility. Device fabrication with mono- and bi- and other multi-layer 2D-phosphane has however been challenging due to a ubiquitous degradation of the layer in air. Here we report on results on this chemistry, which was investigated using in-situ Raman and TEM-EELS. A photo-oxidation initiated by charge transfer to adsorbed oxygen in water is found to be at the origin of the degradation. The oxidation rate is thickness dependent and increases with photon flux and oxygen concentration. Finally, different ways to prevent degradation were used to acquire Raman measurements on mono-, bi- and other multilayer 2D-phosphane in their pristine states. These results as well as signatures of degradation in Raman were determined and they will be discussed here using symmetry analysis. A trend in the intensity ratio of A1g and A2g Raman modes emerges from our data as a useful parameter to assess the oxidation level.

17:00**High Performance X-ray Transmission Windows Based on Graphenic Carbon**Sebastian Huebner¹, Natsuki Miyakawa², Andreas Pahlke², Franz Kreupl¹¹Institute of Hybrid Electronic Systems, Technische Universität München, Arcistr. 21, 80333 Munich, Germany²Ketek GmbH, Hofer Str. 3, 81737 Munich, Germany

A novel x-ray transmission window based on graphenic carbon (GC) has been developed and integrated into a silicon drift detector (SDD) with much better performance than beryllium transmission windows that are currently used in the field [1]. GC integrated on a silicon frame allows for a 7 mm wide window which does not use a mechanical support grid or additional light blocking layers. Compared to beryllium, the novel GC window exhibits an improved x-ray transmission in the important low energy region (0.1 keV - 3 keV) enabling the detection of C and F while demonstrating excellent mechanical stability, as well as light and vacuum tightness. Be-windows with an opening diameter of 7 mm are specified to withstand a differential pressure of 2 bar. The GC window with a thickness of 1 micrometer exceed this requirement. Pressure cycle fatigue for Be-windows is specified to $\sim 20k$ cycles, while GC has already demonstrated more than 4 million pressure cycles without damage. Therefore, the newly established GC window, can replace beryllium in x-ray transmission windows with a nontoxic and abundant material.

[1] S. Huebner et al., accepted for publication in IEEE Trans. on Nuclear Science

17:30**Ion selectivity and water flow in graphene-derived membranes**Slaven Garaj^{1,2}¹Department of Physics, National University of Singapore, Singapore¹Centre for Advanced 2D Materials, National University of Singapore, Singapore

Graphene's unique interaction with water, ions and molecules - with implied superior performance in diverse fields such as next-generation DNA sequencing or water desalination - has attracted a lot of attention from research groups and industrial champions.

We have previously shown that the monoatomic, crystalline graphene membrane in its pristine form is impermeable to water and ions[1]. If modified, graphene membrane could become an effective ionic and molecular sieve, while retaining ultra-high water flux. Two strategies have been applied to that end: (a) perforating graphene with sub-nanometer sized pores[1,2]; and (b) layering graphene-oxide crystallites into a thin laminated membrane[3]. With careful investigation of the ionic flow in graphene-derived membranes, for a range of ionic species, we identified basic mechanisms governing ion-graphene interaction. This insight opens us a new venue for developing desalination membranes with unmatched performance.

[1] S. Garaj et al, Nature 467, 190 (2010).

[2] D. Cohen-Tanugi and J. C. Grossman, Nano Lett 12, 3602 (2012).

[3] R. K. Joshi et al, Science 343, 752 (2014).

18:00**IWEPNM 2015 Conference Summary**C. Stampfer^{1,2}¹JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52056 Aachen, Germany, EU²Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany, EU

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